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Elastic wave propagation in polycrystals

by

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Declaration of Originality

The content of this thesis is my own research work, which was completed under the supervision of Profs Michael J S Lowe and Peter Cawley. Appropriate references have been provided wherever the work of others has been used.

Ming Huang

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Abstract

Scattering occurs as elastic waves propagate through a random polycrystalline medium, exhibiting scattering-induced attenuation and velocity dispersion. These behaviours carry bulk information about microstructure and can therefore be used for microstructure characterisation. The purpose of this thesis is to gain knowledge about the behaviour of elastic waves in polycrystals in order to facilitate the characterisation of microstructure. This thesis contributes mainly in six aspects.

First, a theoretical second-order approximation (SOA) model is developed to calculate the scattering-induced attenuation and velocity dispersion of plane elastic waves in random polycrystals. This model provides solutions of second-order accuracy in material inhomogeneity that are valid across all scattering regimes and partially account for multiple scattering. It applies to statistically equiaxed and elongated grains of arbitrary crystal symmetries, with decoupled geometric and elastic statistics represented respectively by the two-point correlation (TPC) function and the elastic covariance. A simple Born approximation, with a reduced accuracy considering only single scattering, is formulated based on the SOA model, and analytical asymptotes are derived for the low-frequency Rayleigh and high-frequency stochastic regimes.

Second, a three-dimensional (3D) finite element (FE) method is advanced to solve the wave propagation problem in the time domain. This method uses grain-scale spatial representation, in significant sample volumes of large numbers of grains, to describe polycrystalline materials. It captures the exact interactions of waves with grains without low-order scattering approximations. The numerical errors and statistical uncertainties of the FE method are minimized to deliver very accurate calculations of attenuation and phase velocity. The TPC function of the FE model is accurately determined and incor-

porated into the SOA model to enable a direct comparison of both models.

Then, the SOA and FE models are used to study the propagation of plane longitudinal waves in polycrystals with statistically equiaxed grains and greatly differing inhomogeneities. Attenuation exhibits fourth- and second-power dependences on frequency in the Rayleigh and stochastic regimes, while phase velocity is nondispersive in both regimes. Attenuation and phase velocity also show proportionalities to material inhomogeneity, and in the Rayleigh regime, the difference between the SOA and FE models is quadratically related to inhomogeneity for both attenuation and velocity.

The fourth contribution relates to using the SOA and FE models to study plane longitudinal wave propagation in polycrystals with statistically elongated grains. The models are found to agree very well with each other for the studied polycrystals over a wide frequency range. In the Rayleigh regime, attenuation and phase velocity exhibit dependencies on the fourth- and zeroth-power of frequency, show respective proportionalities to the effective volume of the grains and the mean grain radius in the direction of propagation, and both manifest a proportionality to the mode-converted elastic scattering factor. In the stochastic regime, attenuation and phase velocity show dependencies on the second- and zeroth-power of frequency, demonstrate positive and negative proportionalities to the mean grain radius in the direction of propagation, and both are proportional to the same-mode elastic scattering factor.

Subsequently, a practical problem is addressed to represent the actual TPC statistics of polycrystals by a single exponential. A variety of potential parameters are identified for the single exponential and their goodness is evaluated by using the SOA and FE models. It is found that the effective grain radius is an optimal choice for the single exponential to represent the microstructure of a range of polycrystals with greatly differing grain uniformities and to achieve a fairly accurate calculation of attenuation and velocity.

The last contribution concerns the theoretical discovery of three modes for elastic waves in polycrystals. For either longitudinal or transverse propagating waves, three solutions are found in the far-field approximation and the SOA model, indicating that three modes may co-exist. A further study by the spectral function approach reveals that the two non-dominant modes mostly have negligible energy in comparison to the dominant mode.

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Chapter 1

Introduction

1.1 Motivation

Polycrystalline materials are composed of crystallites, also known as grains, of varying shapes, sizes, and orientations. They are the most commonly found materials in inorganic solids and are being very widely used. In particular, many safety-critical components are made from polycrystalline materials in a number of industries, such as aerospace, nuclear, defence, and automotive. For such applications, it is crucial to ensure that the material components perform their function in a durable and safe manner.

The durability and safety of polycrystalline components largely relies on their microstructural parameters. One of the key parameters is the grain size, which determines the total area of grain boundaries per unit volume. Since grain boundaries are known to be pinning points impeding dislocation propagation, a smaller grain size (i.e., a larger grain boundary area) is associated with higher strength and toughness [1,2] and better resistance to fatigue crack initiation and propagation [3]. On the other hand, grain boundaries can increase the rate of diffusional creep by facilitating the movement of lattice vacancies across grains or along boundaries [4]. This means that a larger grain size is needed to achieve a better creep resistance in high-temperature applications such as nickel and titanium alloys used in aero-engines and power plants. The other two important parameters are the shape and crystallographic orientation of the grains, which would cause anisotropy to material performance if they have a preferred alignment or orientation [5]. Therefore,

it is highly desirable to characterise the microstructure of polycrystals in order to ensure that they perform as desired.

Microstructure characterisation can be achieved by using a number of techniques such as optical and electron microscopes. Such techniques perform characterisation on a well-prepared, two-dimensional plane through the three-dimensional component. This process requires very time-consuming surface preparation, and microstructural statistics are thus usually acquired from a single outer surface of the component. When these techniques are used for volumetric characterisation, a destructive serial-sectioning procedure is needed to cut through the component in a layer-by-layer fashion [6, 7].

By contrast, ultrasonic waves (more generally, elastic waves) can be utilized to non-destructively characterise the bulk, volumetric microstructure of polycrystals without the need for careful surface preparation and sample sectioning. The elastic properties within a polycrystal are spatially varied, owing to the differently oriented crystallographic axes of elastically anisotropic grains. Thus, elastic waves are scattered as they propagate through a polycrystal, and the energy transmitted in the main beam of the propagating wave is attenuated and the propagation direction of each beam is deflected, exhibiting scattering-induced attenuation and phase velocity dispersion in the main beam [8, 9]. These wave behaviours depend on the size, shape, and orientation of the grains, and their variations with frequency and direction carry abundant information about these microstructural parameters. Therefore, the microstructure of polycrystals can be inversely determined from attenuation and velocity measurements, which are relatively simple and inexpensive to perform [10–12].

The inverse characterisation of microstructure relies on a clear understanding of the relationship between the wave behaviours and the microstructure of polycrystals. To facilitate microstructure characterisation, this thesis is motivated to study the propagation of elastic waves in polycrystals and to correlate wave behaviours with microstructure.

1.2 Literature review

Extensive research studies have been carried out to understand the behaviours of elastic waves in polycrystals. A brief review of previous work is provided below for polycrystals with statistically equiaxed and elongated grains.

1.2.1 Elastic waves in polycrystals with equiaxed grains

The attenuation and velocity dispersion of waves in polycrystals with statistically equiaxed grains have received extensive attention over the past few decades. Early studies, as reviewed by Papadakis [13], obtained theoretical Rayleigh and stochastic asymptotes for equiaxed grains of cubic, hexagonal and orthorhombic symmetries and described experimental results mainly for cubic polycrystals. Significant progress was achieved by Stanke and Kino [14] who, based on the Keller approximation [15,16], developed a unified second-order approximation (SOA) model that is valid for all frequency ranges for cubic polycrystals with equiaxed grains. An equivalent model was later developed by Weaver [17] based on the Dyson equation with the introduction of the first-order smoothing approximation [18]. These models used a geometric autocorrelation function to describe the microstructure of the polycrystals. They considered untextured polycrystals with single-phase equiaxed grains of cubic crystal symmetry, but they were subsequently extended to a variety of materials with texture, lower crystal symmetries, and duplex microstructures [11,19–28]. The theoretical models are necessarily approximate, and the Stanke and Kino [14] and Weaver [17] models are accurate to the second order of material inhomogeneity perturbations, allowing for the consideration of partial forward multiple scattering. However, only a few extensions [23,26–28] maintained the second-order accuracy in the final results, while others (including Weaver [17]) additionally introduced the Born approximation to deliver explicit expressions for attenuation [11,19,21,22,24,25], limiting their validities to even lower-order scattering at frequencies below the geometric regime.

In contrast to theoretical studies, numerical simulations can be performed without the approximations of low order scattering. A wide range of numerical methods can be employed to achieve such numerical experiments and a summary of them can be found in

Van Pamel et al. [29]. Among these methods, the finite element (FE) method is widely researched for the simulation of elastic waves in complex media [30]. The use of this method for polycrystals has long been limited, by its extreme computational demands, to two-dimensional cases [31–35]. However, the dependence of scattering on spatial dimensionality at certain frequencies [36] means that three-dimensional (3D) simulation is always desirable for understanding real-world wave phenomena. Recent advancements of computer hardware and elastodynamic software, especially the development of the GPU-accelerated Pogo program [37], have enabled the successes of 3D modelling [28, 29, 38, 39]. These 3D simulation studies, with representations of polycrystals at grain scale in realistic sample volumes, addressed a relatively simple case of plane longitudinal waves propagating in polycrystals with macroscopically isotropic elastic properties and equiaxed grains. They have demonstrated that 3D FE simulations can accurately describe the interactions of elastic waves with grains that involve complex multiple scattering.

Whereas this subject of wave propagation in polycrystals with equiaxed grains has received plentiful study, two important topics remain unresolved so far: 1) A theoretical SOA model has not been developed for polycrystals with crystallographic symmetry lower than cubic, in spite of many practically-important alloys having hexagonal or even lower symmetries. 2) The accurate 3D FE method has enabled the evaluation of the approximations of the theoretical models that show generally good quantitative agreement with the FE models across different frequency ranges, crystal symmetries, inhomogeneity levels, and grain size distributions [28, 29, 38, 39]. However, there is an absence of study investigating when the theoretical models break down by their lack of representation of high-order terms on material inhomogeneity perturbation.

1.2.2 Elastic waves in polycrystals with elongated grains

Relatively limited studies have been conducted to understand the propagation of waves in polycrystals with elongated grains, although the grains of most polycrystals in practice tend to be elongated due to material processing like forging, rolling, and extrusion [5, 10, 22, 40]. An early theoretical analysis was performed for elongated polycrystals of cubic crystal symmetry by Ahmed and Thompson [40] by directly extending and numerically

evaluating the Stanke and Kino [14] dispersion equation in its initial general form. This was followed by extensions of the Weaver model [17] to polycrystals of lower crystal symmetries with elongated grains [11, 21, 41] and elongated microtexture regions [24, 25] by Rokhlin and co-authors, but they have invoked the Born approximation and thus limited their analyses to frequencies below the geometric regime. Recently, a far-field approximation (FFA) model was developed by Rokhlin et al. [26] for ellipsoidal grains of general crystallographic symmetry that gives good agreement with the SOA model in all frequency ranges. Furthermore, a spectral function approach for the SOA model was introduced by Calvet and Margerin [42, 43] where the attenuation and velocity are obtained by evaluating the spectral function for cubic polycrystals.

The experimental studies of attenuation in elongated polycrystals were performed in different frequency ranges in prior studies [24, 25, 44–46] where microstructure statistics were determined in different sample directions, but the author is not aware of any experimental study that exhibits sufficient detail and precision in velocity dispersion for elongated polycrystals. In general, experimental studies have a limited ability in quantitative comparison with, and validation of, theoretical predictions. This is due to the experimental difficulty of determining the microstructure statistics for elongated grains, and the difficulty of performing measurements in a sufficiently large frequency range.

Two essential elements are absent in existing studies for wave propagation in polycrystals with elongated grains: 1) A theory maintaining the exact second-order accuracy has not been reported so far for polycrystals with elongated grains. 2) The 3D FE method does not suffer from the above-mentioned experimental limitations because of its full control and knowledge of microstructure statistics and its ability to perform simulations in a large frequency range under plane wave conditions [28]. This method is thus ideal for a better understanding of wave scattering in polycrystals with elongated grains and for a quantitative evaluation of the theoretical models. However, a 3D FE model has not been implemented for the simulation of wave propagation in polycrystals with elongated grains.

1.3 Aim and scope

This thesis aims to address the above-mentioned topics that have not been dealt with by existing studies. This is achieved by developing a theoretical SOA model for elastic wave propagation in polycrystals with equiaxed and elongated grains of arbitrary crystal symmetries, and by implementing a 3D FE method for simulating the same wave propagation problem. Theoretical predictions will be compared with FE results to evaluate the dependence of attenuation and phase velocity on frequency and material inhomogeneity for polycrystals with equiaxed grains, and to assess the potential breakdown condition of the theoretical model. Also, the theoretical and FE models will be employed to study the frequency and angular reliance of attenuation and velocity in polycrystals with elongated grains.

This thesis also aims to evaluate the possibility of representing the spatial autocorrelation of a polycrystal by a single exponential. This is to address the practical need of performing a rapid but fairly accurate calculation of attenuation and velocity based on not-so-accurate autocorrelation data and to provide a foundation for the inverse characterisation of microstructure. In addition, this thesis seeks to report the theoretical existence of three modes for elastic waves in random polycrystals.

In practice, polycrystalline materials may be produced with voids or inclusions inside grains or on grain boundaries, and they may also be generated with multiple phases of different chemical constituents, lattice constants, or crystal structures. However, this thesis does not involve such complex microstructures and its scope is limited to a relatively simple case: 1) the grains of a polycrystal are densely-packed, fully-bonded, and defect-free, 2) the polycrystal has a single phase, meaning that the grains have identical material mass and stiffness properties but different crystallographic orientations, 3) the polycrystal is homogeneous on the macroscopic scale and has untextured, isotropic properties in an ensemble average sense. It is important to note that ignoring crystallographic texture may not be practical for polycrystals with elongated grains. This is because the material processing that produces elongated grains may also create preferred crystallographic orientations, showing anisotropic texture. While studying elongated polycrystals with texture is important, it is useful to separate its effect from that of the grain shape. Such

separation is still practically important because there are application scenarios where preferred crystallographic orientation is partially eliminated by specific material processing while grain elongation remains to affect the scattering of waves. It also allows a better understanding of the effect of model approximations when applied to scattering in elongated grains.

1.4 Thesis outline

Chapter 2 begins with the description of the theoretical SOA model for elastic waves in polycrystals with equiaxed and elongated grains of arbitrary crystal symmetry. Then, the Born approximation of the SOA model is introduced and the analytical Rayleigh and stochastic asymptotes are derived. The far-field approximation is finally outlined.

Chapter 3 reports the 3D FE method for simulating waves in polycrystals with equiaxed and elongated grains. The approaches for determining attenuation and phase velocity and for measuring the spatial autocorrelation function are described. The method for quasi-static simulation is also provided.

Chapter 4 presents researches into maximising the accuracy of FE simulation. First, the two approaches, the through-transmission and fitting, for the determination of attenuation and phase velocity are evaluated. Then, the modelling errors and uncertainties caused by FE approximations and statistical considerations are studied. This is followed by evaluating the effect of symmetry boundary conditions on attenuation and velocity calculations.

Chapter 5 uses the theoretical and numerical models to study wave propagation in polycrystals with equiaxed grains. It first uses a variety of polycrystals of cubic crystal symmetry to evaluate the dependences of attenuation and phase velocity on frequency and material inhomogeneity and to assess the approximations of the theoretical models. Then, the suitability of the theoretical models for triclinic polycrystals is investigated.

Chapter 6 uses the theoretical and numerical models to study wave propagation in polycrystals with elongated grains. It begins with the analysis of the dependences of attenuation on frequency, elastic properties, and grain elongation. Then, a similar analysis is

performed for phase velocity and the quasi-static limit of velocity.

Chapter 7 evaluates the possibility of representing the spatial autocorrelation of a polycrystal by a single exponential. First, the three measurable probability functions for describing the spatial autocorrelation of polycrystals are studied and their mutual relations are investigated. Then, five potential parameters are identified for the single exponential function to replace the actual autocorrelation function. This is followed by evaluating the goodness of the selected parameters in representing attenuation and phase velocity.

Chapter 8 reports the theoretical existence of three modes in the dispersion equation for either longitudinal or transverse waves in polycrystals and discusses the possibility of their co-existence in actual problems. It begins with the discussion of the approximate scalar case and ends with the actual elastic case.

Chapter 9 summarises the key findings and contribution of this thesis and discusses the potential for future work.

Chapter 2

Theoretical models

2.1 Introduction

This chapter describes the theoretical models for the scattering-induced attenuation and phase velocity dispersion of elastic waves in polycrystals. The models are primarily formulated for polycrystals with statistically elongated grains and are conveniently degenerated to the specific case of grains being statistically equiaxed; the crystallographic symmetry of the grains is arbitrary. The polycrystals considered in the theories are composed of single-phase grain aggregates which are densely-packed and fully-bonded. The materials are macroscopically homogeneous and have untextured, isotropic properties in an ensemble average sense.

The theoretical description in this chapter focuses on one of the advanced models, the second-order approximation (SOA) [28], that is applicable in all frequency ranges as the Stanke and Kino model [14]. This SOA model is described in §2.2, which begins with the presentation of its dispersion equation in §2.2.1 that provides a solution to the wave number as perturbed by grain scattering. The real and imaginary parts of this perturbed wave number determine phase velocity and attenuation respectively. Then, the most important term of the dispersion equation, the mass operator, is formulated in §2.2.2 to consider the multiple scattering of waves by the grains. Eventually, §2.2.3 discusses the statistical information, the two-point correlation (TPC) function, as required by the mass operator to describe grain structures. This chapter also formulates the Born approximation of the

SOA model in §2.3, from which the low-frequency Rayleigh and high-frequency stochastic asymptotes are derived. Besides, the far-field approximation is provided in §2.4.

This chapter is largely adapted from the manuscript [P3] that has been submitted for possible publication and [P4] with the permission of AIP Publishing. The derivation of the theoretical models has received valuable assistance from Prof Stanislav Rokhlin and Dr Gaofeng Sha, both are co-authors of the two submitted manuscripts.

2.2 Second-order approximation

2.2.1 Dispersion equation

Elastic wave propagation in polycrystals can be accurately described by the elastodynamic wave equations. However, solving these equations analytically and satisfying boundary conditions on grain interfaces is beyond current theoretical capabilities due to the random packing of anisotropic grains and the different orientation of crystallographic axes. If the polycrystalline medium is statistically homogeneous, i.e. the elastic properties are independent of position on the macroscopic scale, an opportunity exists to solve the problem approximately by replacing the polycrystal with a continuous random medium containing small spatial variations of elastic tensor and considering an ensemble-averaged wave response. The continuous random medium spatially relates to the original polycrystal by the proper selection of spatial TPC functions. An elastic wave propagating in such a medium scatters on elastic perturbations and is represented by the mean field described by a plane propagating wave with an effective perturbed wave number. For a propagating wave of mode M , it leads to the dispersion equation [14,17] for the perturbed wave number k of the propagating wave

$$\omega^2 - k^2 V_{0M}^2 - m_M(\mathbf{k}; \omega) = 0, \quad (2.1)$$

where $\omega = 2\pi f$ is the angular frequency (f is the frequency). $\mathbf{k} = k\mathbf{p}$ is the wave vector, with k being the complex wave number and $\mathbf{p}$ being the unit wave vector in the wave propagation direction as illustrated in Figure 2.1. Note that the wave mode M is implicit

in the wave number k . In elastic solids, the incident wave mode M can be any of the three independent modes: longitudinal (L), fast transverse (T1), and slow transverse (T2). V_{0M} represents the phase velocity of wave M that travels in the reference medium [28], which is a homogenised medium with the elastic property being equal to the Voigt average of the elastic property of the polycrystal. For polycrystals considered in this work, the reference medium is assumed to be isotropic and therefore V_{0M} is independent of wave propagation direction $\mathbf{p}$. $m_M(\mathbf{k}; \omega)$ is the mass operator accounting for scattering events, and its formulation will be given in the following §2.2.2.

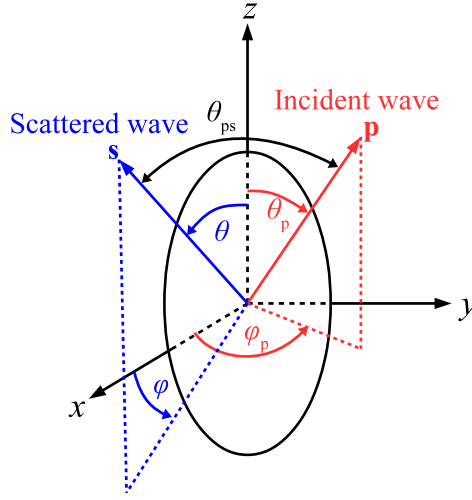


Figure 2.1: Coordinate system for the theoretical models of wave propagation and scattering in polycrystals with statistically ellipsoidal grains. The radii of the ellipsoidal grains are affixed with the axes of the global coordinate system. $\mathbf{p} = (\sin \theta_p \cos \varphi_p, \sin \theta_p \sin \varphi_p, \cos \theta_p)$ and $\mathbf{s} = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)$ represent the propagation directions of the incident and scattered waves, respectively. θ_{ps} is the angle between the two waves.

By solving Equation 2.1, one obtains the perturbed wave number k , which is complex due to scattering; i.e., $k = \text{Re}k + i\alpha$. Then, the effective media parameters, attenuation coefficient and phase velocity, for the plane wave are respectively obtained as $\alpha_M = \text{Im}k$ and $V_M = \omega/\text{Re}k$. Those parameters depend on the wave propagation direction $\mathbf{p}$ due to grain elongation and are thus statistically anisotropic, even though the reference medium with velocity V_{0M} is considered to be isotropic.

2.2.2 Mass operator

The mass operator $m_M(\mathbf{k}; \omega)$ in Equation 2.1 takes into account all possible multiple scattering events. It is understood that [16, 47] this operator cannot be obtained exactly even for scalar cases, and the formulation is generally achieved by introducing approximations to the operator. The second-order approximation (SOA) is adopted in this work to deliver an approximate expression for the mass operator.

This SOA model adopts the first-order smoothing approximation [17, 18] (or equivalently the Bourret approximation [18, 47, 48]) which accounts for double scattering inside each heterogeneity without recurrent visits [28, 47] and the corresponding forward scattering events. The model is applicable to all frequency ranges, but its validity is generally assumed [14, 17] to be limited to cases of small elastic perturbations and short propagation distances, assuring coherency of the incident wave. However, recent 3D FE studies [28, 29, 39] have shown that the SOA model is in very good agreement with 3D FE simulations for equiaxed polycrystals with high grain anisotropy and elastic perturbations, such as Inconel, copper, and triclinic CSP (those conclusions are extended to polycrystals with elongated grains in §6). The wave propagation distances in those 3D FE simulations are on the order of 10 in terms of average grain diameter and wavelength (this translates to about 10 mm in studied metals at the frequency of about 6 MHz).

As in Rokhlin et al. [26], an infinitely small anisotropy is introduced to the reference medium and the mass operator in the SOA model for a given incident wave M is expressed as a sum of three terms representing scattering into longitudinal and two transverse waves with mutually orthogonal polarizations: $m_M(\mathbf{k}; \omega) = \sum_{N=L, T1, T2} m_{M \rightarrow N}(\mathbf{k}; \omega)$, where $m_{M \rightarrow N}(\mathbf{k}; \omega)$ denotes the scattering of waves from mode M to mode N . The incident wave mode M can be one of longitudinal (L), fast transverse (T1), or slow transverse (T2) waves, while all three modes exist for the scattered wave N due to mode conversion on grain boundaries.

Since the reference medium is considered to be isotropic, the two transverse waves approximately have the same velocities but mutually orthogonal polarizations. This allows the two transverse scattering terms, $m_{M \rightarrow T1}$ and $m_{M \rightarrow T2}$ to be combined into a total transverse wave scattering term $m_{M \rightarrow T}$. It is important to emphasise that the phase velocities

of the two transverse waves are slightly different as a result of the macroscopic anisotropy caused by grain elongation [42]. This difference is generally small [42], and therefore the two terms degenerate into one in this thesis.

As a result, the mass operator can be expressed as $m_M(\mathbf{k}; \omega) = \sum_{N=L,T} m_{M \rightarrow N}(\mathbf{k}; \omega)$. Similarly to the representation in Rokhlin et al. [26], the mass operator component $m_{M \rightarrow N}$ is given in the spherical coordinate system as

$$m_{M \rightarrow N}(\mathbf{k}; \omega) = \frac{k^2 k_{0N}^3}{\eta \rho^2 V_{0N}^2} \left\{ \text{P.V.} \int_0^\infty \left[\frac{\xi^4}{1 - \xi^2} \int_0^\pi \int_0^{2\pi} f_{M \rightarrow N}(k, \omega, \xi, \theta, \varphi) \sin \theta d\varphi d\theta \right] d\xi - i \frac{\pi}{2} \int_0^\pi \int_0^{2\pi} f_{M \rightarrow N}(k, \omega, \xi = 1, \theta, \varphi) \sin \theta d\varphi d\theta \right\}, \quad (2.2)$$

where ρ is the mass density and it is constant because the polycrystal is assumed to be composed of single-phase grains. $k_{0N} = \omega/V_{0N}$ is the wave number for mode N in the reference medium. P.V. represents Cauchy principal value and ξ is a dimensionless variable. The factor η is employed to give a unified expression for longitudinal ($M = L$; $\eta = 1$) and transverse ($M = T$; $\eta = 2$) propagating waves.

The factor $f_{M \rightarrow N}$ in Equation 2.2 is the spectral representation of the spatial correlation function, $\langle \delta c_{ijkl}(\mathbf{x}) \delta c_{\alpha\beta\gamma\delta}(\mathbf{x}') \rangle$, between points $\mathbf{x}$ and $\mathbf{x}'$; $\delta c_{ijkl}(\mathbf{x})$ is a small random spatial fluctuation of the elastic tensor $c_{ijkl}(\mathbf{x})$ around its mean $\langle c_{ijkl} \rangle$. The correlation function can be factored into $\langle \delta c_{ijkl}(\mathbf{x}) \delta c_{\alpha\beta\gamma\delta}(\mathbf{x}') \rangle = \langle \delta c_{ijkl} \delta c_{\alpha\beta\gamma\delta} \rangle w(\mathbf{x} - \mathbf{x}')$ for statistically homogeneous media, with the first part representing the elastic covariance and the second part denoting the geometric two-point correlation (TPC) function. The validity of this factorisation has been demonstrated by the direct numerical comparison in [49] for statistically isotropic polycrystals with equiaxed grains. The good agreement between the theoretical and 3D FE models in §6 indirectly supports the applicability of the factorisation to polycrystals with elongated grains that exhibit statistical anisotropy. Similarly, the factor $f_{M \rightarrow N}$ can be factored into two parts in the spectral domain

$$f_{M \rightarrow N}(k, \omega, \xi, \theta, \varphi) = \text{IP}_{M \rightarrow N}(\theta, \varphi) W_{M \rightarrow N}(k, \omega, \xi, \theta, \varphi), \quad (2.3)$$

where $W_{M \rightarrow N}$ is the spectral representation of the geometric TPC function $w(\mathbf{x} - \mathbf{x}')$ and it will be described in the following §2.2.3. $\text{IP}_{M \rightarrow N}$ is the inner product accounting for the

elastic covariance $\langle \delta c_{ijkl} \delta c_{\alpha\beta\gamma\delta} \rangle$ and the propagation and polarization directions of both incident and scattered waves. For the wave propagation setup shown in Figure 2.1, the inner product is given by [11, 26]

$$\text{IP}_{M \rightarrow N}(\theta, \varphi) = A_{MN} + B_{MN} \cos^2 \theta_{\text{ps}} + C_{MN} \cos^4 \theta_{\text{ps}}, \quad (2.4)$$

where the coefficients A_{MN} , B_{MN} and C_{MN} ($M, N \in \text{L, T}$) are invariants [11] and are represented by linear combinations of the seven quadratic invariants. The coefficients are the sums of the quadratic terms of elastic constants, their expressions can be found in Appendix A for arbitrary crystal symmetries. θ_{ps} is the angle between the incident and scattered waves and $\cos \theta_{\text{ps}} = \mathbf{p} \cdot \mathbf{s} = \cos(\varphi - \varphi_{\text{p}}) \sin \theta \sin \theta_{\text{p}} + \cos \theta \cos \theta_{\text{p}}$.

2.2.3 Two-point correlation function

The spectral TPC function $W_{M \rightarrow N}(k, \omega, \xi, \theta, \varphi)$ is represented as $w(\mathbf{r})$ in the spatial domain, which describes the probability of two points $\mathbf{x}$ and $\mathbf{x}'$ separated by a vector $\mathbf{r} = \mathbf{x} - \mathbf{x}'$ being in the same grain.

For statistically equiaxed grains, the TPC function is direction-independent, and thus $w(\mathbf{r}) = w(r)$. This function was conventionally given [14, 17] in the exponential form, $w(r) = \exp(-r/a)$, by assuming that the line intercepts (also known as chord lengths) of equiaxed grains follow Poisson statistics [50]. a is the mean radius of the grains. However, recent studies demonstrated that this form cannot accurately represent actual experimental [51] and simulated [28, 39, 49] microstructures. It was suggested [28] that a better representation can be achieved by using a generalized TPC function. This generalized function is given as the sum of an exponential series: $w(r) = \sum_{i=1}^n A_i \exp(-r/a_i)$. The coefficients A_i and a_i can be obtained by best fitting this function to the TPC data directly measured from real or simulated polycrystals.

For polycrystals with elongated grains, the TPC function is direction-dependent and therefore the polycrystal is statistically anisotropic. For simplicity, this work assumes that the average shape of the elongated grains is ellipsoidal, and the grains are statistically elongated in the same direction. As shown in Figure 2.1, the axes of the average ellipsoidal

grain are affixed, without loss of generality, to the axes of the global coordinate system. In this case, the generalized TPC function of the elongated grains can be given by

$$w(\mathbf{r}) = \sum_{i=1}^n A_i \exp \left[-\sqrt{\frac{r_x^2}{(a_x^i)^2} + \frac{r_y^2}{(a_y^i)^2} + \frac{r_z^2}{(a_z^i)^2}} \right], \quad (2.5)$$

where a_x^i , a_y^i , a_z^i and A_i are the coefficients of the i -th term of the exponential series, which are determined by fitting the actual TPC data of the polycrystal. Only the total TPC function $w(\mathbf{r})$ describes the polycrystal statistics and a physical meaning is not assigned to the individual terms of the series [28]. The transform of the TPC function in the spatial frequency domain [21] is presented as

$$W(\mathbf{k}) = \sum_{i=1}^n \frac{A_i a_x^i a_y^i a_z^i}{\pi^2 [1 + k_x^2 (a_x^i)^2 + k_y^2 (a_y^i)^2 + k_z^2 (a_z^i)^2]^2}, \quad (2.6)$$

where k_x , k_y and k_z are the components of the vector $\mathbf{k}$. Now the spectral TPC function $W_{M \rightarrow N}(k, \omega, \xi, \theta, \varphi)$ in Equation 2.3 can be written as

$$W_{M \rightarrow N}(k, \omega, \xi, \theta, \varphi) = W(\mathbf{k} - \mathbf{k}_N^S) = \sum_{i=1}^n \frac{A_i a_x^i a_y^i a_z^i}{\pi^2 [1 + q_x^2 (a_x^i)^2 + q_y^2 (a_y^i)^2 + q_z^2 (a_z^i)^2]^2}, \quad (2.7)$$

where $\mathbf{k}_N^S = \xi k_{0N} \mathbf{s}$ is the scattered wave vector. $(q_x, q_y, q_z) = \mathbf{k} - \mathbf{k}_N^S$ is the difference between the incident and scattered wave vectors, i.e.

$$(q_x, q_y, q_z) = k(\sin \theta_p \cos \varphi_p, \sin \theta_p \sin \varphi_p, \cos \theta_p) - \xi k_{0N}(\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta). \quad (2.8)$$

While a physical meaning is not assigned to each term of the representation in Equation 2.5, some insights into the meaning of the length scales $a_{x,y,z}^i$ may be gained [28] considering the spatial spectral domain representation in Equation 2.6 and comparing it to the corresponding actual spectral TPC of the polycrystal. Each term of Equation 2.6 essentially modifies the spatial spectrum of the actual TPC, which is eventually represented by the sum of all TPC terms.

2.3 Born approximation and analytical asymptotes

The Born approximation is introduced into the SOA model to obtain explicit expressions for attenuation and phase velocity. This approximation significantly reduces computational complexity and allows the analytical Rayleigh and stochastic asymptotes to be derived for attenuation and phase velocity as provided in the following §2.3.2 and §2.3.3.

2.3.1 Born approximation

In the Born approximation, the perturbed wave vector $\mathbf{k}$ in the mass operator (Equation 2.2) is replaced by the unperturbed reference wave vector $\mathbf{p}k_{0M}$. And the small wave number perturbation $(\omega/V_{0M})^2 - k^2$ in the dispersion equation (Equation 2.1) is substituted by the first-order term $2k_{0M}(k_{0M} - k)$ of its Taylor series about $k = k_{0M}$. These simplifications result in an explicit solution to the perturbed wave number

$$k = k_{0M} - \frac{m_M(\mathbf{p}k_{0M}; \omega)}{2k_{0M}V_{0M}^2}, \quad (2.9)$$

where the mass operator $m_M(\mathbf{p}k_{0M}; \omega) = \sum_{N=L,T} m_{M \rightarrow N}(\mathbf{p}k_{0M}; \omega)$. The component $m_{M \rightarrow N}(\mathbf{p}k_{0M}; \omega)$ is obtained by replacing the wave vector $\mathbf{k}$ in Equation 2.2 by $\mathbf{p}k_{0M}$. Due to this replacement, the factor $f_{M \rightarrow N}$ is now a real function, and the real and imaginary parts of the mass operator can thus be conveniently separated, with the real part being the first term with the triple integral, and the imaginary part the second term with the double integral. This yields the separated expressions for attenuation coefficient $\alpha_M = \text{Im}(k)$ and phase velocity $V_M = \omega/\text{Re}(k)$ as

$$\alpha_M = \sum_{N=L,T} \alpha_{M \rightarrow N}, \quad (2.10)$$

$$V_M = \frac{V_{0M}}{1 + \sum_{N=L,T} \Delta_{M \rightarrow N}}, \quad (2.11)$$

where the attenuation component $\alpha_{M \rightarrow N}$ and the scattering-induced relative velocity change $\Delta_{M \rightarrow N}$ are given by

$$\alpha_{M \rightarrow N} = \frac{\pi \omega^4}{4 \eta \rho^2 V_{0M}^3 V_{0N}^5} \int_0^\pi \int_0^{2\pi} f_{M \rightarrow N}(k_{0M}, \omega, \xi = 1, \theta, \varphi) \sin \theta d\varphi d\theta, \quad (2.12)$$

$$\Delta_{M \rightarrow N} = \frac{-\omega^3}{2 \eta \rho^2 V_{0M}^2 V_{0N}^5} \text{P.V.} \int_0^\infty \frac{\xi^4 d\xi}{1 - \xi^2} \int_0^\pi \int_0^{2\pi} f_{M \rightarrow N}(k_{0M}, \omega, \xi, \theta, \varphi) \sin \theta d\varphi d\theta. \quad (2.13)$$

The triple integral in Equation 2.13 can be written in the following form by substituting Equation 2.3 into the integral and re-arranging its terms

$$\begin{aligned} \sum_{i=1}^n \frac{A_i a_x^i a_y^i a_z^i}{\pi^2} \int_0^\pi \int_0^{2\pi} (A_{MN} + B_{MN} \cos^2 \theta_{ps} + C_{MN} \cos^4 \theta_{ps}) \sin \theta \times \\ \text{P.V.} \int_0^\infty \frac{\xi^4 d\xi}{(1 - \xi^2)(C_0^i - C_1^i \xi + C_2^i \xi^2)^2} d\varphi d\theta, \end{aligned} \quad (2.14)$$

where the functions C_0^i , C_1^i and C_2^i are introduced to simplify notation

$$\begin{aligned} C_0^i &= 1 + k_{0M}^2 \{[(a_x^i)^2 \cos^2 \varphi_p + (a_y^i)^2 \sin^2 \varphi_p] \sin^2 \theta_p + (a_z^i)^2 \cos^2 \theta_p\}, \\ C_1^i &= 2k_{0M} k_{0N} \{[(a_x^i)^2 \cos \varphi \cos \varphi_p + (a_y^i)^2 \sin \varphi \sin \varphi_p] \sin \theta \sin \theta_p + (a_z^i)^2 \cos \theta \cos \theta_p\}, \\ C_2^i &= k_{0N}^2 \{[(a_x^i)^2 \cos^2 \varphi + (a_y^i)^2 \sin^2 \varphi] \sin^2 \theta + (a_z^i)^2 \cos^2 \theta\}. \end{aligned} \quad (2.15)$$

The innermost Cauchy integral in Equation 2.14 is evaluated by using the contour integral and the residue theorem because its integrand approaches zero when $\xi \rightarrow \infty$. This leads to the following solution $\chi(\theta, \varphi)$ for the Cauchy integral

$$\begin{aligned} \chi(\theta, \varphi) = \frac{2\pi(C_0^i)^2}{(D^i)^3[(C_1^i)^2 - (C_0^i + C_2^i)^2]} - \frac{2\pi C_0^i[(C_0^i)^2 - (C_2^i)^2]}{D^i[(C_1^i)^2 - (C_0^i + C_2^i)^2]^2} - \\ \frac{\pi(C_0^i + C_2^i)D^i}{[(C_1^i)^2 - (C_0^i + C_2^i)^2]^2}, \end{aligned} \quad (2.16)$$

where $D^i = \sqrt{4C_0^i C_2^i - (C_1^i)^2}$. Note that the evaluation result is originally complex but only its real part is given in Equation 2.16 because its imaginary part cancels out during

the later double integration over θ and φ . Now the velocity change $\Delta_{M \rightarrow N}$ is given by

$$\Delta_{M \rightarrow N} = \frac{-\omega^3}{2\pi^2 \eta \rho^2 V_{0M}^2 V_{0N}^5} \sum_{i=1}^n A_i a_x^i a_y^i a_z^i \times \int_0^\pi \int_0^{2\pi} (A_{MN} + B_{MN} \cos^2 \theta_{ps} + C_{MN} \cos^4 \theta_{ps}) \chi(\theta, \varphi) \sin \theta d\varphi d\theta. \quad (2.17)$$

The Born approximation only considers single scattering. This limits its validity to frequencies below the geometric regime. To evaluate its range of validity, it is compared with the SOA model in Figure 2.2 for longitudinal wave propagation in polycrystalline Copper Sulfate Pentahydrate (CSP) with elongated grains of triclinic crystallographic symmetry. The grains have an ellipsoid-of-rotation shape on average and the TPC coefficients satisfy $a_x^i = a_y^i$; all parameters are specified in the figure caption. The figure shows that the Born approximation agrees very well with the SOA model at low frequencies, and the difference between the two models increases as frequency approaches the geometric regime. It is clear from the left figure that the stochastic asymptote for the elongated direction approaches the Born approximation only at frequencies significantly above the geometric region transition for the SOA model. This suggests that in this case the stochastic regime is not observed for propagation in the grain elongation direction (it is barely developed in the shortened propagation direction).

2.3.2 Rayleigh asymptotes

Rayleigh attenuation asymptote

The expression for attenuation is simplified in the low-frequency Rayleigh scattering regime. At this low-frequency limit, the wavelength is much larger than the average grain size in any direction of a polycrystal. By considering this fact, the asymptote for attenuation is obtained that provides a better understanding of the scattering phenomenon at a long wavelength.

The low-frequency Rayleigh attenuation asymptote is derived in Appendix B.1 from the Born approximation. For polycrystals with elongated grains of statistically ellipsoidal

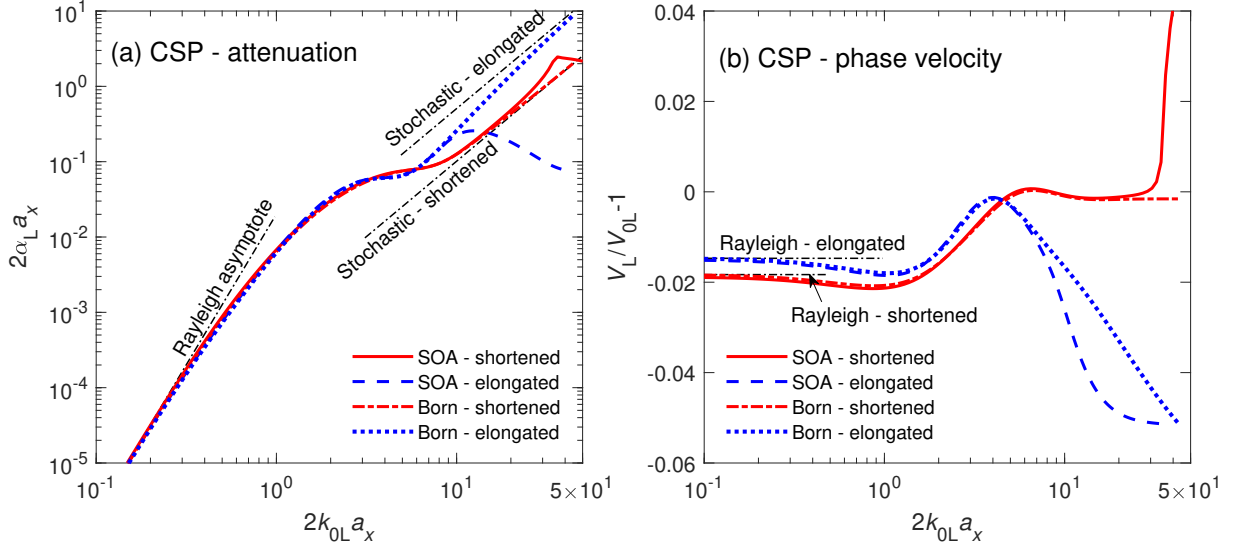


Figure 2.2: Comparison of the SOA model and the Born approximation in all frequency regimes for the normalised (a) attenuation and (b) velocity of longitudinal waves. The results are given for polycrystalline CSP with elongated grains having an elongation ratio of 5. The mean grain radius of the polycrystal in the elongated z -direction, a_z , is 5 times those of the shortened x - and y -directions: $a_z = 5a_x = 5a_y$. The spatial autocorrelation of the polycrystal is represented by the generalized TPC function with coefficients being given in Table 3.3, and in this case, the mean grain radius in the shortened x -direction is determined from the slope at the origin of the generalized TPC function by $a_x = 1/\sum_{i=1}^n (A_i/a_x^i)$ (similarly for a_y and a_z). The elastic properties of the polycrystal are given in Table 3.2.

shape, the attenuation asymptote is given by

$$\alpha_M^R = \frac{1}{2\pi} k_{0M}^4 V_{\text{eff}}^g \left(Q_{MM}^* + \frac{V_{0M}^3}{V_{0N}^3} Q_{M \rightarrow N} \right), \quad (2.18)$$

where $M, N \in \{L, T\}$ and $M \neq N$. V_{eff}^g is the effective grain volume; it is given by $V_{\text{eff}}^g = 8\pi \sum_i A_i a_x^i a_y^i a_z^i$ for elongated polycrystals and $V_{\text{eff}}^g = 8\pi \sum_i A_i a_i$ for equiaxed ones. $Q_{MM}^* = (A_{MM} + B_{MM}/3 + C_{MM}/5)/(4\eta\rho^2 V_{0M}^4)$ is the elastic factor introduced to simplify the above equation. $Q_{M \rightarrow N} = (A_{MN} + B_{MN}/3 + C_{MN}/5)/(4\eta\rho^2 V_{0M}^2 V_{0N}^2)$ is the mode-converted scattering factor following the definition of Rokhlin et al. [26]. The Q factors are for polycrystals of arbitrary crystallite symmetries and their coefficients are summarised in Appendix A.

Equation 2.18 shows that at the low-frequency limit the attenuation obeys a fourth-power dependence on frequency (frequency is implied in the wave number k_{0M}). It is proportional to the effective grain volume and thus independent of grain shape, meaning that

the attenuation is the same in different wave propagation directions. Attenuation also depends on the elastic properties of grains primarily through the scattering factors, Q_{MM}^* and $Q_{M \rightarrow N}$, and the reference wave velocities, V_{0M} and V_{0N} . For longitudinal waves considered later in this thesis, it is worth noting that the factor Q_{LL}^* in Equation 2.18 is small compared to $Q_{L \rightarrow T} V_{0L}^3 / V_{0T}^3$. Thus, the longitudinal attenuation is approximately proportional to $Q_{L \rightarrow T}$ and the third power of the velocity ratio V_{0L} / V_{0T} at the low-frequency limit which is useful for material property normalisation as discussed in §5 and §6.

Rayleigh velocity asymptote

While the above Born approximation is given for elongated grains of generally ellipsoidal shape, here the Rayleigh velocity asymptote (or the quasi-static limit) is only provided for statistically ellipsoid-of-rotation grains, which is the case mainly studied later in this thesis. Based on the Born approximation, the asymptote is given as

$$V_M^R = \frac{V_{0M}}{1 + \sum_{N=L,T} \Delta_{M \rightarrow N}}, \quad (2.19)$$

where $\Delta_{M \rightarrow N}$ represents the relative change of phase velocity at the Rayleigh limit. It is derived in Appendix B.2, and its final expression, which is independent of frequency, is given by

$$\Delta_{M \rightarrow N} = \frac{1}{32\eta\rho^2 V_{0M}^2 V_{0N}^2} \sum_{i=1}^n A_i [\varsigma_0 + \varsigma_2 \cos^2(\theta_p) + \varsigma_4 \cos^4(\theta_p)], \quad (2.20)$$

where θ_p is the angle between the directions of wave propagation and grain elongation, see Figure 2.1. ς_0 , ς_2 , and ς_4 are the shape factors

$$\begin{aligned} \varsigma_0 &= 16A_{MN} + 8B_{MN} \frac{R_i^2 - f(R_i)}{(R_i^2 - 1)} + 3C_{MN} \frac{R_i^2(2R_i^2 + 1) - (4R_i^2 - 1)f(R_i)}{(R_i^2 - 1)^2}, \\ \varsigma_2 &= -8B_{MN} \frac{2 + R_i^2 - 3f(R_i)}{(R_i^2 - 1)} - 6C_{MN} \frac{R_i^2(2R_i^2 + 13) - 3(4R_i^2 + 1)f(R_i)}{(R_i^2 - 1)^2}, \\ \varsigma_4 &= C_{MN} \frac{16 + 83R_i^2 + 6R_i^4 - 15(4R_i^2 + 3)f(R_i)}{(R_i^2 - 1)^2}, \end{aligned} \quad (2.21)$$

and $f(R_i)$ is given by $f(R_i) = R_i/\sqrt{R_i^2 - 1} \operatorname{arccosh} R_i$. $R_i = a_z^i/a_x^i$ is the ratio of the parameters $a_{x,z}^i$ in the fitted exponential series between the elongated z and shortened x directions; note that $a_x^i = a_y^i$ for the statistically ellipsoid-of-rotation grains considered here.

For polycrystals with statistically equiaxed grains, the ratio $R_i = a_z^i/a_x^i$ is unity for all terms. The Rayleigh velocity limit for this equiaxed case is obtained by taking the limit of Equation 2.20 at $R_i \rightarrow 1$ and accounting for that $\lim_{R_i \rightarrow 1} f(R_i) = 1$ and the denominators are cancelled. This results in the expression below

$$\Delta_{M \rightarrow N} = \frac{(A_{MN} + B_{MN}/3 + C_{MN}/5)}{2\eta\rho^2 V_{0M}^2 V_{0N}^2} = \begin{cases} 2Q_{MM}^*, & N = M \\ 2Q_{M \rightarrow N}, & N \neq M \end{cases}. \quad (2.22)$$

A simple Rayleigh velocity limit expression can thus be obtained for equiaxed polycrystals as

$$V_M^R = \frac{V_{0M}}{1 + 2Q_{MM}^* + 2Q_{M \rightarrow N}}, \quad (2.23)$$

where $N \in \{L, T\}$ and $N \neq M$.

For the extreme case of $R_i \rightarrow 0$ that corresponds to the infinitely thin (in the z -direction) pancake-shaped grains, the Rayleigh velocity limit can be obtained by substituting $R_i = 0$ into Equation 2.20, leading to

$$\Delta_{M \rightarrow N} = \frac{A_{MN} + B_{MN} \cos^2 \theta_p + C_{MN} \cos^4 \theta_p}{2\eta\rho^2 V_{0M}^2 V_{0N}^2}. \quad (2.24)$$

For the extreme case of $R_i \rightarrow \infty$ that corresponds to ellipsoid-of-rotation grains with infinitely large axial dimension, its Rayleigh velocity asymptote as obtained from Equation 2.20 is

$$\Delta_{M \rightarrow N} = \frac{8A_{MN} + 4B_{MN} \sin^2 \theta_p + 3C_{MN} \sin^4 \theta_p}{16\eta\rho^2 V_{0M}^2 V_{0N}^2}. \quad (2.25)$$

It is important to realise that the Rayleigh velocity limit as influenced by grain elongation is bounded by the extreme values at $R_i \rightarrow 0$ (Equation 2.24) and $R_i \rightarrow \infty$ (Equation

2.25). Also, it immediately follows from Equations 2.24 and 2.25 that the velocity limit in the larger radius direction is the same for $R_i \rightarrow 0$ and $R_i \rightarrow \infty$: $V_M^{R_i \rightarrow 0}(\theta_p = \pi/2) \equiv V_M^{R_i \rightarrow \infty}(\theta_p = 0)$.

It is clear from Equation 2.23 that the coefficients of the TPC function cancel out for equiaxed polycrystals, suggesting that the phase velocity limit is solely related to the elastic properties of the polycrystals and is independent of grain geometry. As follows from Equations 2.19 and 2.20, however, the phase velocity limit for elongated polycrystals depends on grain shape and is thus dependent on the wave propagation direction θ_p , which will be discussed later in §6. The quasi-static limit is independent of frequency and the absolute values of the correlation radii $a_{x,z}^i$; it depends only on their ratio. The independence of the Rayleigh velocity limit on frequency and its dependence on grain shape are in direct contrast to the Rayleigh attenuation that is dependent on frequency and independent on the wave propagation direction. The analytical work provided here may be useful for investigating the influence of grain shape on static elastic moduli of polycrystals.

2.3.3 Stochastic asymptotes

Stochastic attenuation asymptote

The stochastic attenuation asymptote has been derived by Yang et al. [21] and provided in a normalised form by Li and Rokhlin [11] for elongated polycrystals with TPC statistics being represented by a single exponential (i.e., the summation over i in Equation 2.5 is not present). The derivation was based on the facts that the same mode scattering is dominant at the stochastic limit, namely $\alpha_M^S \approx \alpha_{M \rightarrow M}$, and the forward scattering is dominant in $\alpha_{M \rightarrow M}$. The derivation is not repeated here; readers are referred to Yang et al. [21] for details. This work follows the normalised form of Li and Rokhlin [11] and adapts it to the case of arbitrary crystallographic symmetry and multi-term generalized TPC function as follows

$$\alpha_M^S = k_{0M}^2 a_{CL}(\theta_p, \varphi_p) Q_{M \rightarrow M}, \quad (2.26)$$

where $Q_{M \rightarrow M} = (A_{MM} + B_{MM} + C_{MM}) / (4\eta\rho^2 V_{0M}^4)$ is the elastic scattering factor. $a_{CL}(\theta_p, \varphi_p)$ is the correlation length in the direction of wave propagation (θ_p, φ_p) as illustrated in Figure 2.1. For elongated polycrystals described by the generalized TPC function, it is given as

$$a_{CL}(\theta_p, \varphi_p) = \sum_{i=1}^n \frac{A_i}{\sqrt{\frac{\sin^2 \theta_p \cos^2 \varphi_p}{(a_x^i)^2} + \frac{\sin^2 \theta_p \sin^2 \varphi_p}{(a_y^i)^2} + \frac{\cos^2 \theta_p}{(a_z^i)^2}}}, \quad (2.27)$$

while for polycrystals with equiaxed grains, it is independent of propagation direction and is expressed as

$$a_{CL} = \sum_{i=1}^n A_i a_i. \quad (2.28)$$

Equation 2.26 demonstrates that attenuation obeys a second-power dependence on frequency at the high-frequency stochastic limit. Additionally, attenuation also depends on the elastic scattering factor $Q_{M \rightarrow M}$ and correlation length $a_{CL}(\theta_p, \varphi_p)$. It is important to note that for statistically ellipsoid-of-rotation grains, attenuation asymptote only changes with the angle θ_p because the correlation length a_{CL} is now a univariate function of θ_p .

Stochastic velocity asymptote

In contrast to the above analytical asymptotes, the stochastic velocity asymptote is derived only for polycrystals with equiaxed grains. The derivation is provided in Appendix B.3 and the final expression for the relative change of phase velocity at the stochastic limit is given by

$$\Delta_{M \rightarrow N} = \begin{cases} 5Q_{M \rightarrow M}/2 & N = M \\ 2Q_{MN}^*/(1 - V_{0M}^2/V_{0N}^2) & N \neq M \end{cases}, \quad (2.29)$$

where the elastic scattering factor $Q_{M \rightarrow M}$ has been given above, while $Q_{MN}^* = (A_{MN} + B_{MN} + C_{MN}) / (4\eta\rho^2 V_{0M}^2 V_{0N}^2)$ is an elastic factor introduced for simplification. The phase velocity at the stochastic limit can thus be obtained by substituting $\Delta_{M \rightarrow N}$ into Equation

2.11

$$V_M^S = \frac{V_{0M}}{1 + 5Q_{M \rightarrow M}/2 + 2Q_{M \rightarrow N}^*/(1 - V_{0M}^2/V_{0N}^2)}, \quad (2.30)$$

where $N \in \{L, T\}$ and $N \neq M$.

2.4 Far-field approximation

The above-presented SOA model involves the calculation of the Cauchy integral for the perturbed wave number. This difficulty can be eliminated by utilizing the far-field Green's function of scattered waves and the mean value theorem [26]. This leads to the far-field approximation (FFA) with the mass operator being given as [26]

$$m_{M \rightarrow N}(\mathbf{k}; \omega) = \frac{-k^2 V_{0M}^2 k_{0N}^2 Q_{M \rightarrow N}}{\pi} \int \frac{\exp(ik_{0N}r)}{r} w(\mathbf{r}) \exp(-i\mathbf{k} \cdot \mathbf{r}) d^3r, \quad (2.31)$$

where $\exp(ik_{0N}r)/r$ is the far-field Green's function for a scattered wave N . $Q_{M \rightarrow N}$ is the elastic scattering factor as stated above. $w(\mathbf{r})$ is the generalized TPC function given by Equation 2.5. By substituting the total mass operator, $m_M(\mathbf{k}; \omega) = \sum_{N=L,T} m_{M \rightarrow N}(\mathbf{k}; \omega)$, into the dispersion equation (Equation 2.1), the solutions for attenuation and phase velocity can be obtained. Equation 2.31 is for polycrystals with statistically ellipsoidal grains, and the integral in the equation reduces to a one-dimensional integral [26] for statistically ellipsoid-of-rotation grains. For equiaxed grains, Equation 2.31 further reduces to a closed form

$$m_{M \rightarrow N} = \frac{-8\pi a^2 k^2 V_{0M}^2 k_{0N}^2 Q_{M \rightarrow N}}{a^2 k^2 - (i + ak_{0N})^2}. \quad (2.32)$$

The modification of the mass operator mainly affects the near-field part of the total scattering field on inhomogeneities [26]. This results in a constant phase velocity shift of $V_M^R - V_{0M}$ across the whole frequency range. Thus, the velocity V_M obtained from the FFA model needs to be corrected by adding a constant $V_M^R - V_{0M}$, where V_M^R is the Rayleigh velocity limit of the SOA model as given in Equation 2.19.

The FFA model is valid in all frequency ranges including the geometric regime. In comparison to the SOA model, the FFA model uses additional approximations, making it more computationally efficient. On the other hand, the approximations to some extent reduce the accuracy of the FFA model. The potential reduction of accuracy is evaluated here by comparing it with the SOA model for polycrystalline CSP with elongated grains of triclinic symmetry. The resulting attenuation and phase velocity are provided in all frequency ranges in Figure 2.3(a) and (b) for longitudinal waves in the shortened and elongated directions of the grains; all parameters are specified in the figure caption.

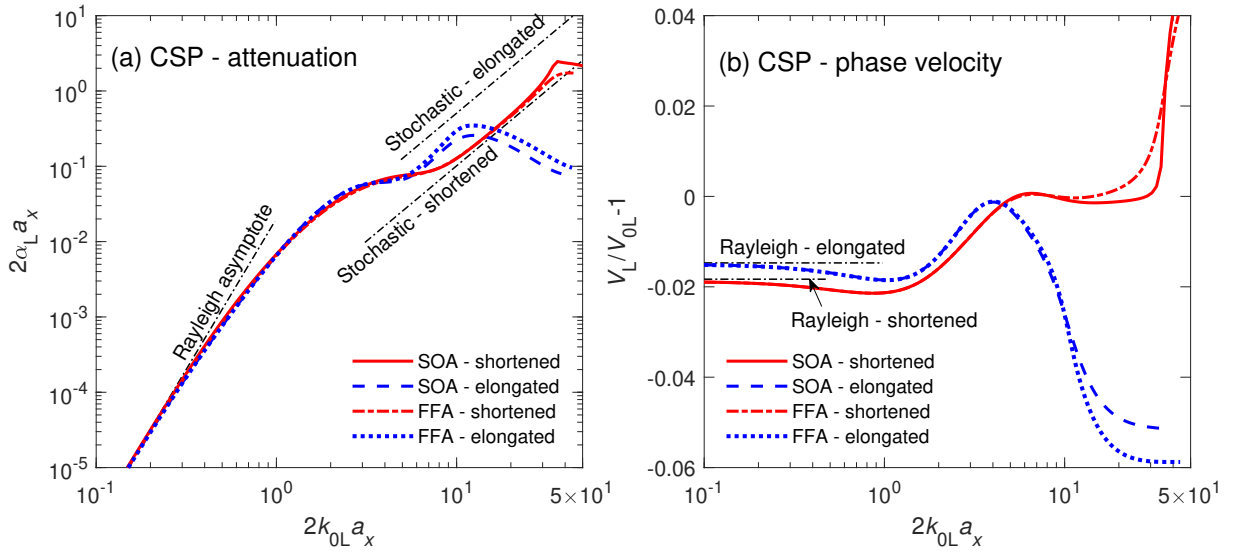


Figure 2.3: Comparison of the SOA and FFA models in all frequency regimes for the normalised (a) attenuation and (b) velocity of longitudinal waves. The results are given for polycrystalline CSP with elongated grains having an elongation ratio of 5. The mean grain radius of the polycrystal in the elongated z -direction, a_z , is 5 times those of the shortened x - and y -directions: $a_z = 5a_x = 5a_y$. The spatial autocorrelation of the polycrystal is represented by the generalized TPC function with coefficients being given in Table 3.3, and in this case, the mean grain radius in the shortened x -direction is determined from the slope at the origin of the generalized TPC function by $a_x = 1/\sum_{i=1}^n (A_i/a_x^i)$ (similarly for a_y and a_z). The elastic properties of the polycrystal are given in Table 3.2. The velocities of the FFA model have been corrected by using the approach provided in the context.

It is shown in the figure that the FFA model has a generally good agreement with the SOA model in the whole frequency range for both attenuation and velocity. The stochastic regime is not pronounced in the elongated direction due to the strong scattering that accelerates the transition to the geometric region. When comparing the results in Figure 2.3 for elongated and shortened grain directions, one needs to remember that the axes are normalised by the grain radius of the shortened direction, a_x , and therefore the transition

to the geometric region for propagation in the elongated grain direction occurs at about $2k_{0L}a_z = 50$ (where $a_z = 5a_x$ is the grain radius in the elongated direction).

As implied in Equations 2.1 and 2.31, the perturbed wave number k in the FFA model is a function of two independent elastic scattering parameters $Q_{M \rightarrow L}$ and $Q_{M \rightarrow T}$, which combine the effect of the 21 elastic constants that appear in the inner products of the SOA model. The excellent agreement between the SOA and FFA models means that the attenuation and velocity obtained from the SOA model also implicitly depend on the same two combinations, $Q_{M \rightarrow L}$ and $Q_{M \rightarrow T}$, of the elastic constants. As discussed later in §6, this allows the equivalency of different material systems to be established in terms of scattering-induced attenuation [26, 46].

2.5 Summary

This chapter first presents the theoretical SOA model for elastic waves propagating in polycrystals with equiaxed and elongated grains of arbitrary crystal symmetry. The model takes the elastic inner product and geometric TPC function of the polycrystals as input and calculates the attenuation and phase velocity of the propagating waves. Then, the Born approximation is introduced into the SOA model to deliver a simpler theoretical calculation and to derive the analytical Rayleigh and stochastic asymptotes. The Born approximation agrees very well with the SOA model at low frequencies but deviates as frequency approaches the geometric regime. Finally, the far-field approximation is outlined which significantly improves calculation efficiency while maintains a very good agreement with the SOA model across the whole frequency range.

Chapter 3

Three-dimensional finite element model

3.1 Introduction

The three-dimensional (3D) finite element (FE) method is presented in this chapter to numerically calculate scattering-induced attenuation and phase velocity dispersion for plane longitudinal waves propagating through polycrystals with statistically equiaxed and elongated grains. In comparison to the preceding theoretical models, the 3D FE method captures the actual wave interactions with grains without low-order scattering approximations, and it thus delivers a more accurate calculation of attenuation and velocity dispersion. This method is generally suitable for polycrystals with any grain shape, but the model description in this chapter focuses on polycrystals with elongated grains of statistically ellipsoid-of-rotation shape, of which polycrystals with statistically equiaxed grains are special cases.

In this chapter, the representation of polycrystals at grain scale is initially introduced in §3.2. This is followed by the description of spatial and temporal discretisation in §3.3 and the excitation of plane longitudinal waves in §3.4. Then, this chapter describes the determination of attenuation and phase velocity for the waves in §3.5 and the measurement of spatial autocorrelation function from the polycrystal models in §3.6. Finally, the quasi-static simulation method is presented in §3.7. The majority of this chapter is adapted from the manuscript [P3] that has been submitted for possible publication, while the description in §3.7 is reproduced from [P1], with the permission of AIP Publishing.

3.2 Representation of polycrystals at grain scale

The 3D FE method starts with the generation of a numerical material model with the dimensions of $d_x \times d_y \times d_z$ along the three coordinate axes. The model is composed of random grains created by the Voronoi tessellation method [52]. The grains are densely packed and fully bonded, and they have statistically equiaxed shape; typical equiaxed grains are shown in Figure 3.1(a). To simulate elongated grains, the equiaxed model is then scaled by using the scale factors of $S_x \times S_y \times S_z = (1 \times 1 \times R)/\sqrt[3]{R}$, leading to a stretched model with the dimensions of $d_x S_x \times d_y S_y \times d_z S_z$. The constituting grains of the stretched model are elongated in the z -direction with an elongation ratio of R and the average shape of the grains is ellipsoid-of-rotation; typical elongated grains are shown in Figure 3.1(b). The scale factors are chosen such that $S_x \cdot S_y \cdot S_z = 1$, which are used to ensure that the volume of each grain remains unchanged during the scaling and to enable a direct comparison between equiaxed and elongated cases.

In order to simulate the wave propagation in the off-symmetry axis direction with an angle of θ_p to the grain elongation direction, the stretched model is rotated about the x -axis with the desired angle θ_p . The outer surfaces of the rotated model are no longer normal to the coordinate axes which complicates wave excitation and monitoring. This problem is averted by creating a sufficiently large equiaxed model and then by cropping its stretched and rotated counterpart to achieve the dimensions of $d_x S_x \times d_y S_y \times d_z S_z$ along the coordinate axes. The models created for this thesis are listed in Table 3.1. For equiaxed polycrystals ($R = 1$), the average grain diameter D in the table refers to the cubic root of average grain volume $\bar{v}$: $D = \sqrt[3]{\bar{v}}$; for elongated ones ($R = 5$), it is direction dependent and is determined by $D(S_x \times S_y \times S_z)$ for the three coordinate axes. This dimensional parameter differs from the extensively-used mean grain radii $a_{x,y,z}$ of this thesis which correspond to the slopes at the origin of the generalized two-point correlation function in the respective directions.

The generated models are further assigned with material properties. This work employs nine single-phase polycrystalline materials with properties being given in Table 3.2. Eight materials possess the highest crystal symmetry of cubic and one material (CSP, copper sulfate pentahydrate) has the lowest symmetry of triclinic; all materials have greatly

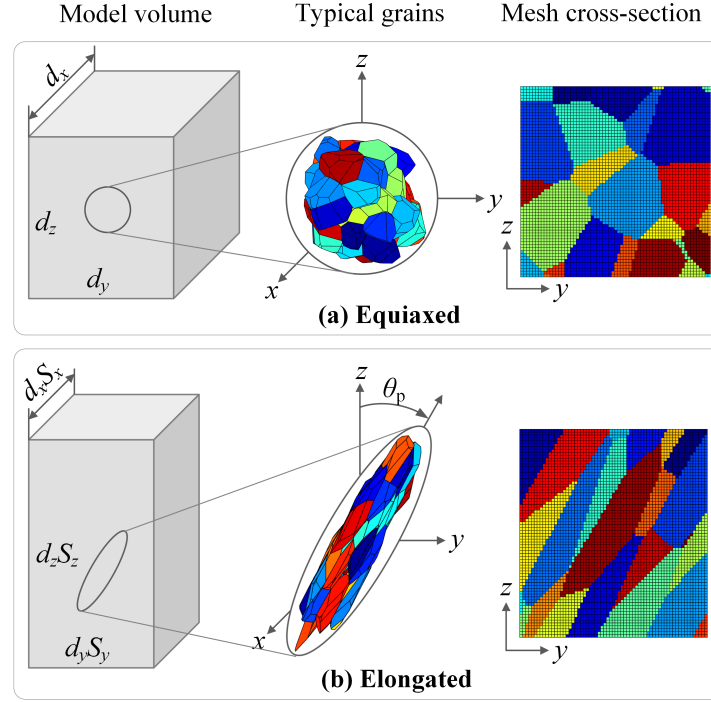


Figure 3.1: Illustration of 3D FE models for polycrystalline materials with statistically (a) equiaxed and (b) elongated grains. The equiaxed model in (a) has the dimensions of $d_x \times d_y \times d_z$. The elongated model in (b) is generated through 1) scaling a large equiaxed model by using the scale factors of $S_x \times S_y \times S_z = (1 \times 1 \times R)/\sqrt[3]{R}$ with an elongation ratio of $R = 5$, 2) rotating the scaled model about the x axis with an angle of θ_p , and 3) cropping the rotated model to the desired dimensions of $d_x S_x \times d_y S_y \times d_z S_z$. The rightmost images show the cross-sections of the grains discretised with uniform 8-node linear "brick" elements.

Table 3.1: Polycrystalline models. Elongation ratio R , dimensions $d_x \times d_y \times d_z$ (mm), average grain diameter D (mm, cubic root of average grain volume), number of grains N , mesh size h (mm), degree of freedom d.o.f..

Model	R	$d_x \times d_y \times d_z$	D	N	h	d.o.f.
N115200	1	$12 \times 12 \times 100$	$0.5 \times 0.5 \times 0.5$	115200	0.05	349×10^6
N11520	1	$12 \times 12 \times 10$	$0.5 \times 0.5 \times 0.5$	11520	0.025	278×10^6
	5	$7.02 \times 7.02 \times 29.24$	$0.29 \times 0.29 \times 1.46$			
N16000	1	$20 \times 20 \times 5$	$0.5 \times 0.5 \times 0.5$	16000	0.02	755×10^6
	5	$11.70 \times 11.70 \times 14.62$	$0.29 \times 0.29 \times 1.46$			
N12250	1	$17.5 \times 17.5 \times 5$	$0.5 \times 0.5 \times 0.5$	12250	0.017	967×10^6
	5	$10.23 \times 10.23 \times 14.62$	$0.29 \times 0.29 \times 1.46$			

differing anisotropy factors. The grains of each model share the same material mass and elastic properties but face different directions in terms of crystallographic orientation. To enable a direct comparison with the theoretical SOA models, each FE model is made

3. Three-dimensional finite element model

statistically homogeneous by uniformly randomly assigning crystallographic orientations to the grains. In this case, a polycrystal model with equiaxed grains exhibits elastic isotropy on the macro scale. However, the randomness in crystallographic orientation does not induce the same isotropy to a polycrystal with elongated grains. Instead, an elongated polycrystal exhibits macroscopic anisotropy as a result of grain elongation, and it is specifically transversely isotropic for a polycrystal with ellipsoid-of-rotation grains as addressed in the present FE model.

Table 3.2: Polycrystalline materials. Elastic constants c_{ij} (GPa), density ρ (kg/m³), Voigt velocities V_L and V_T (m/s), anisotropy factor A [53], universal anisotropy factor A^U [54], elastic scattering factors $Q_{L \rightarrow L}$ and $Q_{L \rightarrow T}$ ($\times 10^{-3}$). CSP is short for Copper Sulfate Pentahydrate [26, 55].

		c_{11}	c_{12}	c_{44}	ρ	V_L	V_T	A	A^U	$Q_{L \rightarrow L}$	$Q_{L \rightarrow T}$
Cubic symmetry	Aluminium	103.4	57.1	28.6	2700	6318	3128	1.24	0.05	0.08	0.33
	A1.5	262.1	136.5	95.3	8000	6001	3207	1.52	0.21	0.39	1.43
	A1.8	251.7	141.7	100.5	8000	6001	3207	1.83	0.45	0.76	2.79
	A2.4	237.1	149.0	107.8	8000	6001	3207	2.45	1.03	1.49	5.48
	Inconel	234.6	145.4	126.2	8260	6025	3366	2.83	1.42	2.26	7.59
	Copper	169.6	122.4	74.0	8935	4847	2455	3.14	1.75	1.76	7.19
	A5.0	210.6	162.1	121.0	8000	6000	3207	5.00	3.84	3.44	12.66
	Lithium	13.4	11.3	9.6	534	6157	3402	9.14	8.70	5.44	18.70
Triclinic symmetry	CSP	c_{11}	c_{12}	c_{13}	ρ	V_L	V_T	A	A^U	$Q_{L \rightarrow L}$	$Q_{L \rightarrow T}$
		56.5	26.5	32.1	2286	4874	2303	-	0.95	3.23	7.19
		c_{14}	c_{15}	c_{16}	c_{22}	c_{23}	c_{24}	c_{25}	c_{26}	c_{33}	c_{34}
		-3.3	-0.8	-3.9	43.3	34.7	-0.7	-2.1	2.0	56.9	-4.4
		c_{35}	c_{36}	c_{44}	c_{45}	c_{46}	c_{55}	c_{56}	c_{66}		
		-2.1	-1.6	17.3	0.9	0.3	12.2	-2.6	10.0		

3.3 Discretisation of polycrystals in space and time

The generated models are spatially discretised in order to be solved by the FE method. This thesis uses a structured mesh that subdivides a spatial model into uniform 8-node linear "brick" elements. Example cross-sections of the 3D meshes are illustrated in Figure 3.1(a) and (b) for equiaxed and elongated grains, respectively. For the models involved in this thesis, their mesh sizes h (the edge sizes of the elements) are provided in Table

3.1. The choice of mesh size depends on two determining factors. The first is to minimise numerical errors, and a satisfactory mesh size is chosen to be smaller than one tenth of the simulated wavelength [38], which will be studied in-depth in §4. The second factor is to ensure that grain geometries are accurately characterised by the structured mesh. In this thesis, the element size is chosen to be twenty times smaller than the average grain diameter D (the cubic root of average grain volume). For equiaxed grains, it has been shown [38] that this choice makes the structured mesh perform equally as well as an unstructured mesh that is capable of perfectly describing planar grain boundaries. For elongated grains, however, a possibility exists that such a mesh size choice may not be able to properly describe their sharp tips. Thus, it is essential to evaluate this possibility in order to deliver a satisfactory representation.

The model N11520 with elongated grains is used for the evaluation because it has the largest mesh size among the models adopted for simulating elongated polycrystals. The evaluation utilizes grain cross-sectional area as a measure to identify the difference of grain geometry before and after discretisation. The measured statistics are plotted in Figure 3.2. In the figure, the x -axis represents the grain cross-sectional area A_g as normalised by the area $A_e = 0.025 \times 0.025 \text{ mm}^2$ of an element face. The y -axis indicates the probability p of occurrence of a given cross-sectional area. The lines and points are measured on the models before and after discretisation, respectively. For each coordinate direction of the un-discretised model, 1000 cross-sections normal to this direction are randomly chosen. The intersections of the grains and the chosen cross-sections are identified and the areas A_g of the intersections are then counted to acquire the statistics. For each direction of the discretised model, the acquisition visits all discrete cross-sections that are perpendicular to the given direction and similarly counts the intersected areas between the grains and the cross-sections. For both cases, their z -direction statistics (dash-dotted line and triangles) are further normalised before plotting: the area A_g is multiplied by the elongation ratio $R = 5$ and the probability p is divided by the same ratio.

The figure shows that the statistics for individual directions are overlapped, meaning that the desired grain elongation has been well reproduced in both un-discretised and discretised models. A clear difference between the lines and points can be observed from the figure at cross-sectional areas A_g below $3A_e$. This is because some very small grain

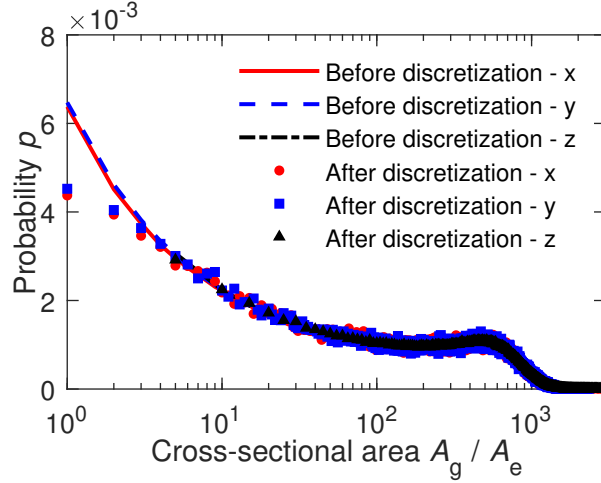


Figure 3.2: Comparison of grain cross-sectional area statistics measured before and after discretisation. The model N11520 with elongated grains is used for the measurement of the shown statistics. A_g represents the cross-sectional areas of the grains and A_e the area of an element face. Lines and points are measured on the models before and after discretisation, respectively. z -direction statistics (dash-dotted line and triangles) have been normalised: the A_g on the horizontal axis is multiplied by the elongation ratio $R = 5$ and the probability p on the vertical axis is divided by the same ratio.

cross-sections, closer to the sharp tips of the grains, or simply in small grains in the un-discretised material model, are underrepresented in the discretised model, since the elements of the discretised model are uniformly sized cubes. However, according to the mesh convergence study by Van Pamel et al. [38], this underrepresentation of small grain cross-sections by structured meshes only induces a very small simulation uncertainty to attenuation and phase velocity. It was shown [38] that attenuation converges to within 1% (velocity has a better convergence) when the number of elements per average grain diameter is approximately 10 ($D/h \approx 10$), while in this work there are at least 11.70 elements per grain diameter even for the shortened direction (for N11520 with the coarsest mesh, $(D/\sqrt[3]{R})/h = 11.70$). Nonetheless, it is important to note that there might be a few very sharp tips in the elongated direction that can hardly be represented by structured meshes; this needs further investigation.

In addition to spatial discretisation, the sampling of time is also necessary for the elastodynamic FE method. For this purpose, time is partitioned into discrete instances having a uniform step Δt between adjacent instances. The time step is defined by the Courant-Friedrichs-Levy condition: $\Delta t = Ch/V_{\max}$. C is the Courant number and it being not

greater than unity, namely $C \leq 1$. $V_{\max}$ is the peak phase velocity of a polycrystalline material. This condition designates the time step being at most equal to the smallest propagation time within the discrete space, and it ensures incremental solution of the elastodynamic problem, stably and accurately.

3.4 Excitation of plane longitudinal waves

This work simulates the propagation of plane longitudinal waves within the above generated polycrystal models. Without loss of generality, the wave vector direction is confined to the z -direction. To achieve the plane wave modality, symmetry boundary conditions (SBCs) are applied to the four outer x - z and y - z surfaces of a cuboid model to constrain their out-of-plane motions. These mirror-like outer surfaces repeatedly mirror the FE model along the surfaces and it effectively represents an infinite volume through which plane waves can be transmitted.

To excite a longitudinal wave propagating in the z -direction, a three-cycle Hann-windowed toneburst signal is applied as a uniformly distributed force in the z -direction to all of the nodes on the x - y surface at $z = 0$. As mentioned in §3.2 and will be demonstrated in §6, an FE model exhibits transverse isotropy on the macro scale as a result of grain elongation, even when the material crystallography is macro-isotropic; it will be observable also that the effective macroscopic anisotropy caused by grain elongation is frequency dependent. Thus, for the wave excitation in the off-symmetry axis directions ($\theta_p \neq 0^\circ, \theta_p \neq 90^\circ$; see Figure 3.1(b)), the actual FE particle displacements are not aligned strictly to the z -direction of wave propagation. As a result, the longitudinal wave manifests as a quasi-longitudinal wave with a skew angle between the polarization and propagation directions [56]; and, in addition to the plane quasi-longitudinal wave, small amplitude quasi-transverse modes may be excited in this setup. However, the effect of quasi-transverse waves is negligible in the studied cases as the elastic anisotropy caused by grain elongation is small (for reference, the largest skew angle for the studied materials is estimated to be smaller than 0.1° at the quasi-static limit). In fact, we were unable to determine any effect of this mode impurity in the results of the FE simulations. Ideally, when the z -axis is directed off the grain elongation axis, exciting a pure longitudinal wave propagating in

the z -direction would require the application of forces in both parallel and perpendicular directions to the z -direction. This exact loading condition, however, is not pursued in this work because the motion perpendicular to the z -direction has been constrained on boundaries associated with the SBCs.

3.5 Determination of attenuation and phase velocity

The setup of the FE models is now complete and the models can be solved with the elastodynamic time marching method. While the spatial problem is represented by finite element discretisation using first-order 8-node regular hexahedral elements, the time-stepping solution is based on the finite difference method, using the well-known equilibrium equation

$$\mathbf{M} \frac{\mathbf{U}^{n+1} - 2\mathbf{U}^n + \mathbf{U}^{n-1}}{\Delta t^2} + \mathbf{K}\mathbf{U}^n = \mathbf{F}, \quad (3.1)$$

where $\mathbf{F}$ is the dynamic load vector describing externally applied forces at individual degrees of freedom. $\mathbf{M}$ and $\mathbf{K}$ are the mass and stiffness matrices, so $\mathbf{K}\mathbf{U}^n$ is the elastic force vector, with $\mathbf{U}^n$ representing the global displacement vector at time step n . $\mathbf{M}\ddot{\mathbf{U}}^n$ is the inertia force, and the acceleration vector $\ddot{\mathbf{U}}^n$ therein is represented by a standard central difference as $(\mathbf{U}^{n+1} - 2\mathbf{U}^n + \mathbf{U}^{n-1})/\Delta t^2$. The equilibrium equation establishes the relation of displacements at three time steps $n - 1$, n , and $n + 1$. Re-arranging the equation allows the displacements at step $n + 1$ to be determined explicitly from those already known at the two preceding steps. Material damping is neglected in this work.

Equation 3.1 is solved by using the FE program Pogo [37], which is tailored for fast, large-scale elastodynamic simulations via parallel GPU computing. Over the course of simulation, the z -direction displacements are monitored across all nodes and at all time steps on the transmitting, $z = 0$, and receiving, $z = d_z$, surfaces. Spatial averaging these two sets of displacements over the respective nodes at each time step leads to the coherent transmitted and received signals, denoted as $U(0; t)$ and $U(d_z; t)$. The frequency-domain signals, $U(0; f)$ and $U(d_z; f)$, are then obtained by Fourier transforming the windowed time-domain signals. Frequency-dependent attenuation is then obtained by comparing

the amplitudes of the signals: $\alpha(f) = -\ln[A(d_z; f)/A(0; f)]/d_z$, where A denotes the amplitude part of U . Similarly, the frequency-dependent phase velocity is calculated by comparing the phases of the signals: $V(f) = 2\pi f d_z / [\phi(0; f) - \phi(d_z; f)]$, where ϕ represents the unwrapped phase of U . The determination of attenuation and phase velocity will be further studied in §4, in which typical coherent signals, attenuation and phase velocity results will be provided.

It is important to realise that different models are used in different frequency ranges to achieve a similar calculation accuracy across the entire frequency range; the centre frequencies used for the models are provided in Table 3.1. Also, a large number of grains are included in each FE model, ensuring the attenuation and phase velocity determined from a single FE material model will incorporate a significant amount of scattering information. Despite this statistical significance of a single model, a combination of multiple realizations (unless otherwise specified, this thesis uses 15 realizations) is used to get converged phase velocity and attenuation results for a given material in a given frequency range. For each case, the multi-realizations are generated by using the same grain structures and re-randomizing the crystallographic orientations of the grains. This approach has been shown to preserve the same statistical variability as the ideal approach of re-randomizing both grain structures and grain orientations [29]. Therefore, one may be confident to use this method to save the intensive computational costs used to re-mesh the spatial models.

3.6 Generalized representation of two-point correlation function

It has been mentioned above that the geometric characteristics of polycrystals are represented by the two-point correlation (TPC) function. This function needs to be accurately determined from the FE material models such that it can be incorporated into the theoretical models for direct comparison.

The procedure for measuring TPC data from 3D FE material models has been previously reported for equiaxed grains [28]. The measurement randomly drops a large number of point pairs into a polycrystal model. The two points of each pair are separated by a

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distance of r . The measurement then counts the number of pairs whose two points occur in the same grain and compares this number to the total number of pairs to obtain the correlation probability $w(r)$. A significant number of tests are generally required to obtain a statistically converged probability and a satisfactory convergence is found in the present study by using 1 million tests per discrete r . For the model N11520 with equiaxed grains, its TPC data is given in Figure 3.3 as rectangular points. This TPC data will also be used to represent other equiaxed material models of this thesis, because all models have sufficiently large numbers of grains and their TPC statistics are fundamentally the same. This also applies to the elongated material models discussed below.

The above procedure can be easily extended to 3D FE material models with statistically elongated grains. The TPC function is now a function of vector distance $\mathbf{r} = r(\sin \theta_p \cos \varphi_p, \sin \theta_p \sin \varphi_p, \cos \theta_p)$. For convenience, the angles θ_p and φ_p describing the direction of incident wave (see Figure 3.1) are used here to define the orientation of two test points. For statistically axisymmetric grains simulated in this thesis, the TPC function only depends on angle θ_p when the elongated direction is aligned with the z -axis of the coordinate system. As shown later in §6, this thesis simulates wave propagation at eight different angles of 0° , 15° , 18.75° , 30° , 45° , 60° , 75° , and 90° . To maintain consistency with actual simulations, the TPC function is also measured at these angles from the FE material system. For each angle θ_p , the correlation probability $w(r, \theta_p, \varphi_p = 0)$ is determined in the same way as the above equiaxed case, except that the orientation of every test pair is confined to the given angle. For the model N11520 with elongated grains, its TPC statistics are provided in Figure 3.3 as circular points. For a clean presentation, the figure only provides statistics for the angles of 0° , 15° , 30° , 45° , and 90° .

It is important to note that the measurements are performed on the FE material models before their discretisation. §3.3 has demonstrated that the small cross-sections of the elongated grains are not well represented by structured meshes. This raises a question of whether the TPC data measured on an un-discretised model also accurately delivers the information of its discretised counterpart. To answer this question, the TPC statistics are also numerically measured from the discretised N11520 model at the angles of 0° and 90° . The resulting TPC data points are indistinguishable from those shown in Figure 3.3 for both angles, indicating the validity of using the TPC data of an un-discretised model

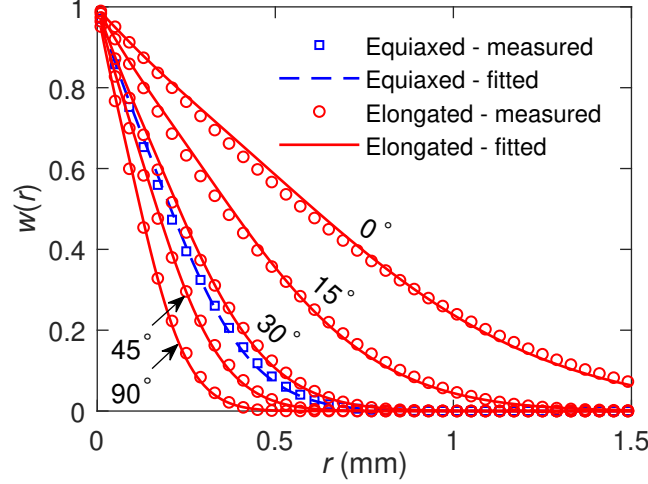


Figure 3.3: Two-point correlation (TPC) functions for polycrystals with equiaxed and elongated grains. The rectangular and circular points are measured from the model N11520 with equiaxed and elongated grains, respectively. For a clean presentation, data points are only shown for the angles of 0° , 15° , 30° , 45° and 90° , and not for 18.75° , 60° , 75° although they are used as propagation angles in FE simulations. The dash and solid lines denote the fitted TPC functions for the equiaxed and elongated polycrystals, respectively.

to describe its discretised counterpart.

Measured TPC data needs to be fitted into a mathematical function so that it can be incorporated into theoretical models. For equiaxed grains, a multi-term exponential series, $w(r) = \sum_i A_i \exp(-r/a_i)$, was used to best fit the measured data [28]. Although special care should be taken in using this exponential fitting [57], satisfactory coefficients A_i and a_i can be found for an equiaxed case that assure proper TPC decay outside of the fitting range. For the model N11520, its fitted TPC function is plotted in Figure 3.3 as a dash line and it is clear that this function matches very well with the original rectangular points of the actual TPC. The coefficients of the fitted function are given in Table 3.3.

For elongated grains, the TPC function can be similarly obtained by fitting an exponential series to the measured data. However, the extra dependence of the TPC function on θ_p complicates the fitting process, and it generally requires a significant number of trial and error calculations to get a good fit. This difficulty is avoided in this work by utilizing the fact that elongated grains are generated by scaling equiaxed ones as described in §3.2. As a result of this scaling, the TPC function of the elongated case is directly obtained from that of the equiaxed case by using the same scaling law.

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Table 3.3: Coefficients of generalized two-point correlation functions for polycrystals with equiaxed and elongated grains. For the elongated case, its coefficients A_i are the same as those of the equiaxed case, while its coefficients a_x^i , a_y^i , and a_z^i are scaled from the equiaxed counterparts a_i by $(a_x^i, a_y^i, a_z^i) = a_i(1, 1, R)/\sqrt[3]{R}$, $R = 5$.

TPC terms	Equiaxed case		Elongated case			
	A_i	a_i	A_i	a_x^i	a_y^i	a_z^i
1	-2922.66	0.1157	-2922.66	0.0677	0.0677	0.3384
2	-10.62	0.1722	-10.62	0.1007	0.1007	0.5036
3	3914.37	0.1108	3914.37	0.0648	0.0648	0.3240
4	-3305.68	0.1032	-3305.68	0.0604	0.0604	0.3018
5	696.92	0.0910	696.92	0.0532	0.0532	0.2662
6	54.36	0.1523	54.36	0.0890	0.0890	0.4452
7	-42.47	0.0724	-42.47	0.0423	0.0423	0.2116
8	1616.78	0.1108	1616.78	0.0648	0.0648	0.3240

Following the scaling law, the TPC function of the elongated case is given as

$$w(r, \theta_p, \varphi_p) = \sum_i A_i \exp \left(-r \sqrt{\frac{\sin^2 \theta_p \cos^2 \varphi_p}{(a_x^i)^2} + \frac{\sin^2 \theta_p \sin^2 \varphi_p}{(a_y^i)^2} + \frac{\cos^2 \theta_p}{(a_z^i)^2}} \right), \quad (3.2)$$

where the coefficients A_i are the same as those of the equiaxed case. The coefficients a_x^i , a_y^i , and a_z^i are scaled from those of the equiaxed case a_i by using the scale factors: $(a_x^i, a_y^i, a_z^i) = a_i(1, 1, R)/\sqrt[3]{R}$.

The resulting coefficients of the TPC function of the elongated case are given in Table 3.3. The scaled TPC function is plotted in Figure 3.3 as solid lines for the angles θ_p where the measured data points from the FE material model are also provided. The figure shows that the scaled function agrees very well with the measured data points for the shown angles, indicating the effectiveness of the scaling approach.

3.7 Quasi-static simulation

The quasi-static phase velocity limit of a polycrystal is related to the macroscopic effective elastic constants of the medium. This velocity limit can be determined by obtaining effective stiffness from static FE analyses, but it requires the solution (equivalent to inversion) of the full stiffness matrix, which is beyond possibility with the large FE models.

However, it was previously reported [28] that the elastodynamic FE solver [37] can be applied in a special way to determine the quasi-static velocity. This thesis further elaborates this methodology, and in particular reports on its accuracy.

In comparison to the above outlined dynamic models, four changes are made to achieve quasi-static modelling. First, an additional boundary condition is defined for the outer surface $z = d_z$ by constraining the z -displacements of the nodes on the surface. Second, a distinct loading condition is used to emulate static loading and deformation while retaining the time marching elastodynamic solution methodology. This is achieved by gradually applying a load to the FE model and keeping the final state of this load as a constant. The load is applied as a uniformly distributed force in the z -direction to all of the nodes on the x - y surface at $z = 0$. Then, material damping is introduced to allow a steady state to be reached after a sufficient period of time. In order to reach the desired steady state as fast as possible, an optimal damping factor is selected such that the compression mode of the simulated model is nearly critically damped. Lastly, the z -displacement is monitored only on the transmitting surface, $z = 0$, since the opposite surface, $z = d_z$, is now being constrained. Typical signals for applied load and displacement response are illustrated in Figure 3.4, which are spatially averaged over the transmitting surface. Upon obtaining the steady-state load F and displacement u , the stress and strain of a simulated model are determined by $\sigma = F/A$ and $\varepsilon = u/d_z$, where A is the surface area of the model at $z = 0$ while d_z is the length of the model. Consequently, the longitudinal modulus is obtained as $C_{11} = \sigma/\varepsilon$ and the longitudinal wave velocity is calculated by $V_L^{\text{st}} = \sqrt{C_{11}/\rho}$. To illustrate its accuracy, this method is utilized to calculate the quasi-static velocity of

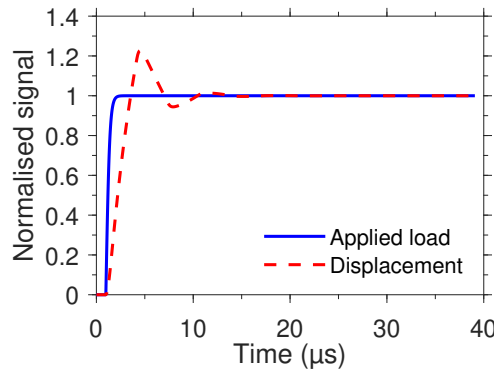


Figure 3.4: A typical example of loading and displacement in quasi-static modelling for CSP.

the homogeneous, isotropic steel ($E = 210$ GPa, $\nu = 0.3$, $\rho = 8000$ kg/m³) with the FE model N115200 as provided in Table 3.1. The resulting quasi-static longitudinal velocity is 5944.0796 m/s, which only has a very small relative difference of 0.0063% as compared to the exact velocity of 5944.4544 m/s. This indicates that the quasi-static FE method can deliver a highly accurate prediction of static velocities.

3.8 Summary

In this chapter, a 3D FE model is implemented for plane longitudinal waves propagating in polycrystals with statistically equiaxed grains and elongated grains with an average shape of ellipsoid-of-revolution. Each realisation represents a material volume comprising specific randomly shaped grains that are contiguous without gaps or overlaps. It simulates wave propagation in realistic sample volumes of a significant number of grains and considers the contribution of all possible multiple scattering. It outputs the attenuation and phase velocity of the propagating waves by post-processing the coherent signals measured during FE simulations. The spatial autocorrelation of the FE material models can be accurately determined and mathematically represented by generalized TPC functions, which can be further incorporated into theoretical models for a direct comparison of the theoretical and FE models. Also, the FE model is modified in order to calculate the quasi-static limit of phase velocity, showing a good accuracy for a homogeneous material example.

Chapter 4

Maximizing the accuracy of the finite element model

4.1 Introduction

Due to the flexibility and accuracy of the 3D FE method, a surge of modelling studies is expected in the future to understand and optimize practical inspection problems, and to evaluate the approximations of theoretical models for model-based applications, such as the inverse characterisation of microstructure. However, even for the relatively simple cases addressed so far [28, 29, 38, 39], some essential topics are not yet understood well enough to allow confidence that the best accuracy of simulation is being achieved. The author has been investigating this challenge, and the purpose of this chapter is to report on important topics of modelling methodology for which new knowledge will inform a reliable quality of simulation performance.

The first topic is the determination of effective media parameters, namely attenuation and phase velocity, from the simulation results. As stated in §3.5, one can perform the determination in a through-transmission configuration, which is commonly used in actual experiments where access is limited to sample surfaces and which has also seen wide applications in previous simulations [28, 29, 38]. Alternatively, one can also determine the parameters by best fitting the waves acquired on multiple surfaces within the simulation volume that are parallel to the transmitting surface. This fitting method was first used in

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a recent work [39] and it is made possible by the intrinsic advantage of FE modelling that waves inside a sample can be easily measured. Each of these two methods has its own advantages: the through-transmission method is consistent with physical experimental configurations, so it is conceptually attractive, and it requires relatively little measured data, while the fitting method can potentially provide more abundant information about wave-microstructure interaction. However, these two methods have not been compared in actual simulations to identify their ranges of application and their possible advantages and drawbacks. It is important to recognize that while the difference between these methods would be trivial for a homogeneous material, this is not the case for a polycrystal: the grain scattering creates high levels of noise in the measurements of the coherent signals as well as local influences of multiple scattering, both of which bring significant uncertainty to the measurements.

The second topic concerns the errors and uncertainties of the determined scattering parameters. It is known that numerical approximations, including the space and time discretization in the FE method and the inexactness in finite-precision computations, can cause numerical errors. In addition, statistical considerations, involving the random distribution of grain structures and the stochastic pattern of wave scattering, can induce both statistical errors and uncertainties. For numerical errors, studies so far were partly limited to homogeneous and isotropic materials [58,59] and were partly qualitative when they went to polycrystalline materials [29,38]; while for statistical errors and uncertainties, attention has not yet been turned to the specific problem of wave propagation within polycrystals.

The third of the three topics of study involves the evaluation of the performance of theoretical models using the simulation data of 3D FE modelling. The simulations are ideal for the evaluation of the effects of the approximations of theoretical models, as they can be fully controlled, and their errors and uncertainties can to some extent be estimated. The evaluation requires the statistical information of FE material systems being measured and being put into theoretical models. As demonstrated in §3.6, such information is represented by the two-point correlation (TPC) function for widely used theoretical models, like the second-order [14,17,28,39] and far-field [26] approximations. Previous studies [28,39] have been successful in incorporating the TPC function of polycrystal models into theoretical models, and have shown good agreement between FE and theoretical results in

terms of scattering parameters. However, these studies neglected in their TPC functions the fact that symmetry boundary conditions actually mirror the boundary grains of FE models and thus make the grains doubled in volume.

This chapter presents a thorough discussion of the above-mentioned topics, with the aim to solve them appropriately. The discussion focuses on the propagation of plane longitudinal waves in polycrystals with untextured properties and equiaxed grains, while the ultimate goal is to lay a foundation for the general cases of arbitrary wave modalities in any polycrystalline material system. §4.2 deals with the determination of effective media parameters. §4.3 presents a systematic study of errors and uncertainties, with discussions on how to suppress them. §4.4 provides a comprehensive discussion covering the proper consideration of symmetry boundary conditions in the TPC function. This chapter is reproduced from [P2], with the permission of AIP Publishing.

4.2 Determination of attenuation and phase velocity

4.2.1 Coherent waves

To calculate attenuation and phase velocity, displacements are numerically measured on planes normal to the propagation direction. In the case of plane longitudinal waves travelling in the z -direction as addressed in this thesis, z -displacements are acquired on cross-sections normal to the z -direction. Note that the displacement needs to be divided by 2 if the cross-section is the stress-free end at $z = d_z$, as the displacement is the sum of the incident and (equally) reflected waves. For an arbitrary cross-section $z = z_0$, the obtained displacement field is denoted as $u(x, y, z_0; t)$. The model length d_z for the z -direction will be used repeatedly hereafter, and for brevity, it will be simplified as d .

As a result of grain scattering, the phase of the wave $u(x, y, z_0; t)$ varies across points on the cross-section. The coherent part of this wave can be obtained by averaging this wave across the cross-section [60]; i.e. $U(z_0; t) = \langle u(x, y, z_0; t) \rangle_{x,y}$, where $\langle \cdot \rangle_{x,y}$ represents the spatial average over all points on the surface $z = z_0$. In the case of FE modelling, a significant number of nodes across the wavefront $z = z_0$ contribute to the average and thus

4. Maximizing the accuracy of the finite element model

significant wave information is included in the coherent wave. Fourier transforming this coherent wave with respect to time t leads to its counterpart $U(z_0; f)$ in the frequency domain. Upon obtaining the coherent waves for two or more cross-sections, the two effective media parameters can be conveniently calculated which will be discussed in the following subsection.

In addition to the coherent part, there is the incoherent, fluctuation part in the total field $u(x, y, z_0; t)$ which scatters with a random phase across the wavefront and therefore its average over the cross-section is zero [60]. Although this fluctuation part is discarded in the calculation of effective media parameters, it is used below to demonstrate the level of scattering over a cross-section. For a clearer demonstration, the fluctuation part is normalised by the coherent part and denoted as $u_f(x, y, z_0; t) = [u(x, y, z_0; t) - U(z_0; t)] / U(z_0; t)$.

Here an example is used to illustrate coherent waves and fluctuations on wavefronts. The example simulates a plane longitudinal wave travelling in the model N11520 (Table 3.1) using the material properties of Inconel (Table 3.2). The wave is excited with a centre frequency of 5 MHz. The z -displacement fields are recorded and denoted as $u(x, y, 0; t)$ and $u(x, y, d; t)$ for the transmitting $z = 0$ and receiving $z = d$ surfaces, respectively.

In the time domain, the spatial averages of the displacement fields, namely $U(0; t) = \langle u(x, y, 0; t) \rangle_{x,y}$ and $U(d; t) = \langle u(x, y, d; t) \rangle_{x,y}$, are calculated and plotted in Figure 4.1(a). For these two coherent signals, Figure 4.1(b) and (c) provide their corresponding fluctuations $u_f(x, y, 0; t_1)$ and $u_f(x, y, d; t_2)$ at the time instances of $t_1 = 0.30 \times 10^{-6}$ s and $t_2 = 1.98 \times 10^{-6}$ s, respectively. As shown in Figure 4.1(a), the time instances t_1 and t_2 are chosen such that the coherent signals are at their maxima.

To obtain the spectral fields $u(x, y, 0; f)$ and $u(x, y, d; f)$, the time-domain fields are cropped by using the time windows that span from $t = 0$ to the vertical marks shown in Figure 4.1(a) and then transformed to the frequency domain by utilizing the Fourier transform. Spatial averaging these spectral fields leads to the coherent parts $U(0; f) = \langle u(x, y, 0; f) \rangle_{x,y}$ and $U(d; f) = \langle u(x, y, d; f) \rangle_{x,y}$, whose amplitude spectra are plotted in Figure 4.1(d). At the frequency of f_0 where the transmitting amplitude is at its maximum, the amplitude fluctuations $u_f(x, y, 0; f_0)$ and $u_f(x, y, d; f_0)$ are illustrated in Figure 4.1(e) and (f).

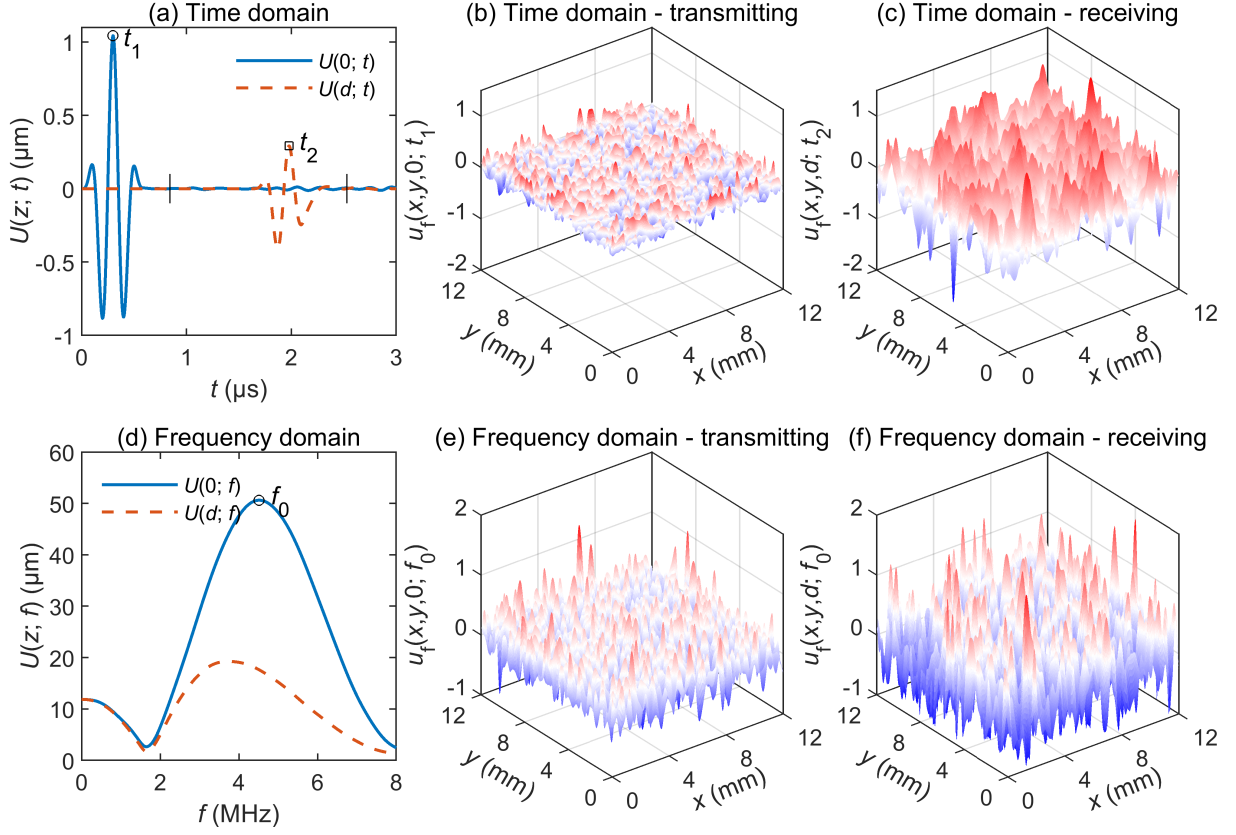


Figure 4.1: Illustration of coherent waves (a, d) and wavefront fluctuations (b, c, e, f) in the time (a-c) and frequency (d-f) domains, using the model N11520 with the material Inconel. The z -displacements are acquired on the transmitting $z = 0$ and receiving $z = d$ surfaces, leading to wave fields $u(x, y, 0; t)$ and $u(x, y, d; t)$. The solid and dashed lines in (a) are the spatial averages of these fields. (b) and (c) show normalised fluctuations $u_f(x, y, 0; t_1)$ and $u_f(x, y, d; t_2)$ for the transmitting and receiving surfaces, respectively; the time instances t_1 and t_2 are marked in (a). Similarly, (e) and (f) provide the normalised amplitude fluctuations at the frequency of f_0 , which is marked in (d); these are obtained by performing Fourier transforms of the received signals at all points on the two cross-sections.

It is clear from Figure 4.1(b) and (e) that the transmitting wavefront at $z = 0$ is not planar. This is because forces are applied while displacements are measured on the plane where random elastic deformations occur immediately upon application of forces. As a result of scattering, the field fluctuation on the receiving wavefront (Figure 4.1(c) and (f)) is substantially larger than that of the source, leading to a smaller coherent wave (spatial average) on the receiving surface, as was seen in Figure 4.1(a) and (d). As previously explained, the change of a coherent wave with propagation distance is represented by attenuation and dispersive phase velocity. The calculation of these parameters from the evolution of coherent waves will be addressed in the following subsection.

4.2.2 Determination by through transmission method

Before determining the scattering parameters, the change of coherent waves with propagation distance is illustrated. In Figure 4.2, example coherent waves in polycrystalline aluminium and Inconel are given as functions of propagation distances z . In the figure, a coherent wave $U(z; f)$ is normalised by its corresponding initiating wave $U(0; f)$, and the amplitude and phase parts of the normalised coherent wave, $U(z; f)/U(0; f)$, are denoted as $A(z; f)$ and $\varphi(z; f)$, respectively. These two parts are shown separately in the (a) and (b) panels of the figure.

Despite the large wavefront fluctuations (illustrated in Figure 4.1), the figure shows that the amplitude and phase parts of the coherent wave change exponentially and linearly with propagation distance, respectively. It is important to emphasise that these exponential and linear relations are nearly perfectly described by their corresponding fitted straight lines (the goodness of fit is characterised by the annotated R^2 measure, and $R^2 = 1$ corresponds to a perfect fit). This is an essential evidence that the change of the coherent wave with distance can be very well represented by the effective media parameters, namely attenuation coefficient $\alpha(f)$ and phase velocity $V(f)$, by the following relations

$$A(z; f) = e^{-\alpha(f)z}, \varphi(z; f) = \frac{2\pi fz}{V(f)}, \quad (4.1)$$

It is clear from Equation 4.1 that attenuation coefficient and phase velocity can be determined in two different ways. The first way is to use only $U(0; f)$ and $U(d; f)$, which are collected on the transmitting $z = 0$ and receiving $z = d$ surfaces, see Figure 2.1. This method is consistent with experiments where measurements can only be made on free boundaries. This method is named the through-transmission method in this thesis and the two scattering parameters can be given explicitly as

$$\alpha(f) = -\frac{\ln A(d; f)}{d}, V(f) = \frac{2\pi fd}{\varphi(d; f)}, \quad (4.2)$$

where $A(d; f)$ and $\varphi(d; f)$ are the amplitude and phase parts of $U(d; f)/U(0; f)$, respectively. This method is graphically shown in Figure 4.2 as the solid (for aluminium) and dash (for Inconel) lines connecting the transmitting points at $z = 0$ to the receiving ones

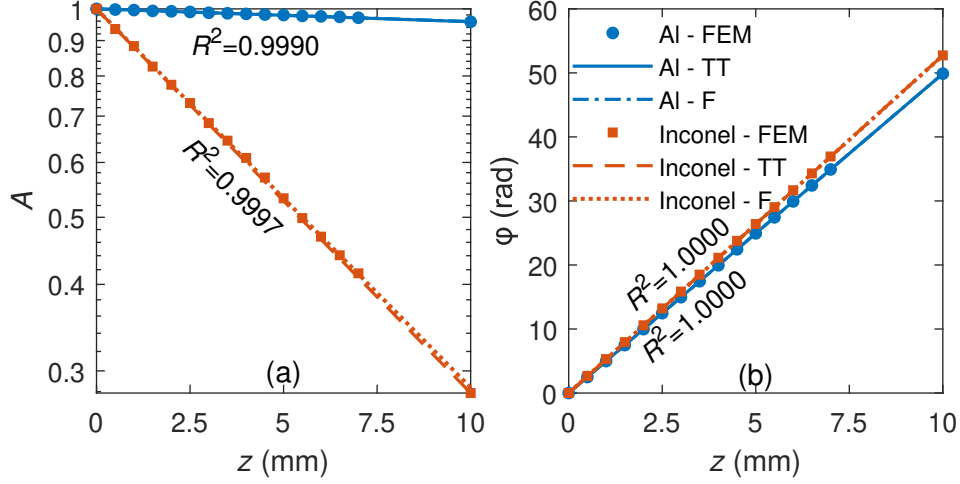


Figure 4.2: Amplitude and phase of typical coherent signals of polycrystalline aluminium and Inconel, normalised by the corresponding initiating waves $U(0; f)$. The signals are acquired from the model N11520 at the frequency of $f = 5$ MHz. (a) and (b) show the respective amplitude A and phase φ parts of the coherent waves. The solid (for aluminium) and dash (for Inconel) lines indicate the through-transmission (TT) method, and the dash-dotted (for aluminium) and dotted (for Inconel) represent the fitting (F) method in a least-squares sense. The through-transmission (TT) and fitting (F) lines are mostly overlapped. Part (a) of the figure uses the same legend as (b) and it uses a logarithmic y-axis scale. R^2 denotes the coefficient of determination that measures how successful a fitting (F) line is in explaining the variation of its corresponding FEM points ($R^2 = 1$ means a perfect fit).

at $z = d = 10$ mm.

4.2.3 Determination by fitting method

The second way to measure attenuation and phase velocity is to use all the coherent waves, measured on the free boundaries as well as inside the models. This can be fairly easily achieved by fitting Equation 4.1 to all the coherent waves, using attenuation coefficient $\alpha(f)$ and phase velocity $V(f)$ as fitting parameters. Similarly, this method is shown in Figure 4.2 as the dash-dotted (for aluminium) and dotted (for Inconel) lines which best fit all the data points in a least-squares sense.

4.2.4 Comparison of the two determination methods

Previously, Lowe and co-authors [28, 29, 36, 38] used the through-transmission method, while Rzyzy et al. [39] employed the fitting method. In comparison, the results in Figure

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4.2 show a very small but visible systematic difference for Inconel. The methods are further compared in Figure 4.3 for aluminium and Inconel over the frequency range of 3-6 MHz; details of the models are given in the caption. Subtle differences can be observed between the two methods: for attenuation coefficient the relative difference is smaller than 2% and for phase velocity it is smaller than 0.04%. Although the differences are small, it seems that the through-transmission method gives systematically larger attenuation coefficients and smaller phase velocities than the fitting method. Thus, it is important to understand the reason for this seemingly systematic difference.

There are two key differences between these methods. 1) The through-transmission method uses waves collected on traction-free boundaries, while the majority of the waves of its counterpart are acquired inside the models; this difference is illustrated in Figure 4.4. Examples are provided in Figure 4.5 to illustrate the difference between measurements made on the boundaries and inside the models. In the figure, circular data sets are acquired inside the model N11520 at the frequency of 5 MHz, with each point and error bar representing the mean and standard deviation of 15 realizations. Square data sets are collected on the same surfaces and under the same modelling conditions, but the collection surfaces are free boundaries that are formed by truncating the model N11520 at these measuring surfaces. Thus, the grains are identical for each of the two models under comparison at each propagation distance. The figure shows that the signal amplitudes on free boundaries are mostly smaller than those inside models, hence the resulting attenuation coefficient from the through-transmission method is inevitably larger than that from the fitting.

This difference is due to the fact that on the boundaries and inside the models, incoherent waves contribute to the coherent signals differently, see Figure 4.4. It is not hard to imagine that on a measuring surface the incoherent waves induced by early arrivals enter the coherent part of the arrival signals. Inside the models, coherent waves harvest incoherent ones in both forward- and backward-propagating directions, while on free boundaries incoherent backward-scattered waves are the only contributors. As a result, coherent waves collected inside models have slightly larger amplitudes than those acquired on the corresponded surfaces that are traction-free. Also, additional mode conversion of scattered waves on a free boundary may contribute to the difference. The incidence of random waves

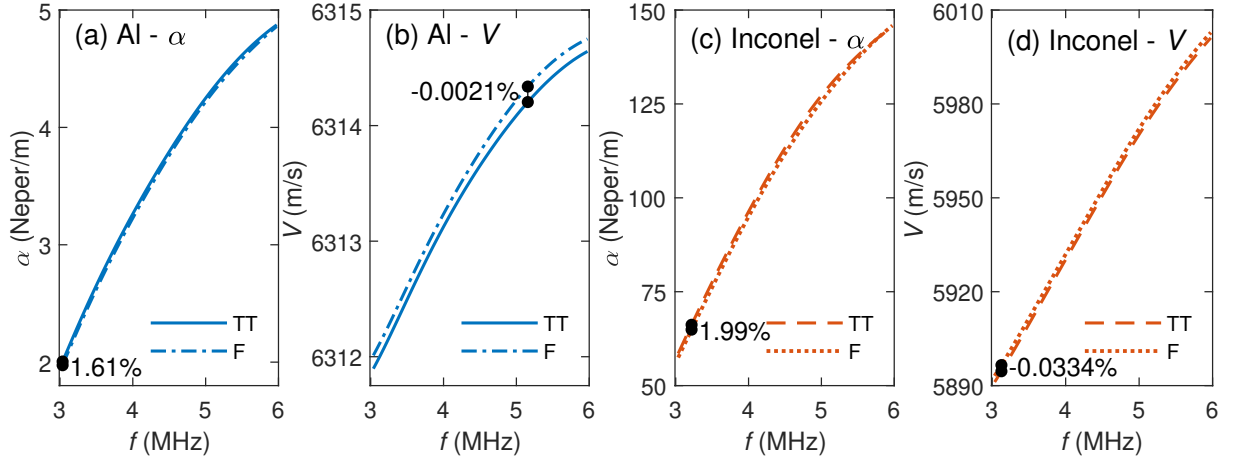


Figure 4.3: Longitudinal wave attenuations (a, c) and velocities (b, d) for polycrystalline aluminium and Inconel determined by the through-transmission (TT) and fitting (F) methods. Each material uses 15 realizations of the model N11520 to get the averaged data as shown in the figure, and simulations are for a plane longitudinal wave with a centre frequency of 5 MHz. The marks followed (or preceded) by percentages show the maximum discrepancies between the through-transmission (TT) and fitting (F) methods, with the fitting method as reference.

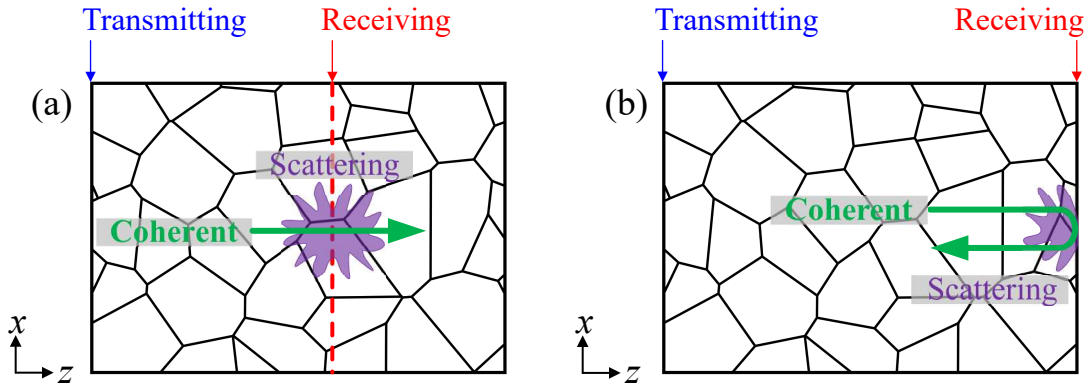


Figure 4.4: Illustration of collecting waves (a) on an internal cross-section and (b) on a free boundary. The shown Voronoi diagram is the sectional view of a 3D polycrystal on the x - z plane. The transmitted coherent wave travels in the z -direction. In (a), the coherent wave received on the internal cross-sections acquires energy from the scattered waves that travel in both forward and backward directions. In (b), the coherent wave received on the free end is the sum of the incident and (equally) reflected waves, and this coherent part only incorporates the scattered waves that travel in the backward direction. Note that the number of grains in an actual simulation is far greater than that of the shown Voronoi diagram.

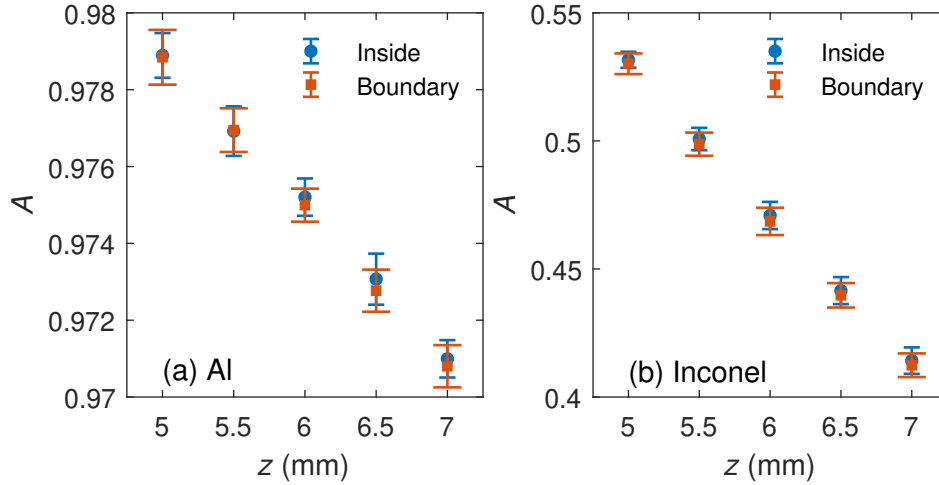


Figure 4.5: Coherent amplitudes of polycrystalline (a) aluminium and (b) Inconel measured inside FE models and on free boundaries. Amplitudes are plotted versus propagation distance at the frequency of $f = 5$ MHz. Each material uses 15 realizations of the model N11520 to get the averaged data as shown in the figure. The circles represent signals collected inside the models, and the squares are collected on the same surfaces but the models are truncated at these surfaces to form traction-free boundaries.

on complex free boundaries, with spatially-varied elastic properties, produces complicated reflections that involve mode conversions. Such mode conversions occur differently on a free boundary compared to the equivalent plane inside the material.

2) The second aspect is that the through-transmission method reflects the overall scattering behaviour of the whole cuboid of a polycrystal medium, while its counterpart is largely influenced by the smaller subsets of the medium. It suggests that these two methods may have different statistical significances in representing the target polycrystal. This volume effect, however, is not the main cause of the difference between the two methods. The reason can be clearly seen from Figure 4.5 which illustrates the use of identical volumes at each propagation distance still leads to statistically different results between the two methods.

However, it is important to realise that the difference between the two methods is generally within the range of error bars as shown in Figure 4.5. This suggests that the through-transmission and fitting methods are practically equivalent and both can be used. In this work, the through-transmission method is used in later discussions due to its convenience in the collection of waves and the calculation of scattering parameters.

4.3 Numerical errors and statistical uncertainties

It is certainly true that disagreement exists between the results calculated by the FE method and the reality. This disagreement should be estimated to establish the validity of the FE model and to aid improvement of its accuracy and precision.

In the case of modelling elastic wave propagation in polycrystals, the disagreement can be divided into two parts. One part is the systematic difference between an FE result and the exact solution, and another is the random variation around the FE result. These two parts are denoted as error and uncertainty, respectively. As mentioned in §3.5, an FE result is obtained by averaging those of multiple FE realizations that are independently generated but follow the same microstructure statistic. Error in this case is the difference between the average result and the exact solution, while uncertainty is the standard deviation of the multiple results relative to the average. Error and uncertainty arise in the FE model mainly as results of numerical approximations and statistical fluctuations.

Numerical approximations include two major facets: one is the approximation of an exact wave propagation problem by an FE model that is discretised in space and time, and another is the truncation or rounding of an exact number to a computer number that has a finite precision. These approximations cause numerical errors, and the estimation of these errors will be provided in §4.3.1.

Statistical fluctuations relate to the random nature of the polycrystalline microstructure and the stochastic scattering it causes. A combination of multiple realizations is used in the FE model to average out the fluctuations and thus to obtain statistically meaningful FE results. Such statistical considerations are accompanied by statistical errors and uncertainties, which will be estimated in §4.3.2

Following the estimations of errors and uncertainties, §4.3.3 examines the propagation of errors and uncertainties through coherent waves to effective media parameters, namely attenuation coefficient and phase velocity. Finally, §4.3.4 and §4.3.5 provide examples to suppress numerical velocity and attenuation errors. In this work, absolute and relative errors are denoted respectively as Δ and δ , while absolute and relative uncertainties are denoted as σ and ε .

4.3.1 Errors in numerical approximations

The spatial and temporal discretisation approximations in the FE method introduce numerical errors, and this work looks at both space and time. The interest of this work is to establish knowledge of the underlying errors in amplitude and in wave velocity that come from the FE discretisation of the propagation behaviour; key to this is whether these errors are significant in comparison with, respectively, the changes of amplitudes due to scattering induced attenuation and the changes of phase velocity due to dispersion by the polycrystal. Such errors, if sufficiently understood, may also be used in practice in order to make corrections to simulated results. Therefore, this work chooses to assess the errors in a homogeneous isotropic domain, being the background on which the polycrystal behaviour will be built, keeping with the same meshes and time-stepping schemes of the latter. This work recognizes that this omits possible errors that might be specific to the discretisation of the spatial changes in the polycrystal, but this work suggests that the target of achieving good recommendations for choices of mesh and time step is addressed most usefully by studying the non-specific homogeneous background case. Furthermore, this work believes that a good discretisation for the homogeneous background will automatically ensure good representation in the polycrystal case because it is already well established that the wave behaviour is not sensitive to specific features at the space scale of the crystal boundaries, and indeed the analytical models do not include information about these boundaries at all.

The evaluation of the accuracy of FE models for wave propagation is a highly developed subject with a long history. Considerations of phase velocity dispersion in particular have motivated many different spatial and temporal schemes; dispersion is strongest for coarse meshes, so the challenge is to achieve the best efficiency for the desired performance in modelling short-wavelength waves. The monograph by Bathe [61] provides an excellent description and evaluation of the basic methodologies of the main schemes in use for time-domain simulation. A variety of studies of performance of these and their variants, limiting to relevance to the method used in the present work, can be found in, e.g., [59, 62–70].

This work limits its reporting here to its specific choice of scheme and includes results in brief for the benefit of modellers in the applications context of this article, leaving detailed

evaluation of the mathematics and performance of the scheme to the cited literature. The specific choice is the central difference explicit scheme, using lumped mass matrices, no material damping, and a structured mesh of identically-sized cube-shaped linear hexahedral elements. The basis of this choice has been optimised and explained in previous studies [29, 38].

The exact solution to the propagation of elastic plane waves within an isotropic non-damping material is given by $\mathbf{u}(\mathbf{x}, t) = \mathbf{p}_0 \exp[i(\mathbf{k}_0 \mathbf{x} - 2\pi f t)]$, where $\mathbf{p}_0$ and $\mathbf{k}_0 = k_0 \mathbf{n}$ are the exact polarization and wave vectors, respectively. It is implied in the solution that the displacement amplitude is unity. There is no dissipation and the wave number $k_0 = 2\pi f/V_0$ is thus a real number, where V_0 is the exact phase velocity.

Due to numerical approximations, the FE solution to the same problem is approximate. At a given node $\mathbf{x}$ and time instance $t = n\Delta t$, the approximate solution $\mathbf{u}_{\mathbf{x}}^n$ takes a similar form to the exact one

$$\mathbf{u}_{\mathbf{x}}^n = \mathbf{p} e^{i(\mathbf{k} \cdot \mathbf{x} - 2\pi f n \Delta t)}, \quad (4.3)$$

where $\mathbf{p}$ and $\mathbf{k} = k \mathbf{n}$ are the approximate polarization and wave vectors. Numerical attenuation α , if any, and phase velocity V are included in the complex wave number k , i.e. $k = 2\pi f/V + i\alpha$. By using Equation 4.1, the wave number can be further related to amplitude and phase changes via $k = \varphi/d - i \ln A/d$, where d is the wave propagation distance. Thus, the estimation of amplitude and phase errors depends on the solution of wave number k .

The central difference explicit scheme is known to be non-dissipative, correctly conserving the energy of the propagating waves [69, 70], although the literature devotes little attention to the details of this, concentrating in preference to the real concern, which is the velocity dispersion. Here this work suggests it is useful to think a bit more about the non-dissipative property before evaluating the dispersion.

The non-dissipative property can be examined by looking at the numerical wave propagation solution for a monochromatic plane wave in an infinite domain (see also, e.g., [63, 70]). The elements are all identical, so this work arbitrarily considers a single node, with waves propagating in the z -direction and no external forces. The scheme requires only local in-

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formation at each time step, so only information from the eight elements that adjoin this node needs to be considered. This local assembly has mass $\mathbf{M}$ and stiffness $\mathbf{K}$ matrices with 81×81 coefficients, as defined in §3.5.

Substituting Equation 4.3 into Equation 3.1 gives a system of 81 equations. However, the eight-element assembly only carries complete information about nodal connectivity for the target node. As a result, only the three equations which correspond to the degrees of freedom of this target node are meaningful in terms of describing wave motion, and, considering compression waves, only the displacement in the chosen coordinate z relates to the example wave propagating along z . Simplifying this equation results in

$$(e^{-i2\pi f\Delta t} + e^{i2\pi f\Delta t} - 2)h^2 - (e^{-ikh} + e^{ikh} - 2)V_0^2\Delta t^2 = 0, \quad (4.4)$$

and solving this equation leads to

$$k = \frac{1}{h} \arccos \left[\frac{\cos(2\pi f\Delta t) - 1}{V_0^2\Delta t^2} h^2 + 1 \right]. \quad (4.5)$$

It is clear from Equation 4.5 that k is a real number. This confirms the non-dissipative nature of the solution, which holds for plane waves that are continuous in space and time. A similar analysis would show the same for shear waves.

Equation 4.5 also shows the relative phase error, which is given by $\delta_\varphi = (k - k_0)/k_0$. Here the spatial sampling and Courant numbers are defined with respect to the longitudinal phase velocity $V_0 = V_L$, i.e. $S = V_L/(fh)$ and $C = \Delta t V_L/h$. Considering these relations, the relative phase error can be expressed as

$$\delta_\varphi = \frac{S}{2\pi} \arccos \left[\frac{\cos(2\pi C/S) - 1}{C^2} + 1 \right] - 1. \quad (4.6)$$

The equation shows that the phase error is directly related to spatial sampling number S and Courant number C , which correspond to spatial discretisation and time stepping respectively. It follows now that there is also an anisotropic behaviour because, however well the element behaves for waves at different angles, the spatial sampling is certainly different in different directions; this is a well-known property of these solutions [59, 63, 67]. Thus a perfect preservation of the amplitude of monochromatic plane waves is expected.

ted, but a frequency-dependent error of phase velocity. The latter will imply that the amplitude of the envelope of a wave packet in the time domain will in general exhibit distortion as it travels. This performance will be evaluated in simulation studies in the following.

A simple cuboid model, with the dimensions of $d_x \times d_y \times d = 12 \times 12 \times 10$ mm, is established using isotropic steel, with Young's modulus $E = 210$ GPa, Poisson's ratio $\nu = 0.3$ and density $\rho = 8000$ kg/m³. The longitudinal wave velocity of this material is $V_L = 5944.45$ m/s. Similar to the FE model given in §3, the model is discretised with uniform eight-node cube elements and configured to accommodate a plane longitudinal wave that has the centre frequency of 5 MHz. The transmitting and receiving waves, $U(0, f)$ and $U(d, f)$, are collected and the relative phase error is thus obtained as $\delta_\varphi = \varphi/(2\pi f d/V_L) - 1$, where φ is the phase part of $U(d, f)/U(0, f)$.

Figure 4.6 compares the actual simulations with analytically predicted results from Equation 4.6. The left panel (a) assesses the influence of spatial discretisation, as characterised by the sampling number S , while the right panel (b) evaluates the impact of time stepping, as characterised by the Courant number C . Model details are given in the figure caption. The figure shows that the actual phase errors can be well represented by Equation 4.6.

A key observation from the figure is the high degree of accuracy of the calculated phase. The lowest sampling number, S , in the results in part (a) of the figure is 10 elements per wavelength, for which the phase error (and thus velocity error) is about 0.5%, and this error is reduced to 0.1% by increasing S to 20 elements per wavelength. Thus, the policy of using at least 10 elements per wavelength is justified for all routine analysis by this method unless particularly high precision is to be pursued.

The figure also defines the two approaches to reduce phase errors, pertaining to spatial discretization and time sampling, respectively. The first is to use finer meshes, which can be discovered from the left panel (a) that phase error decreases exponentially ($\delta_\varphi \propto \exp(-2S)$) as spatial sampling number increases. The second approach is to use larger Courant numbers, which can be found from the right panel (b). When this number is at its limit of unity, phase error can nearly be removed. However, for stability reasons, it is not recommended to use $C = 1$ because the actual C in a simulation could be greater

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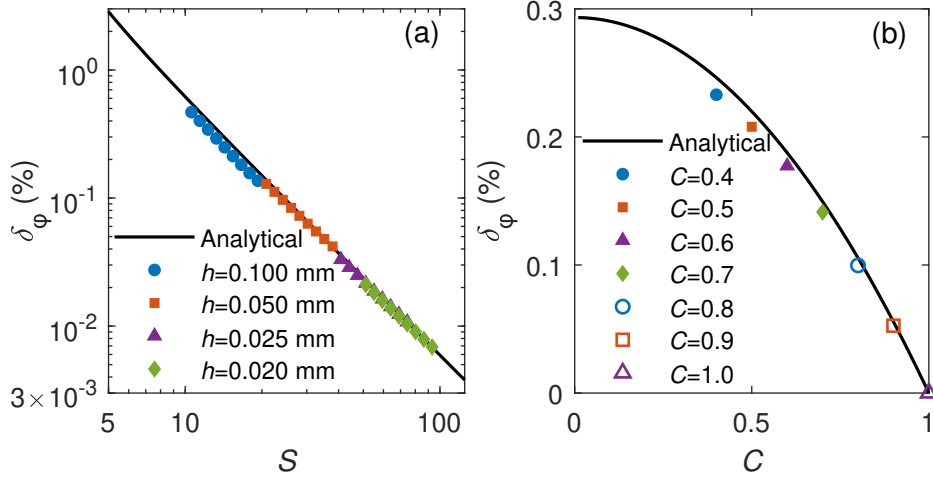


Figure 4.6: Evaluation of numerical phase errors. (a) and (b) assess the influences of spatial sampling number S and Courant number C , respectively. (a) uses four models with different mesh sizes, $h = 0.100, 0.050, 0.025, 0.020$ mm, and fixed Courant number, $C = 0.8$. The resulting relative phase errors (points) are plotted against their sampling numbers S in the frequency range of $f = 3 - 6$ MHz. (b) uses seven models with fixed mesh size, $h = 0.025$ mm, and different Courant numbers, $C = 0.4, 0.5, \dots, 1.0$. Their relative phase errors (points) are plotted versus their Courant numbers at the frequency of $f = 5$ MHz. The solid lines in (a) and (b) are analytically predicted errors from Equation 4.6. Note that the vertical y axes in the figure panels show the percentage error over the propagation distance of 10 mm.

than 1 (thus violate the stability condition) as a result of accelerated wave velocity caused by numerical dispersion, and also this condition cannot be achieved for all waves when there are spatial variations of material properties or multiple wave modes. An important implication of the second approach is that a structured mesh is likely to perform better than a free mesh in this analysis. This is because the free mesh has a range of element sizes and the range can be very wide for sharp spatial features, and therefore it is impossible to achieve the same Courant number everywhere, even if there is only one wave mode and material present. In §4.3.4, examples will be given to show actual errors in phase velocity calculations and to illustrate the corrections of these errors by using the two approaches discussed here.

This work further uses the same models as for Figure 4.6(a) and calculates their relative amplitude errors by $\delta_A = A - 1$, where A is the amplitude of $U(d, f)/U(0, f)$ and its exact solution is unity in the absence of amplitude error. In the frequency range of $f = 3 - 6$ MHz, the errors are plotted against frequency in Figure 4.7.

Figure 4.7 shows that the amplitude errors of the FE simulations are small, and that they

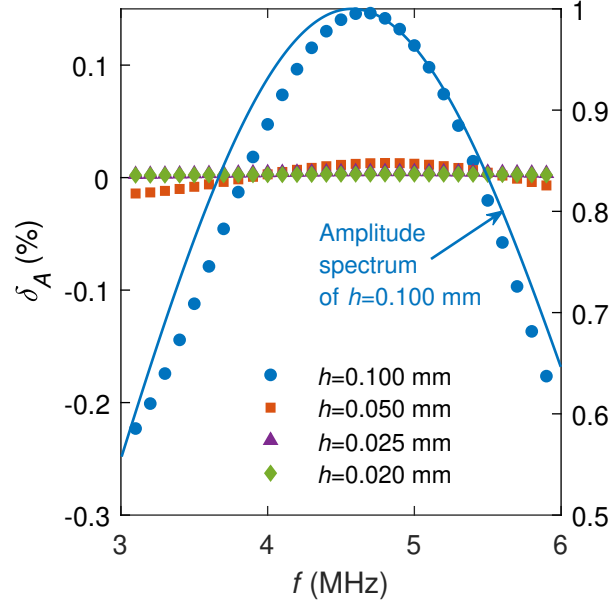


Figure 4.7: Evaluation of numerical amplitude errors. The evaluation utilizes the four FE models that are used in Figure 4.6(a). The points represent the relative amplitude errors and they use the left y -axis. The solid line is the normalised amplitude spectrum of the transmitting wave for the model with the mesh size of $h = 0.100$ mm and it uses the right y -axis. Note that the vertical y axes in the figure panels show the percentage error over the propagation distance of 10 mm.

reduce as the mesh is refined, but they are not zero. It is important to recall here that zero loss is expected for monochromatic plane waves, but that analysis did not include the FE calculations for the transient behaviour of a wave packet. Critically, it is needed to distinguish here between energy loss, which would violate the non-dissipative nature, and signal distortion without loss of energy. Therefore, the integral of the energy content is calculated for the whole wave packet in each case and this revealed that the energy loss is negligible, at around 10^{-4} % for the coarsest mesh. Thus, the energy is correctly retained and the solution is convincingly non-dissipative, but that there is some small distortion of the amplitude spectrum, resulting in time-shifting of some spectral amplitudes in the wave packet.

For interest, Figure 4.7 also shows the normalised amplitude spectrum of the transmitting wave for the model with the mesh size of $h = 0.100$ mm, which can be seen, when scaled appropriately (right y -axis), to match the same shape as the spectrum of the distortion. Further work on this observation could be academically interesting, but this would be beyond the present scope. For now, it is noted that the wave packet does not dissipate

energy, but that there is a small distortion across the amplitude spectrum; furthermore, the latter is very small (0.2%), even for the coarsest mesh ($S = 12$ elements per wavelength at centre frequency), while for the preferred finer meshes it is below 0.003% across the bandwidth ($S = 60$ elements per wavelength at centre frequency). These are very small numbers compared to the scattering induced attenuation in the polycrystal.

Thus the analysis and practice both show that the amplitude errors are insignificant in comparison to the phase errors. Therefore it is expected that limitations of the FE modelling will impact the predicted phase velocity but have a negligible influence on the wave amplitude when reported in the frequency domain. The key result to achieve accurate simulation is the phase error in Figure 4.6(a), showing dramatic improvement as the number of elements per wavelength, S , is increased. However, this is in direct conflict with the desire to minimise S for large models and high-frequency simulations.

4.3.2 Errors and uncertainties in statistical considerations

Generally, one aims to simulate polycrystals of prescribed statistical properties. A single FE model is not capable of fully describing one of such polycrystals, due to its relatively small sample volume and finite number of grains. Instead, the statistical combination of the results of multiple realizations that are randomly generated following the same statistical property is desirable to draw meaningful conclusions about the given polycrystal.

The effectiveness of using multiple realizations to achieve statistical convergence is exemplified here. The model N11520 is used to simulate polycrystalline aluminium and Inconel that have statistically isotropic and macroscopically homogeneous properties. Due to random scattering, the wave field $u(x, y, d; t)$ on the receiving plane $z = d$ should be randomly distributed. This means that at a given time instance of $t = t_0$ the fluctuation $u_f(x, y, d; t_0)$, which is defined in §4.2, should follow the Gaussian distribution. However, the actual distribution of a single realisation differs from the Gaussian for both aluminium and Inconel, which are respectively shown in Figure 4.8(a) and (b) as probability density histograms. Instead, the combination of multiple realizations (15 in this example) delivers satisfactory distributions that agree very well with the Gaussian. Thus, a combination of multiple realizations can be regarded as a confident description of the target polycrystal.

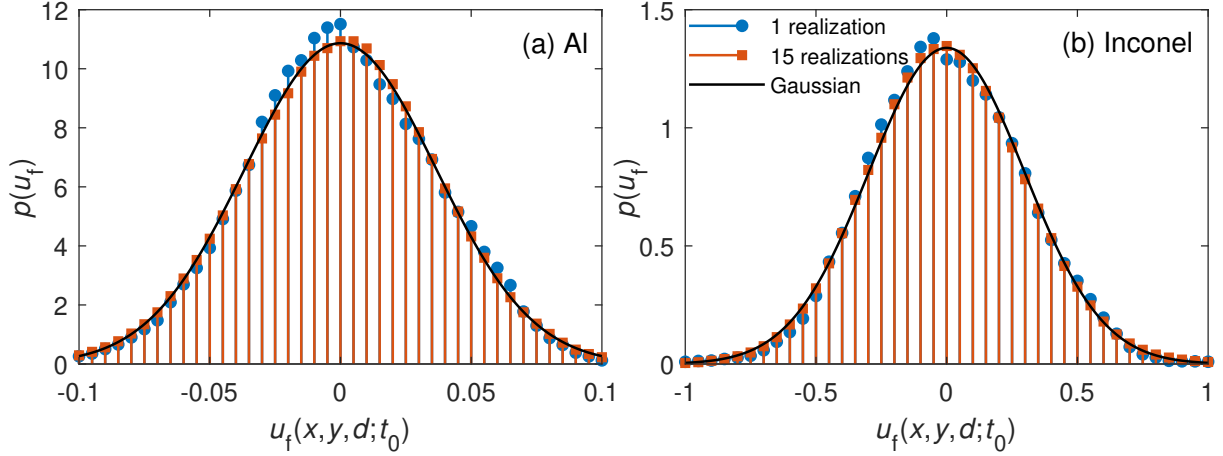


Figure 4.8: Probability density of the normalised receiving fluctuation fields of (a) aluminium and (b) Inconel. The materials are simulated using the model N11520 with the centre frequency of 5 MHz. Each realisation is independently generated by randomizing its crystallographic orientations. The fluctuation $u_f(x, y, d; t_0)$ of each realisation is collected at all nodal points on the receiving plane $z = d$. The time instances t_0 for aluminium and Inconel are 1.88×10^{-6} and 1.98×10^{-6} s respectively, which correspond to the maxima of their coherent waves $U(d; t)$. Note the order of magnitude difference in the horizontal scale indicating significantly stronger scattering for Inconel. Part (a) uses the same legend as (b).

As mentioned in §4.2, the coherent wave of a model is used to calculate effective media parameters. In the case of multiple realizations, the calculation needs to use the average of the multiple coherent waves that can be denoted as $\mu(z; f) = \langle U_i(z; f) \rangle_i$, where $U_i(z; f)$ is the coherent wave of the i -th realisation. As prescribed by the central limit theorem, the multiple coherent waves follow the Gaussian distribution because the multiple realizations are independently randomly generated. And, the average $\mu(z; f)$ is an appropriate estimate of the true coherent wave, and this estimation includes statistical uncertainty and error as discussed below.

Uncertainty is characterised by the standard deviation $\sigma(z; f)$ of the coherent waves. Here the 15-realisation example of Figure 4.8 is used to investigate the uncertainties associated with the simulations. For the received coherent waves $U_i(d; f)$ ($i = 1, 2, \dots, 15$), their uncertainties are calculated and split into amplitude σ_A and phase σ_φ parts, respectively; normalisation by their respective mean values results in relative uncertainties $\varepsilon_A = \sigma_A/\mu_A$ and $\varepsilon_\varphi = \sigma_\varphi/\mu_\varphi$. The results show that Inconel has a larger uncertainty than aluminium, which is consistent with Figure 4.8. This means that uncertainty is positively correlated with material anisotropy. In addition, the amplitude uncertainty is around 10 times larger

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than that of phase. This is opposite to what has been found for numerical errors which was that amplitude error is in general smaller than phase error; this was shown in Figures 4.6(a) and 4.7.

Error in this case is termed the standard error of the mean. It is a statistical error between the mean and the true value, and it can be probabilistically estimated by $\sigma_\mu = \sigma/\sqrt{N}$, where N is the number of realizations.

It is important to realise that uncertainty cannot be suppressed, but rather it can be better determined by using more realizations for example. For standard error, however, its expression indicates that it can be reduced by increasing the number of realizations N . Practically, a simple trial-and-error process can be employed to suppress standard error to a satisfactory extent. This process increases the number N until the relative standard error of either amplitude or phase ($\delta_\mu = \varepsilon_{A,\varphi}/\sqrt{N}$) is below a set threshold (e.g. 0.1%).

4.3.3 Propagation of errors and uncertainties

It is known that errors and uncertainties propagate through independent variables to dependent ones. Thus, those of coherent waves discussed in §4.3.1 and §4.3.2 will be brought into scattering parameters, namely attenuation coefficient and phase velocity, via Equation 4.2.

Given that propagation distance and frequency are accurate, the attenuation coefficient in Equation 4.2 is a univariate function of amplitude. Amplitude error is denoted as $\Delta_A = A - A^T$, where A^T is the true amplitude and A is its estimation given by the mean of multiple realizations. Replacing A by A^T in Equation 4.2 and expanding this equation about the point A in a Taylor series, the relative error of attenuation coefficient can then be obtained as

$$\delta_\alpha = -\frac{e^{\alpha d}}{\alpha d} \Delta_A + O[\Delta_A^2], \quad (4.7)$$

where α is the true value of attenuation coefficient; frequency f is implicit. In general, the true attenuation coefficient α is unknown, so instead it is approximately replaced by the mean value of multiple realizations. Note that only the first-order term of the

Taylor expansion is used in the equation, by assuming that amplitude error is small. Higher-order terms should be included if this assumption does not hold. For uncertainty, the attenuation coefficient of each realisation needs to be expressed as a Taylor series. Substituting the expansion into the formula of standard deviation, the relative uncertainty can then be obtained

$$\varepsilon_\alpha = \frac{e^{\alpha d}}{\alpha d} \sigma_A + O[\sigma_A^2], \quad (4.8)$$

where σ_A is amplitude uncertainty. Similarly, assuming that phase error and uncertainty are small, then their propagation from phase to velocity can be easily obtained from Equation 4.2

$$\delta_V = \frac{V}{2\pi f d} \Delta_\varphi + O[\Delta_\varphi^2], \quad \varepsilon_V = \frac{V}{2\pi f d} \sigma_\varphi + O[\sigma_\varphi^2], \quad (4.9)$$

where V is the true phase velocity that is approximated to the mean value of multiple realizations.

As shown in Equations 4.7 and 4.8, the error and uncertainty of attenuation coefficient are related to those of amplitude by the same factor, $F_\alpha = \exp(\alpha d)/(\alpha d)$. Due to the lack of true values, such propagation of error cannot be evaluated. However, it is easy to do so for uncertainty. For this purpose, σ_A and ε_α are calculated from 15 realizations and the actual propagation factor is calculated from their division. The resulting factor is plotted against αd in Figure 4.9(a) for aluminium and Inconel, and each material covers a wide frequency range by using three models: N115200, N11520, and N16000. The actual uncertainty propagation can be seen to be very well represented by the analytical factor F_α , and this should always be valid as long as amplitude uncertainty is small. Likewise, this factor is also applicable to error propagation on the same condition that amplitude error is small. The figure conveys important information that the propagation factor is at its minimum of $e = 2.72$ when $\alpha d = 1$ Neper. Thus, in order to suppress the magnification of error and uncertainty, the total attenuation αd should be kept around 1 Neper [71]. Practically, this work has observed that moderate magnifications can be achieved by maintaining αd between 0.01 and 6 Neper.

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For phase velocity, Equation 4.9 shows that the same factor $F_V = V/2\pi fd = 1/\varphi$ governs both error and uncertainty propagation. Similarly, uncertainty propagation is evaluated in Figure 4.9(b) by using the same models as its left panel. The figure shows that the factor F_V agrees very well with actual simulations, and it is no doubt that it is also valid to error propagation. An elaborate analysis would suggest that error and uncertainty are naturally suppressed during their propagation. This is based on the fact that achieving a good statistical significance requires waves to propagate at least a quarter of wavelength, which means $\varphi \geq 2\pi/4 = \pi/2$ and further leads to $F_V = 1/\varphi \leq 2/\pi < 1$. Note that in Figure 4.9(b) the phase φ on the horizontal axis is in the range from 10 to 1000 and the propagation factor F_V on the vertical axis is not greater than 0.1. It is also important to emphasise that better suppression can be achieved by using a longer model length d . However, increasing d often makes it difficult to meet the condition of αd being close to 1 Neper, which is necessary to suppress the error and uncertainty of attenuation. It is thus advised to only consider the suppression condition exerted to attenuation and that of phase velocity should be fulfilled accordingly.

4.3.4 Suppression of numerical velocity errors

The preceding studies have provided a variety of ways to understand and then suppress errors and uncertainties. Following these studies, this section and the subsequent section present some typical examples to demonstrate the practical use of the suppression methods in actual simulations.

Suppressing statistical error and uncertainty is relatively simple, and it is thus not exemplified in this subsection. As illustrated in §4.3.2, a statistical error can be reduced to a satisfactory extent by increasing the number of realizations N , while uncertainty cannot be suppressed and can only be better determined through the use of large N . For all simulations considered in this work, $N = 15$ is used to achieve a satisfactory statistical error of at most 0.1% and a sufficiently good determination of uncertainty. §4.3.3 further suggests that the propagations of statistical error and uncertainty can be effectively suppressed by minimizing the factors F_α and F_V , respectively. But because such minimization equally suppresses numerical errors, its discussion is left to the following example suppressions of

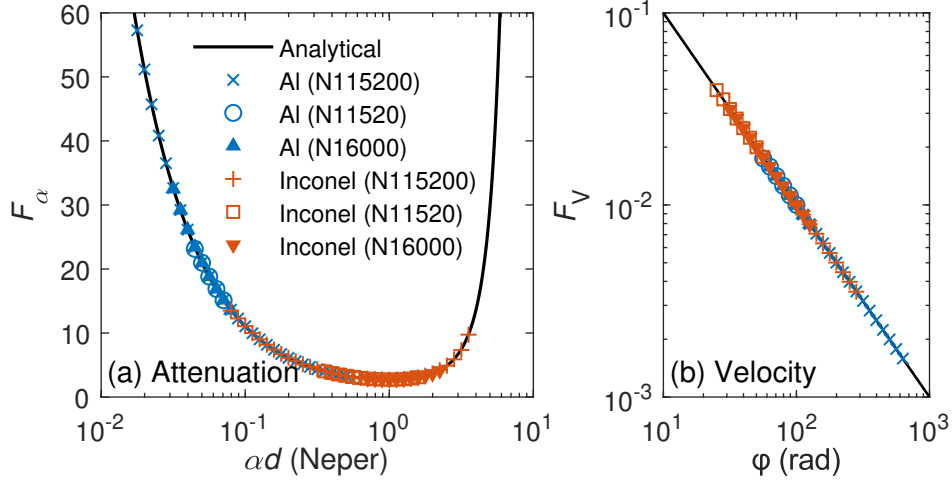


Figure 4.9: Propagation factors for the uncertainties of (a) attenuation and (b) phase velocity. Lines represent analytically derived factors, while the points are obtained from 15 FE realizations. For aluminium, the models N115200, N11520, and N16000 cover the frequency ranges of 1-6.5, 6.5-13.5, and 13.5-25 MHz, respectively. For Inconel, the ranges are 1-2.5, 2.5-6.5, and 6.5-23 MHz. Part (b) of the figure uses the same legend as (a).

numerical errors.

Suppressing numerical errors requires a good combination of modelling parameters, and the suppression approach differs from phase velocity to attenuation. Thus, this section and the subsequent section give suppression examples separately for velocity and attenuation.

As shown in Equation 4.9, the relative error of phase velocity δ_V is the product of phase error Δ_ϕ and propagation factor F_V . Thus, reducing either of these two parts leads to the suppression of velocity error. For F_V , §4.3.3 infers that it naturally reduces errors as it is smaller than unity. This factor can be further reduced by using a longer model length d . However, this work does not aim to do so, because d is a critical parameter for suppressing attenuation error.

For Δ_ϕ , its analytical expression has been obtained for isotropic materials as given in Equation 4.6. Although this work has not seen a means yet to extend it analytically to polycrystals, it will be demonstrated later that the conclusions drawn from it can be quantitatively applied to polycrystals for error suppression. To use this equation for polycrystals, the spatial sampling number S is defined with respect to the Voigt velocity V_{0L} , i.e. $S = V_{0L}/(fh)$, and its Courant number C with respect to the peak velocity $V_{\max}$, namely $C = \Delta t V_{\max}/h$. For cubic materials considered in this work, the

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Voigt and peak velocities are given respectively as $V_{0L} = \sqrt{(3c_{11} + 2c_{12} + 4c_{44})/(5\rho)}$ and $V_{\max} = \sqrt{(c_{11} + 2c_{12} + 4c_{44})/(3\rho)}$ [72].

Reducing phase error Δ_φ can be achieved by using the two approaches summarised in §4.3.1. The first approach is to use a larger spatial sampling number S . However, this approach is practically difficult for the present example. This is because the three material models (Table 3.1) used in this work are already very big in terms of their required computational resources, and further increasing their S requires the use of even finer meshes that would easily exceed the current computer capability. Instead, this first approach is substituted by a correction approach that uses the numerical phase error predicted from Equation 4.6 to correct the error included in the simulation result. The second approach is to control phase error Δ_φ by using a Courant number which is as close to unity as possible.

Examples are provided in Figure 4.10 to illustrate these two approaches. The examples use the same FE models and configurations as Figure 4.9. In the figure, the phase velocities obtained from FE simulations are provided as discrete points, and theoretically predicted results are given as lines. The accurate statistical information of the FE material models is incorporated into the theoretical curves, and these curves are of good accuracy for the studied materials and frequency ranges. In particular, the curve of aluminium in panel (a) is very accurate because the underlying theory can take almost all its weak scattering into consideration. This curve can thus be used as a reference to evaluate the error suppression approaches.

For the first approach of error correction, phase velocities before correction are provided as hollow circles and corrected ones as solid circles. In this case, small Courant numbers (0.81 for aluminium and 0.86 for Inconel) are used in order to get large phase errors and thus to show clear effects of correction. The correction is achieved by subtracting the numerical phase error $\varphi\delta_\varphi$ (δ_φ is the relative phase error calculated by Equation 4.6) from the simulation result φ and then calculating the corrected phase velocity by $V = 2\pi fd/(\varphi - \varphi\delta_\varphi)$. It is obvious that before correction, the three models (N115200, N11520, N16000) do not give consistent velocities as expected at the transitions between individual models. Note that the transitional inconsistency is less clear for Inconel (panel

(b) of the figure) because its y -axis scale is too large to show this. This inconsistency is nicely averted in the corrected results, implying the effectiveness of the correction approach. And by comparing the hollow and solid circles with the theoretical curve of aluminium (panel (a)), it is also observable that the use of the correction approach significantly suppresses numerical phase velocity errors.

For the second approach of error control, both aluminium and Inconel use a large Courant number of $C = 0.99$. This is the largest C number attempted in this study that does not encounter stability issues; the Courant numbers above $C = 0.99$ were tested but led to unstable FE computations for both aluminium and Inconel. The velocity results are provided in the figure as solid squares. The results show good consistencies at model transitions, but not as good as the corrected results of the first approach. The theoretical curve of aluminium in panel (a) is also closer to the corrected points, suggesting that the correction approach performs better than the control approach. This error control approach, however, may be more advantageous for practical simulations as it requires less post-simulation calculation compared to the correction approach.

4.3.5 Suppression of numerical attenuation errors

Equation 4.7 indicates that the relative error of attenuation δ_α is the multiplication of amplitude error Δ_A and propagation factor F_α , and thus reducing either of these two parts leads to the suppression of attenuation error. It is suggested in §4.3.1 that amplitude error Δ_A can be reduced by using either a larger spatial sampling rate S (thus a finer mesh size h) or an appropriate spectrum range that is in close proximity to its maximum. And §4.3.3 indicates that propagation factor F_α can be suppressed by limiting αd to a certain range in the vicinity of 1 Neper.

Thus, three opportunities are available to suppress numerical attenuation errors. For the first opportunity of using a larger spatial sampling rate S , §4.3.4 has mentioned that the three models utilized in this work are already very computationally intensive, and therefore this work does not aim to further increase their sampling rates. For the third opportunity of using a αd being close to 1 Neper, the creation of the currently used FE models has ensured that this condition can be relatively easily satisfied. It is certainly

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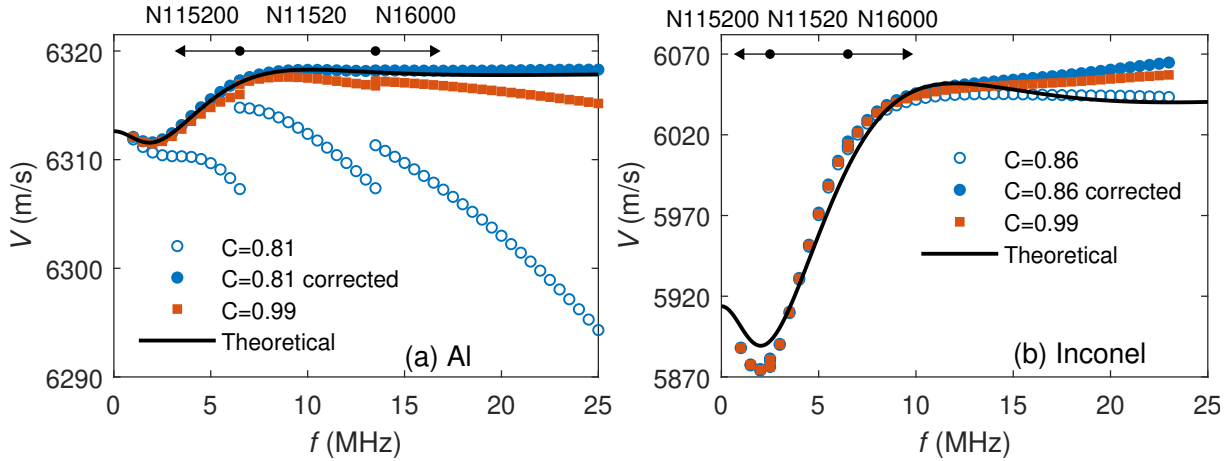


Figure 4.10: Example suppression of numerical velocity error for polycrystalline (a) aluminium and (b) Inconel. Lines represent theoretically predicted [28] phase velocities, while points are obtained from 15 FE realizations. Hollow circles represent un-corrected results and their corrected ones are shown as solid circles. Solid squares represent results obtained by using larger Courant numbers. For aluminium, the models N115200, N11520, and N16000 cover the frequency ranges of 1-6.5, 6.5-13.5, and 13.5-25 MHz, respectively. For Inconel, the ranges are 1-2.5, 2.5-6.5, and 6.5-23 MHz.

true that more models can be created to accommodate different modelling frequencies and polycrystalline media, such that an optimal suppression condition of $\alpha d \approx 1$ Neper can be achieved. But such treatment would introduce huge computation and time costs, and therefore it is not pursued in this example. Instead, this example uses a combination of all three opportunities, rather than any single one, to reduce attenuation errors.

The principle of combining suppression opportunities is relatively simple. For a given material, trial simulations (or theoretical predictions) are first conducted to determine the frequency range of each FE model in which αd is within a bound of 1 Neper, e.g. $0.01 \leq \alpha d \leq 6$ Neper. If there is an overlapped frequency range between two models, the overlapped range is designated to the model with either a larger sampling rate S , a closer attenuation αd to 1 Neper, or both. Finally, within the chosen frequency range of each model, transmitting centre-frequencies are tailored to ensure that the whole range uses appropriate spectra of the waves.

Here an example is provided in Figure 4.11 to demonstrate an incorrect combination of suppression opportunities and the corrected combination that appropriately reduces numerical attenuation errors. The example is given for the material aluminium. In the frequency range of 6.5-13.5 MHz, panel (b) shows that the models N11520 (solid

triangles) and N16000 (hollow circles) both satisfy the condition of $0.01 \leq \alpha d \leq 6$ Neper ($2.72 \leq F_\alpha \leq 101.00$). The incorrect combination chooses the model N16000 to cover this frequency range because it has a larger sampling rate S than N11520, which is shown in panel (c). To save modelling costs, the incorrect combination excites a transmitting wave, in the form of a three-cycle Hann-windowed toneburst, with a centre frequency of 20 MHz to provide a wide frequency coverage. In this case, the range of 6.5-13.5 MHz is far away from the maximum of the transmitted amplitude spectrum as shown in panel (d). This deviation from spectral maximum may cause a relatively small amplitude error Δ_A , but the error is significantly magnified by the large propagation factor F_α . This leads to incorrect attenuation results (hollow circles) as shown in panel (a). Instead, the corrected combination uses the model N11520 having smaller propagation factors in the frequency range of 6.5-13.5 MHz as shown in panel (b) and performs the FE simulations in an appropriate spectral range as shown in panel (d). The corrected results (solid triangles in panel (a)) agree very well with the theoretical curve, which is very accurate in the range of concern as explained in §4.3.4, while the incorrect results deviate substantially from both corrected and theoretical results. It is important to realise that the peak difference between the incorrect and corrected results, with the latter as reference, is as large as -54.78% occurring at the frequency of 6.5 MHz, see Figure 4.11(a).

4.4 Effect of symmetry boundary conditions

The preceding FE method is capable of performing numerical experiments with fully-controlled conditions, and from the experiments, effective media parameters can be ideally measured with errors and uncertainties being appropriately estimated. Thus, this method is well suited to evaluating theoretical models that are generally approximate due to the use of assumptions and simplifications. However, there remains one more challenge for accurate simulations, which is to determine the set of characteristics that are defined by a chosen FE model. Clearly, the choices of most parameters, such as, density, dimensions, or crystal properties, are simply recorded. But the spatial characteristics, represented by the geometric two-point correlation (TPC) function, of the grains are a product of the creation of the polycrystal domain, and these need to be measured from the FE model.

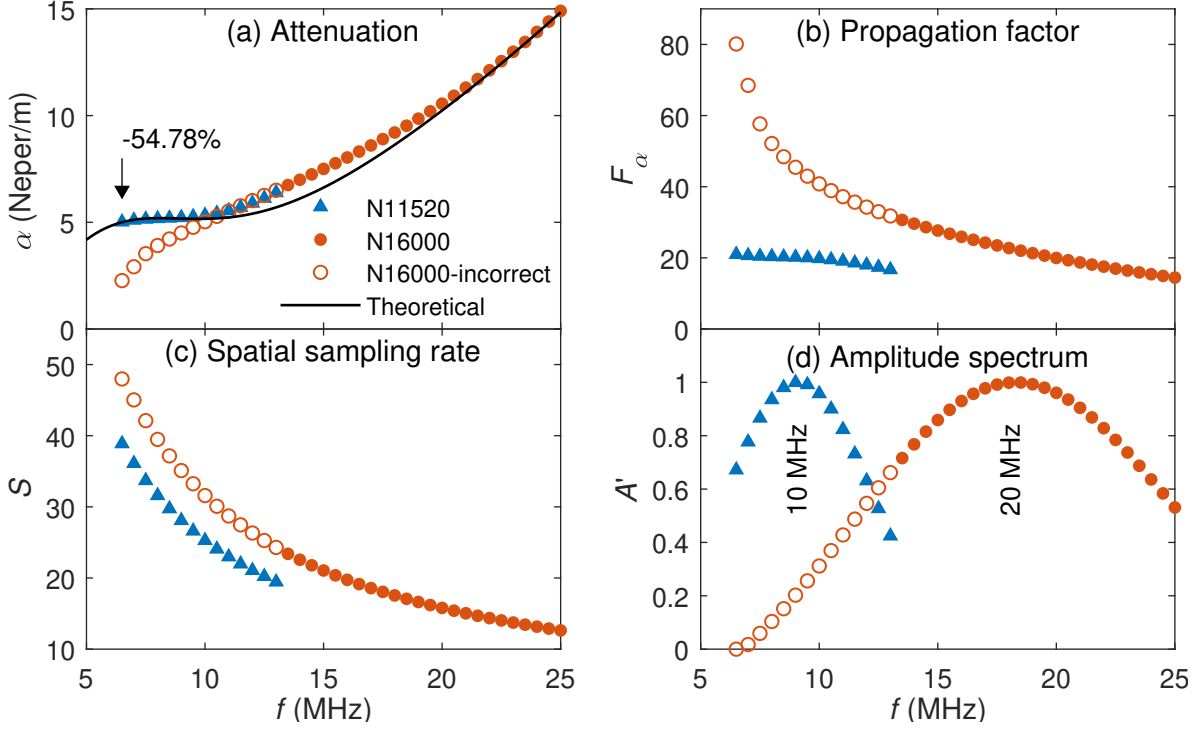


Figure 4.11: Example suppression of numerical attenuation error for aluminium. (a) shows attenuation coefficients obtained from FE models (points) and a theoretical model [28] (solid line). Solid points represent satisfactory results with attenuation errors being appropriately suppressed, while incorrect results are plotted as hollow circles. (b) gives the error propagation factors for the FE models, $F_\alpha = \exp(\alpha d)/(\alpha d)$. (c) plots the spatial sampling rates $S = V_L/(fh)$ and (d) the normalised transmitting amplitude spectra $A' = A(0; f)/\max(A(0; f))$. All panels (b)-(d) use the same legend as given in (a). Each FE model uses 15 realizations to get the averaged result as shown in the figure.

This is a vital step for any comparative studies with theoretical models, to ensure that these properties are represented properly in parallel in the FE and analytical models.

4.4.1 Effect on two-point correlation function

As introduced in §3.6 and the literature [28, 39], the determination of a TPC data point $w(r)$ involves dropping a large number of random pairs of points, each pair being separated by a distance of r , into a polycrystal model. The determination then counts the number of pairs whose two points occur in the same grain and compares this number to the total number of pairs to obtain the probability $w(r)$. As shown in Figure 4.12(a), this approach has limited both points of a random pair to the inside of a model, and thus consider only the statistical information within the cuboid of the model. Nonetheless, it is mentioned in

§3.4 that symmetry boundary conditions (SBCs) are utilized to emulate polycrystal media of infinite size in the transverse direction to that of wave propagation. Such conditions mirror the boundary grains that are associated with the SBCs, which is demonstrated in Figure 4.12(b), and these grains are therefore likely to be larger on average than the grains located within the body of the model. And in the FE computations, this results in stronger scattering of propagating waves when they encounter enlarged boundary grains. Thus, it might be desirable to consider this mirroring effect in the measurement of TPC data with a goal to evaluate, by comparison with the FE results, which TPC is more appropriate for evaluating theoretical results.

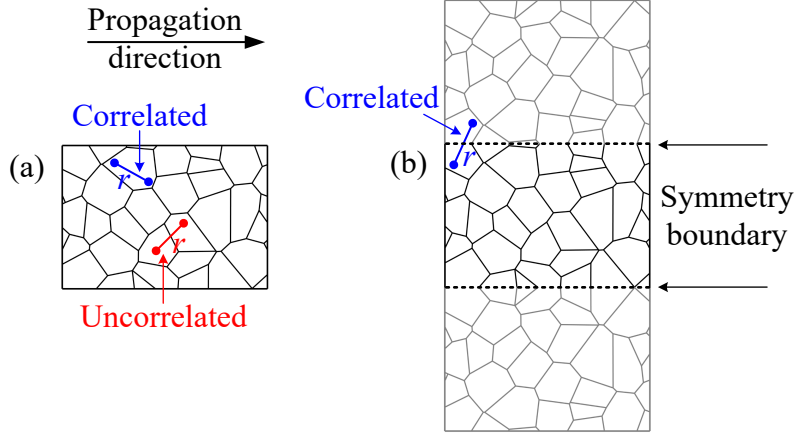


Figure 4.12: Illustration of (a) the measurement of two-point correlation function $w(r)$ and (b) the effect of symmetry boundary conditions. $w(r)$ is the probability that two points separated by a distance of r are correlated. Previous measurement procedures [28, 39] only use internal points, which is shown in (a), to determine $w(r)$. In this case, two points are deemed correlated if they are in the same grain. As shown in (b), the use of symmetry boundary conditions in the FE simulations leads to the mirroring of boundary grains. Due to this mirroring effect, two points are also deemed correlated if they are in the same extended boundary grain.

It can be inferred from the illustration in Figure 4.12(b) that the statistical significance and impact of the boundary grain mirroring increases as the proportion of boundary grains grows. Based on this inference, the actual effect of SBCs on the TPC function is evaluated here. Achieving this evaluation requires the grains associated with SBCs being parametrically described and the TPC functions with consideration of SBCs being numerically measured.

To describe the grains associated with SBCs, three parameters are used: the number fraction NF and volume fraction VF describing respectively the relative number and

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volume of boundary grains to all grains within the model, and the surface area to volume ratio SA:V representing the amount of symmetry boundary area per unit model volume. These parameters are calculated for the models given in Table 3.1 and the results are provided in Table 4.1 with each of the coordinate axes being wave propagation direction. The table shows that for the provided models having significant numbers of grains, these three parameters are actually equivalent, with NF and VF being approximately equal to each other and being proportional to SA:V. It is important to realise that NF is slightly smaller than VF because the grains generated by the Voronoi tessellation do not have uniform volume, but rather boundary grains are to some degree larger than internal grains. Since these three parameters are equivalent, the following evaluation only uses the surface area to volume ratio SA:V to represent SBCs, because this parameter can be easily calculated without the knowledge of actual grains. And the studies reported below just consider, for the sake of clarity, the five cases in Table 4.1 with unique SA:V values: N115200- x , N11520- x , N11520- z , N16000- x , and N16000- z . Here the label of each case is composed of its model name and propagation direction.

To measure the TPC functions with consideration of SBCs, this study uses a procedure that is mostly the same as the one summarised in §3.6 except for the two treatments adopted to consider SBCs. The first treatment is that for a pair of random points only one of them is confined within the model, while the other is completely random as long as their distance is r , meaning that the latter point can be outside of the model. Given a sufficiently large number of pairs, this allows the ergodicity to be satisfied, as the pairs can

Table 4.1: Parameters of the grains associated with symmetry boundary conditions. The parameters are given for three models, with information being provided in Table 3.1, of waves propagating in three coordinate axes. NF and VF are the number and volume fractions, describing respectively the relative number and volume of symmetry boundary grains to all grains within a model. SA:V is the surface area to volume ratio, representing the amount of symmetry boundary area per unit model volume.

Model	x -direction			y -direction			z -direction		
	NF	VF	SA:V	NF	VF	SA:V	NF	VF	SA:V
N115200	0.086	0.090	0.187	0.086	0.090	0.187	0.148	0.154	0.333
N11520	0.158	0.171	0.367	0.161	0.168	0.367	0.146	0.156	0.333
N16000	0.224	0.232	0.500	0.226	0.233	0.500	0.090	0.096	0.200

cover the entire space of infinite lateral extents that are prescribed by SBCs. The second treatment involves the counting of correlated pairs. As illustrated in Figure 4.12(b), an extra situation of two points being correlated may occur when the second point is outside of the model. In this case, a pair is considered to be correlated if one point occurs in a symmetry boundary grain and the other falls into its mirrored counterpart. By using this measurement procedure, the TPC data of the five cases given above are obtained and plotted in Figure 4.13(a) as hollow points (the data points for the case N115200- z are also given in the figure for later use). To evaluate the influence of SBCs, the TPC statistics neglecting SBCs are also provided as solid points in the figure.

The simulated waves travel in the z -direction, meaning that the consideration of SBCs involves only the cases associated with z -direction: N115200- z , N11520- z and N16000- z . It is shown in Figure 4.13(a) that these three cases are quite close to each other, but N11520- z has the largest tail and thus the strongest SBC effect. Therefore, this case is used in the following as an example for the consideration of SBCs, and it is further plotted in Figure 4.13(b) as hollow circles. For the case of neglecting SBCs, the TPC data of the three models (Figure 4.13(a)) are nearly identical. Thus, their average, provided in Figure 4.13(b) as solid circles, is employed to describe the case of neglecting SBCs.

It would be practically meaningful to reduce the impact of SBCs such that measuring TPC data can be performed in a simpler way by neglecting SBCs. This can be achieved by using smaller SA:Vs due to the positive correlation between TPC data and SA:V. It is shown in Table 4.1 that the way to get a smaller SA:V is through widening the lateral dimensions of polycrystal models, and in extreme cases, the effect of SBCs can be negligible if the lateral dimensions are sufficiently wide. However, the models adopted in the present work are already very big, and increasing their lateral dimensions will lead to added challenges to the computation resources. In addition, an alternative possibility of minimizing SBCs effect is to reduce the average size of the symmetry boundary grains such that the mirrored grains would have similar sizes to internal grains. It is practically difficult to generate grains with such a distribution but implementing a method for this aim would be very useful.

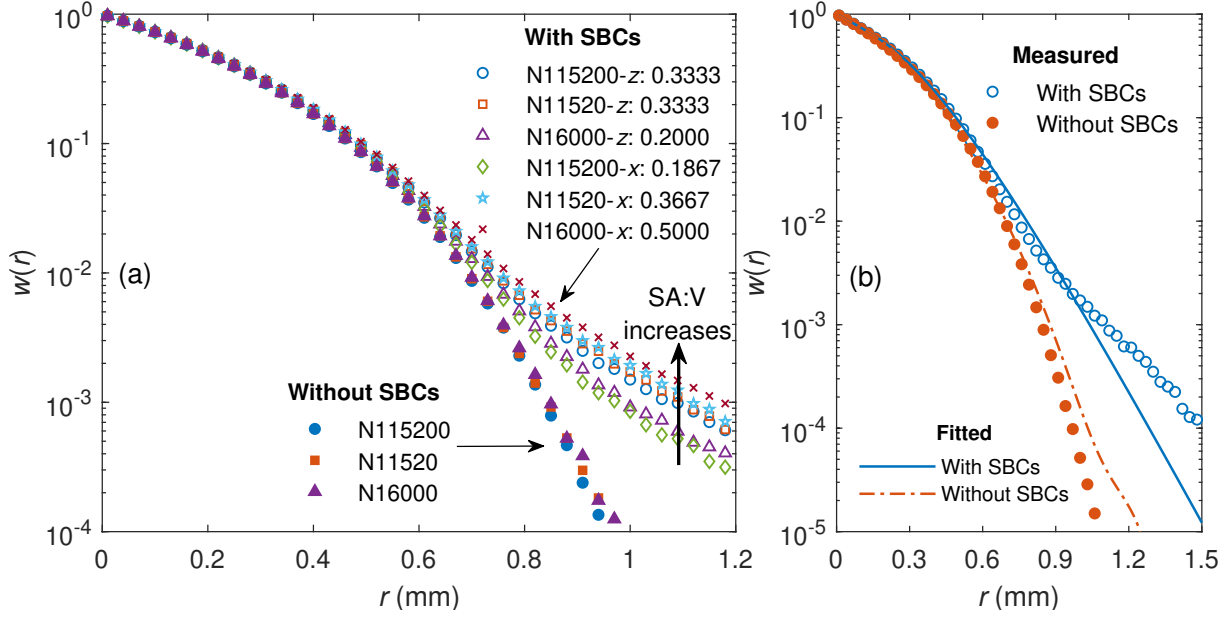


Figure 4.13: Two-point correlation data numerically measured from FE models (a) and those related to actual FE simulations of this work (b). In (a), hollow points are collected with consideration of symmetry boundary conditions (SBCs), while solid points ignore this SBCs effect. The label of hollow points, N115200-z: 0.3333 for example, is started with model name (N115200), followed by wave propagation direction (z), and ended with surface area to volume ratio SA:V (0.3333). In (b), hollow points correspond to those of N11520-z: 0.3333 in (a), and solid points are the averages of the solid ones in (a). These two sets of discrete data are fitted into mathematical functions and are shown as lines. For better visualisation, only every third point of measured data points are shown in the figure.

4.4.2 Effect on attenuation and phase velocity calculation

Having demonstrated in the preceding examination that SBCs have a significant effect on TPC functions, it is now essential to identify if SBCs would equally affect effective media parameters in terms of attenuation coefficient and phase velocity. For this purpose, the TPC functions, with and without consideration of SBCs, are put into one of the advanced theoretical models, the second-order approximation (SOA), to calculate the parameters. The degrees of agreement between the resulting parameters and FE results are then estimated to assess the improvement brought in by the consideration of SBCs.

Incorporating TPC functions into the SOA model requires the two sets of data in Figure 4.13(b) to be fitted to mathematical forms. The case without consideration of SBCs has been fitted in §3.6 and the coefficients of the fitted function are repeated in Table 3.3. Similarly, the case with SBCs is fitted and the results are shown in the same table.

The fitted functions are further plotted in Figure 4.13(b), showing a reasonably good agreement with the data points.

Substituting the two fitted functions into the SOA model and solving the equation results in the theoretical solutions to attenuation and phase velocity. Inconel is used here as the material input to calculate theoretical solutions; the properties of Inconel are given in Table 3.2. The resulting attenuation and velocity curves are plotted in Figure 4.14(a) and (b), respectively. In the figure, the corresponding FEM results are also provided as baseline data to evaluate the approximations of these solutions.

It is shown in Figure 4.14(a) and (b) that the overall agreement between the theoretical and FEM results is very good, no matter whether SBCs are considered in the TPC functions or not. However, there are clear differences between the theoretical results, which demonstrates that the SBCs effect is actually prominent. In most frequency regions, the curves with consideration of SBCs agree better with FEM points, conveying an essential message that the FEM results are influenced by the doubling of grain size at symmetry boundaries. It is also important to notice that the theoretical and FEM results are not perfectly matched even when boundary grains are considered. This is because in the FEM results the SBCs affect scattering only at boundaries, while in the theoretical model the effect is not reproduced exactly as the TPC function assumes random, homogeneous distribution of those grains.

There is no doubt that the TPC function with SBCs should be selected for the material systems when evaluating the theoretical model. To quantify the improvement of theoretical prediction brought in by the consideration of SBCs, the relative differences of theoretical curves to the FEM points are calculated and plotted in Figure 4.14(c) and (d). The agreement is clearly better at all frequencies for the TPC function with SBCs.

This investigation concludes that it is best to consider the SBCs effect in the TPC function. In practice, however, it is always desirable to reduce the effect of the boundaries to a negligible level by making a model as wide as possible. It is important to do so, because one of the key interests of FE modelling at the moment is to check the significance of assumptions in analytical models, and thus there is a strong motivation to eliminate this TPC source of differences from the modelling.

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Table 4.2: Coefficients of mathematically fitted two-point correlation functions. A_i and a_i are coefficients of the i -th term of the mathematically fitted function $w(r) = \sum_i A_i \exp(-r/a_i)$.

Terms	Without SBCs		With SBCs	
	A_i	a_i	A_i	a_i
1	-2922.66	0.115726	-129.485	0.1280002
2	-10.6181	0.172221	-388.413	0.1279995
3	3914.370	0.110790	797.091	0.1517330
4	-3305.68	0.103201	-1372.040	0.1898924
5	696.919	0.0910265	1982.690	0.1867733
6	54.3582	0.152263	694.300	0.1242404
7	-42.4732	0.0723540	-469.525	0.1279995
8	1616.78	0.110790	-1113.610	0.1709402

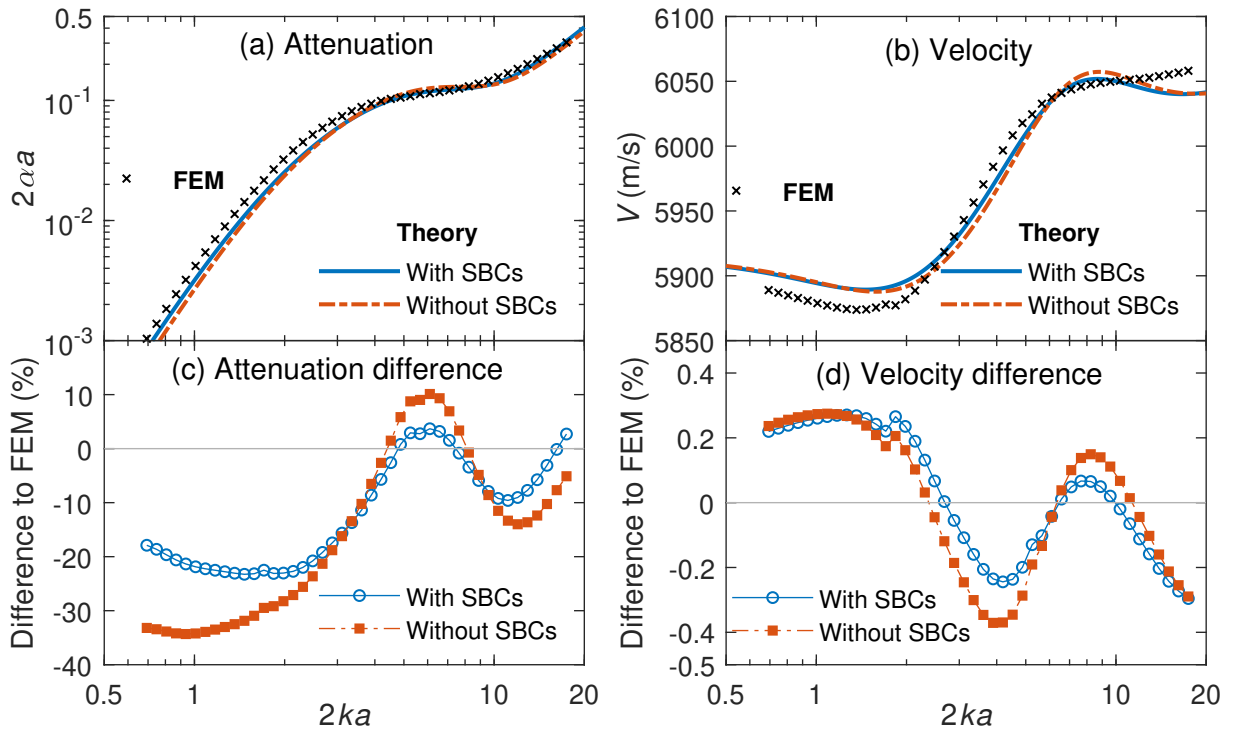


Figure 4.14: Comparison of theoretically predicted effective media parameters with FEM results for Inconel: (a) attenuation, (b) phase velocity, (c) relative difference of attenuation, and (d) relative difference of phase velocity. In (a) and (b), lines represent the theoretical solutions of the SOA model which uses the two-point correlation functions with (solid lines) and without (dash-dotted lines) consideration of symmetry boundary conditions (SBCs). Crosses denote the FEM results obtained from the models N115200, N11520, and N16000. Each model uses 15 realizations to obtain the averaged results shown in the figure. For better visualisation, only every ten points of FEM data are shown here. In (c) and (d), the relative differences are computed by subtracting FEM results from theoretical predictions and then dividing by FE results.

4.5 Summary

This work presents a thorough study to maximize the accuracy of the finite element (FE) method for the propagation and scattering of elastic waves in polycrystals. Specifically, this work addresses the following three topics that have not been covered by the modelling studies so far but are essential to future FE simulations.

The determination of effective media parameters, namely attenuation and phase velocity, is first discussed. These parameters describe the amplitude and phase changes of a plane wave as it travels through a polycrystalline medium. It is demonstrated that the travelling wave essentially does not have a planar wavefront, which is caused by random scattering. However, it is demonstrated that the coherent part, belonging to the plane wave, can be conveniently calculated as the spatial average of the wavefront. From a set of coherent waves, attenuation and phase velocity can be determined in two ways. The through-transmission approach uses the coherent waves measured on two external surfaces: the transmitting surface and its opposite receiving surface. In addition to the two waves used in the through-transmission method, the fitting approach also utilizes extra coherent waves collected inside a FE model. These two approaches are found to be practically equivalent and can thus be used interchangeably. The through-transmission method might be preferable in actual simulations due to its ease of wave collection and calculation.

The estimation and suppression of the errors and uncertainties of effective media parameters are then attempted in this study. It is found that two factors can cause errors and uncertainties: numerical approximations and statistical considerations. Numerical approximations only cause errors, while statistical considerations involve both errors and uncertainties. For numerical errors, both attenuation and velocity errors can be suppressed by the use of a larger spatial sampling number S (thus a finer mesh size h) if computational capability allows. In addition to this, numerical attenuation and velocity errors can also be reduced in different ways: 1) Numerical attenuation error can be suppressed by using an appropriate spectrum range that is in close proximity to its maximum, or by limiting attenuation αd to a certain range in the vicinity of 1 Neper. 2) Numerical velocity error can be controlled by using a large Courant number C that is close to unity, and can also be corrected by utilizing the analytically predicted error from Equation 4.6.

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For statistical errors and uncertainties, the suppression approaches developed for numerical errors also ensure that they can be satisfactorily controlled to a certain extent. The only requirement is that a sufficiently large number N of realizations has to be used to obtain a reasonably small statistical error and a fairly converged statistical uncertainty.

The incorporation of FE model information into theoretical models is finally discussed. It is indicated that the two-point correlation (TPC) function is the statistic required to put into theories. The symmetry boundary conditions (SBCs), employed to emulate infinitely wide media that can hold plane waves, have a considerable effect on the TPC function and on the theoretically predicted attenuation and velocity. Thus, this SBCs effect needs to be considered in the TPC function for a more accurate incorporation of statistical information.

The FE method discussed in this work focuses on the specific case of plane longitudinal waves travelling in untextured polycrystals with equiaxed grains. However, it is expected that the principle established in this work may be extended reliably to more general cases, for example to elongated grains and preferred crystallographic texture materials.

Chapter 5

Elastic waves in polycrystals with equiaxed grains

5.1 Introduction

This chapter studies the attenuation and phase velocity dispersion of plane longitudinal waves in polycrystals with equiaxed grains. The polycrystals are statistically isotropic and homogeneous on the macroscopic scale, and two types of such polycrystals are considered in this chapter.

The first type has the highest crystal symmetry, i.e., cubic, for the constituting grains. This type of material has been studied previously by using the theoretical SOA and Born models with comparison to 3D FE simulations [28, 29, 39]. The theoretical models were shown to agree very well with FE results in a wide frequency range for a variety of materials with the Zener anisotropy factor A [53] varying from 1.24 (Al) to 3.14 (Copper), indicating that wave scattering by polycrystals can generally be properly accounted for by the theoretical models. However, the studies also demonstrated a slightly degenerated agreement as A increases. This is not surprising since the theoretical models better describe materials of low material inhomogeneity due to their lack of representation of high order terms on inhomogeneity in the theoretical models. This chapter aims to evaluate how the theoretical models behave when A is much higher than previously considered and thus to establish the range of validity of those models. Since the elastic scattering factors

$Q_{L \rightarrow T}$ and $Q_{L \rightarrow L}$ [26] are more accurate and contain more information than the anisotropy factor A , they will be used to characterise the level of material inhomogeneity for the low-frequency Rayleigh and high-frequency stochastic regions, respectively. This part of work will be presented in the following §5.2, and it is being prepared for publication [P5].

The second type of polycrystal has the lowest symmetry, namely triclinic, for the constituting grains. Although prior works have studied polycrystals of symmetry lower than cubic using the theoretical Born and FFA models [11, 26, 46, 73], the studies involving the development of the SOA model and the comparison with FE simulations were limited to polycrystals of cubic symmetry [14, 17, 19, 28, 29, 39]. Moreover, many practically-important polycrystalline materials have symmetries lower than cubic, e.g., titanium alloys generally have a hexagonal symmetry [74] and α/β colonies in aerospace titanium alloys form effective grains of monoclinic symmetry [75]. To fill this gap, this chapter seeks to use the SOA model as formulated in §2 and the 3D FE model as implemented in §3 to study the most general case of a polycrystalline material having the lowest triclinic symmetry that needs to be described by 21 independent elastic constants. This part of the work will be reported below in §5.3. It has been reproduced from [P1], with the permission of AIP Publishing; the theoretical curves were originally generated by Dr Gaofeng Sha as a co-author of the publication.

5.2 Polycrystals of cubic crystal symmetry

This section studies equiaxed polycrystals of cubic symmetry, investigating their attenuation and velocity dispersion for plane longitudinal waves propagating within them. The purpose is to evaluate the change of wave behaviours with material inhomogeneity and establish the range of validity of the theoretical SOA and Born models by comparing to numerical FE simulations. The eight cubic materials given in Table 3.2 are considered and their anisotropy factors A vary from 1.24 to 9.14. Initially, this section compares the theoretical and numerical FE results for attenuation and velocity and discusses their frequency dependences. This is followed by analysing the influence of material inhomogeneity on the results. The approximations of the theoretical models are then evaluated against the FE model. Lastly, the quasi-static velocity limit is investigated.

5.2.1 Frequency dependence of attenuation and velocity

Figure 5.1 shows the normalised attenuation $2\alpha_L a$ in (a-b) and the normalised phase velocity $V_L/V_{0L} - 1$ in (c-d) versus the dimensionless frequency $2k_{0L}a$ for the eight polycrystalline materials. Each material utilizes the equiaxed FE models N115200, N11520 and N16000 given in Table 3.1, combined with multiple modelling centre frequencies, to cover a wide frequency range. The choice of FE material models and their modelling parameters has ensured a satisfactory numerical accuracy across the covered frequency range. A combination of 15 realizations has been used for each modelling case to achieve statistically meaningful results. The FEM points in the figure show the averages of multi-realisation cases; standard deviations are not provided since the corresponding error bars are smaller than, or comparable to, the size of the point markers. The theoretical SOA (solid) and Born (dash) curves have incorporated the TPC function as accurately measured from the FE material models; the coefficients of the TPC function are given in Table 3.3. The normalisation factor a is determined from the slope at the origin of the TPC function, representing the mean linear size of the grains.

The Rayleigh and stochastic attenuation asymptotes are given for aluminium; for clarity of the plots, those of other materials are not provided. The asymptotes approach the theoretical and numerical results of aluminium in the low- and high-frequency ranges, and they are clearly parallel to the results of other materials. It can thus be inferred from the asymptote expressions, Equations 2.18 and 2.26, that attenuation has fourth- and second-power dependences on frequency in the two regimes. Between the Rayleigh and stochastic regimes, frequency dependence transits from fourth to second power and a hump behaviour can be consistently seen from the theoretical and numerical results for all materials. As a unique feature of longitudinal waves, this hump behaviour is caused by the transition of dominant scattering from the $L \rightarrow T$ component in the Rayleigh regime to $L \rightarrow L$ in the stochastic regime [14]. Also, it is observable that for a material with a higher inhomogeneity, the stochastic regime is less pronounced and the geometric regime (seemingly flat attenuation) occurs earlier in frequency as can be more clearly seen from the SOA curve for lithium.

For phase velocity, the theoretical and numerical results tend to approach the Rayleigh and

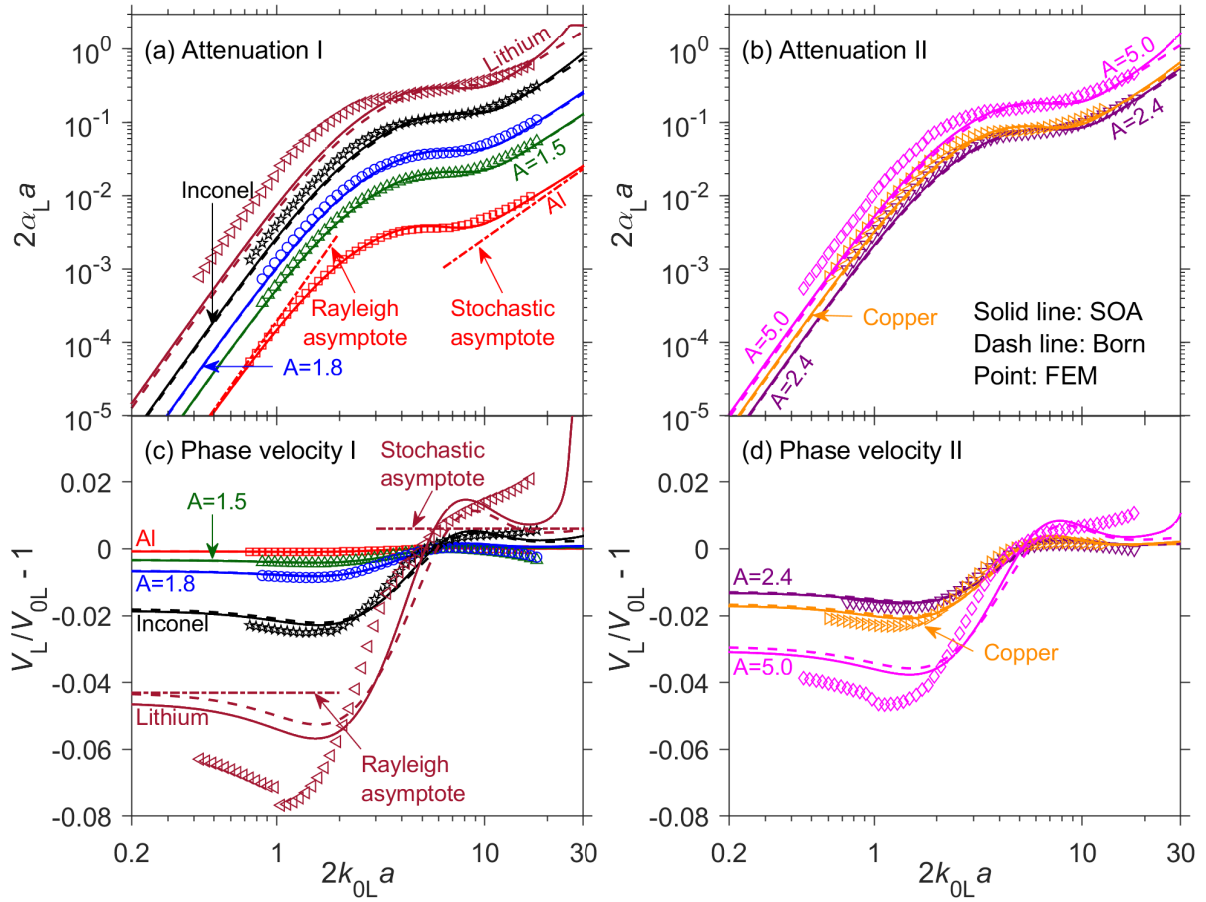


Figure 5.1: Normalised (a-b) attenuation and (c-d) phase velocity versus normalised frequency for longitudinal waves in equiaxed polycrystals comparing theoretical SOA and Born predictions with numerical FEM results. All FEM points are obtained by averaging the results of 15 FE realizations; the corresponding error bars are not shown since they are smaller than the size of the point markers. The theoretical SOA and Born curves have used the TPC function (Table 3.3) as accurately measured from the FE models. The properties of the polycrystalline materials are given in Table 3.2, and their inhomogeneities (characterised by the elastic scattering factors $Q_{L \rightarrow T}$ and $Q_{L \rightarrow L}$) have the relationship of $Al < A=1.5 < A=1.8 < A=2.4 < Copper < Inconel < A=5.0 < Lithium$.

stochastic asymptotes in the low- and high-frequency ranges, respectively. For clarity of the plots, the asymptotes are provided for lithium only. The asymptotes are independent of frequency, meaning that phase velocity is non-dispersive in these two frequency ranges. In the transition region, a dispersive behaviour occurs as a result of dominant scattering transition as mentioned above. It is also supported by the phase velocity results that the stochastic regime gets shorter as the material inhomogeneity becomes larger. The FEM points for the materials $A=5.0$ and lithium do not show frequency-independent parts in the range where the stochastic regime is expected. This may be attributed to the

relatively larger numerical errors involved in the results or the complete disappearance of the stochastic regime due to the strongly scattering nature of the materials.

In addition to the frequency dependences, attenuation and phase velocity also show reliance on material inhomogeneity. This is manifested as a larger material inhomogeneity being accompanied by a higher level of attenuation and a larger deviation of phase velocity to the Voigt velocity. These inhomogeneity dependences will be further discussed in the following §5.2.2.

The theoretical SOA and Born models have a high quality of agreement with the 3D FE results, especially for materials of relatively low inhomogeneity. The agreement between the theoretical and numerical models and its degeneration with the increase of material inhomogeneity will be evaluated in-depth in §5.2.3.

5.2.2 Inhomogeneity dependence of attenuation and velocity

Figure 5.1 has shown that attenuation and phase velocity vary across different materials, exhibiting dependences on material inhomogeneity. These dependences are more prominent in relatively low- and high-frequency ranges. For this reason, two normalised frequencies, $2k_{0L}a = 1$ and $2k_{0L}a = 12$, are chosen in these two ranges to quantitatively evaluate the dependences. At these two frequencies, normalised attenuation and phase velocity points are extracted from Figure 5.1 and plotted versus material inhomogeneity in Figure 5.2. The choice of the two material inhomogeneity factors, $Q_{L \rightarrow T}$ and $Q_{L \rightarrow L}$, in the figure is based on the asymptotes of the Rayleigh and stochastic regimes where the two frequencies roughly fall into. At the Rayleigh limit, $Q_{L \rightarrow T}$ is the dominant elastic factor affecting attenuation and velocity: 1) The elastic dependence of the Rayleigh attenuation in Equation 2.18, $\alpha_L \propto Q_{LL}^* + V_{0L}^3/V_{0T}^3 Q_{L \rightarrow T}$, can be reduced to $\alpha_L \propto Q_{L \rightarrow T}$ since Q_{LL}^* is generally negligible while V_{0L}^3/V_{0T}^3 just differs slightly from one material to another; 2) The Rayleigh velocity in Equation 2.23 can be approximated to $V_L/V_{0L} - 1 \approx -2Q_{LL}^* - 2Q_{L \rightarrow T} \approx -2Q_{L \rightarrow T}$ since the elastic factors Q_{LL}^* and $Q_{L \rightarrow T}$ are far smaller than unity and the former is generally negligible. Likewise, $Q_{L \rightarrow L}$ governs the level of scattering at the stochastic limit: 1) the stochastic attenuation in Equation 2.26 satisfies $\alpha_L \propto Q_{L \rightarrow L}$; 2) the stochastic velocity in Equation 2.30 can be approximated to

$$V_L/V_{0L} - 1 \approx -5Q_{L \rightarrow L}/2 + 2Q_{LT}^*/(V_{0L}^2/V_{0T}^2 - 1) \propto Q_{L \rightarrow L}.$$

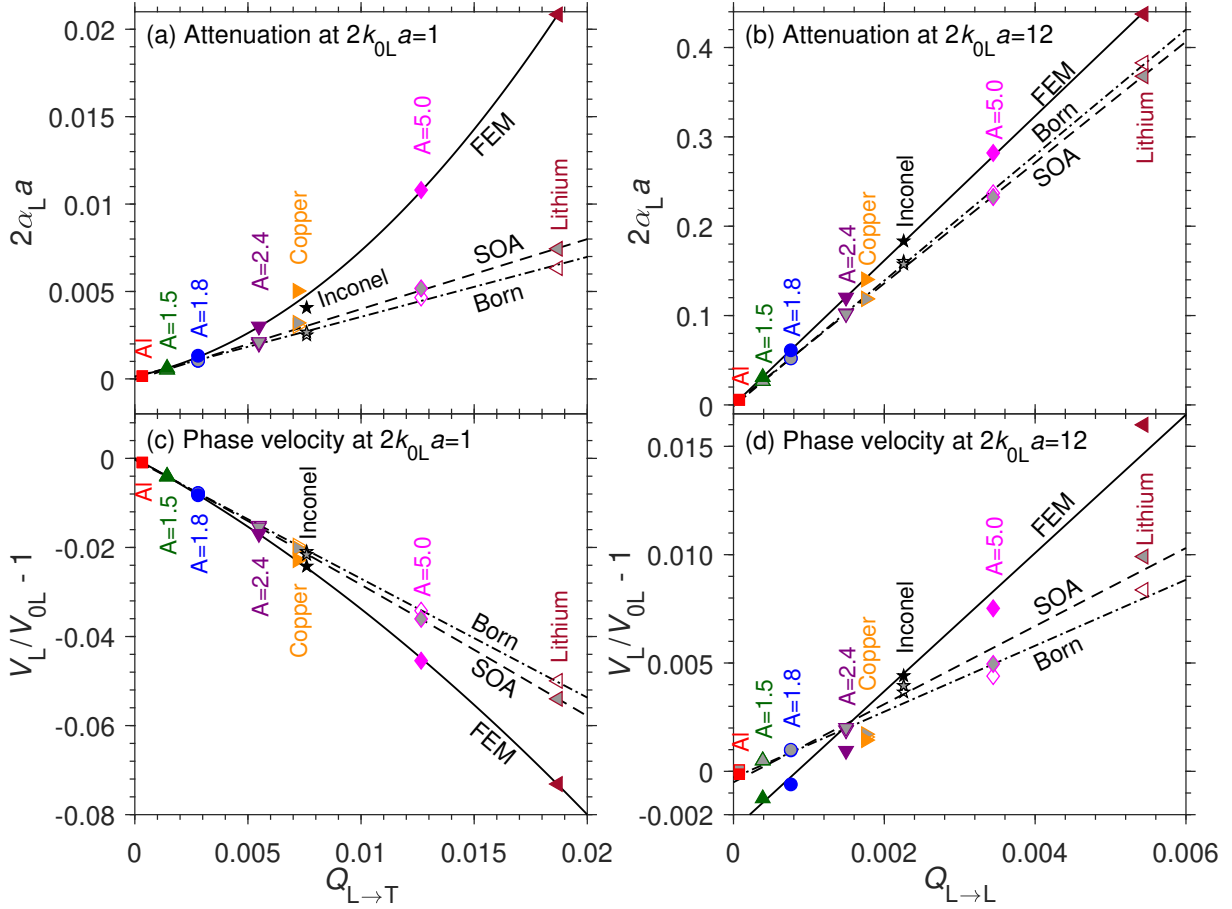


Figure 5.2: Normalised (a-b) attenuation and (c-d) phase velocity versus material inhomogeneity for longitudinal waves in equiaxed polycrystals comparing theoretical SOA and Born predictions with numerical FEM results. The FEM (solid), SOA (shaded) and Born (hollow) points are taken from Figure 5.1 at the normalised frequencies of (a,c) $2k_{0L}a = 1$ and (b,d) $2k_{0L}a = 12$. The two selected frequencies fall roughly into the Rayleigh and stochastic regimes, respectively. The elastic scattering factors, $Q_{L \rightarrow T}$ and $Q_{L \rightarrow L}$, are used as the material inhomogeneity parameters for the x -axes of the plots. The solid and dash lines in (a) and (c) are quadratic fits of the points, while the rest lines in the figure are linear fits.

At the low-frequency $2k_{0L}a = 1$, the numerical FE points show a distinct quadratic relationship with the inhomogeneity factor $Q_{L \rightarrow T}$ for both attenuation and phase velocity. Quadratic fits are produced for the data points and plotted in the figure. The theoretical SOA predictions also have a quadratic dependence on inhomogeneity; their quadratic fits, however, have much smaller quadratic terms than linear ones, manifested as the nearly straight lines in the figure. Also, the SOA model predicts smaller attenuation and velocity change than the FE model, suggesting that only a limited amount of multiple scattering is considered by the former in comparison to the consideration of all scattering

possibilities in the latter. The theoretical Born predictions exhibit a linear dependence (quadratic fits were generated for them, but the quadratic terms are nearly zero) on material inhomogeneity, which is consistent with its linear approximation made in the derivation. Since the Born model only considers single scattering, the extra attenuation and velocity obtained from the FE model may be attributed to the contribution of multiple scattering. Also, it is important to note that the attenuation points for copper and Inconel in panel (a) deviate slightly from the fitted lines because the factor $Q_{L \rightarrow T}$ is not fully representative of the degrees of inhomogeneity for these two materials; nearly perfect fits can be obtained if the complete factor $Q_{LL}^* + V_{0L}^3/V_{0T}^3 Q_{L \rightarrow T}$ is used for material inhomogeneity.

At the high frequency $2k_{0L}a = 12$, all results have a linear dependence on the material inhomogeneity factor $Q_{L \rightarrow L}$, as is more evident from attenuation results shown in panel (b). Nonetheless, it is worth emphasizing that this assertion of linear dependence may not be appropriate. This is due to the possibility that not all evaluated materials are consistently in the stochastic regime at $2k_{0L}a = 12$: weakly scattering materials are yet to enter the stochastic regime while the strongly scattering ones are already transiting into the geometric regime. Thus, several different scattering mechanisms may be involved at $2k_{0L}a = 12$ across different materials and the finding from the evaluation may not be conclusive.

Consistently for both the low- and high-frequency cases, the level of scattering gets stronger with the increase of material inhomogeneity, leading to a larger attenuation and a greater deviation of phase velocity to the Voigt velocity. In order to visually observe the growth of scattering with inhomogeneity, wavefront fluctuation fields are provided in Figure 5.3 for the eight materials at the low frequency of $2k_{0L}a = 1$, with details in the caption. A fluctuation field records the relative variation of wave motion to the coherent wave that represents the spatial average of wave motion over the wavefront. The way to obtain a fluctuation field can be referred to §4.2.1.

It is demonstrated in Figure 5.3 that wavefront fluctuation intensifies as material inhomogeneity increases. This is to say that a wavefront degenerates and scatters more energy locally into incoherent components as scattering gets stronger. The magnitude of fluctu-

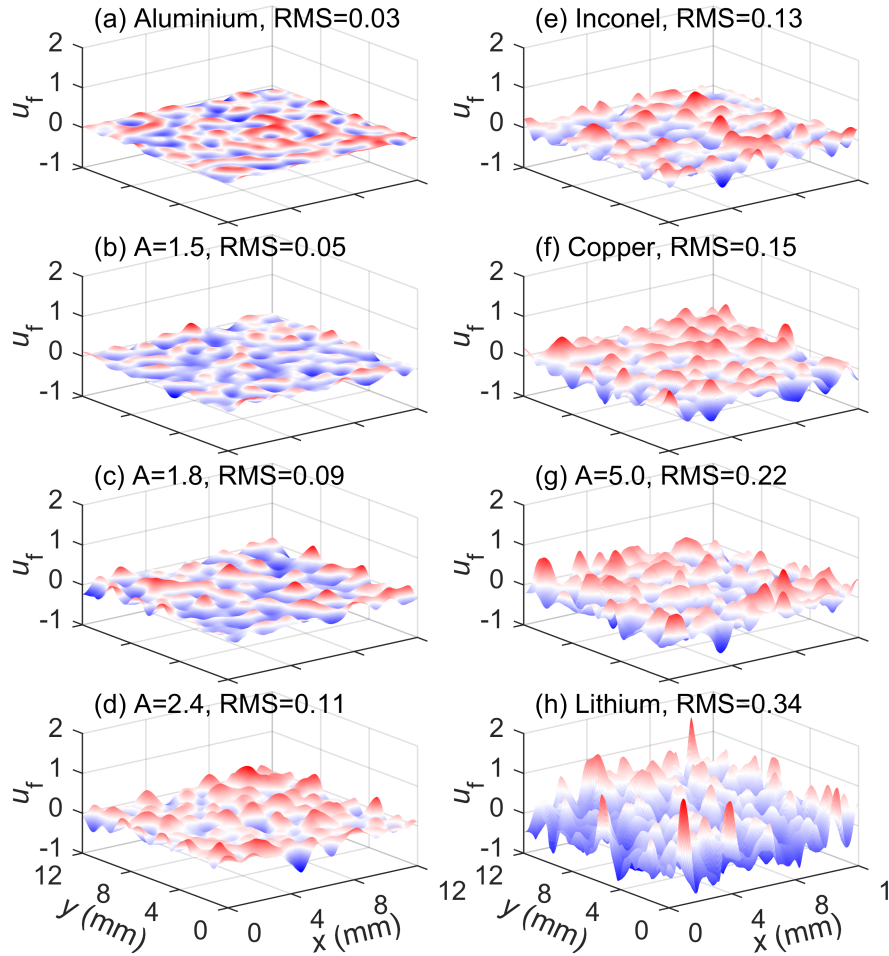


Figure 5.3: Normalised wavefront fluctuations for longitudinal waves in equiaxed polycrystals at the normalised frequency of $2k_{0L}a = 1$. Each plot is obtained by monitoring the displacement field $u(x, y; t)$ on the receiving end $z = d_z$ of the N115200 model, and in the spectral domain, the normalised amplitude fluctuation is calculated by $u_f(x, y; f) = u(x, y; f) / \langle u(x, y; f) \rangle_{x,y} - 1$, where $\langle \cdot \rangle_{x,y}$ represents spatial averaging over all x and y points. The root-mean-square (RMS) values of the fluctuations are annotated in the plots.

ation is very small as compared to the coherent wave for materials of low inhomogeneity such as aluminium, but it can be twice the magnitude of the coherent part for the most strongly scattering material, lithium, as considered in this thesis. This change of fluctuation with inhomogeneity can be more clearly seen from the root-mean-square (RMS) values of the fluctuations as annotated in the plots. The RMS values of individual materials are further plotted against their inhomogeneity factors in Figure 5.4. It is evident that fluctuation RMS exhibits a quadratic relationship with the inhomogeneity factor $Q_{L \rightarrow T}$, which is consistent with that for the corresponding attenuation and velocity as demonstrated above.

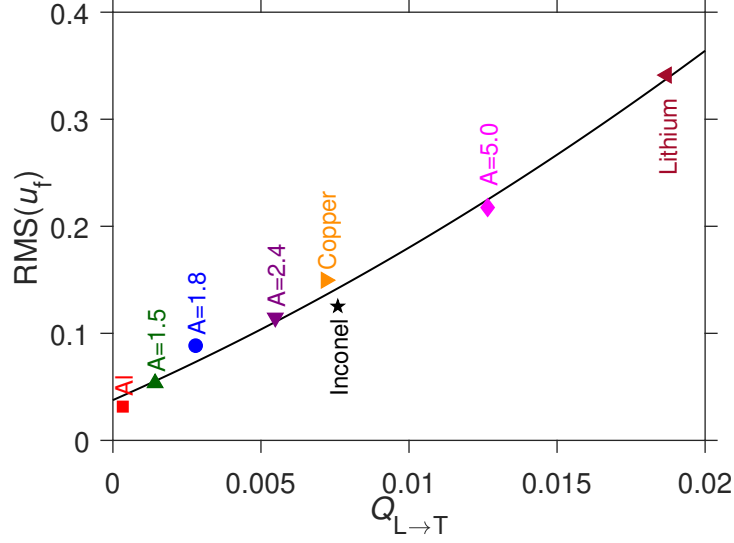


Figure 5.4: Root-mean-square (RMS) of normalised wavefront fluctuation versus material inhomogeneity $Q_{L \rightarrow T}$ at the normalised frequency of $2k_{0L}a = 1$. The RMS points are taken from Figure 5.3, and the line represents their quadratic fit expressed as $RMS = 206.96Q_{L \rightarrow T}^2 + 12.18Q_{L \rightarrow T} + 0.04$ with the goodness-of-fit of $R^2 = 0.99$.

5.2.3 Evaluation of the approximations of the theoretical models

As mentioned in §5.2.1, the FE simulation of waves in polycrystals has achieved a very high degree of accuracy by using a proper combination of FE material models and modelling parameters. The FE simulation results can thus be employed as reference to evaluate the approximations of the theoretical SOA and Born models that consider only a limited amount (or none) of the multiply scattered waves. In order to achieve this evaluation, the relative differences between the theoretical curves and the FEM points shown in Figure 5.1 are quantitatively analysed and plotted in Figure 5.5. The solid and dash lines in the figure represent the relative differences of the SOA and Born predictions to the FE results, respectively.

In the figure, the quality of agreement between the theoretical and FE models is very good in comparison to that between the theoretical and experimental results as observed in the early work [13]. The largest differences for attenuation and phase velocity are found to be around -70% and 3%, both for lithium. As can be found from both attenuation and phase velocity curves, the differences are mostly smaller for the SOA model than for the Born model, correctly reflecting the different degrees of assumptions and approximations made in the derivations of these models.

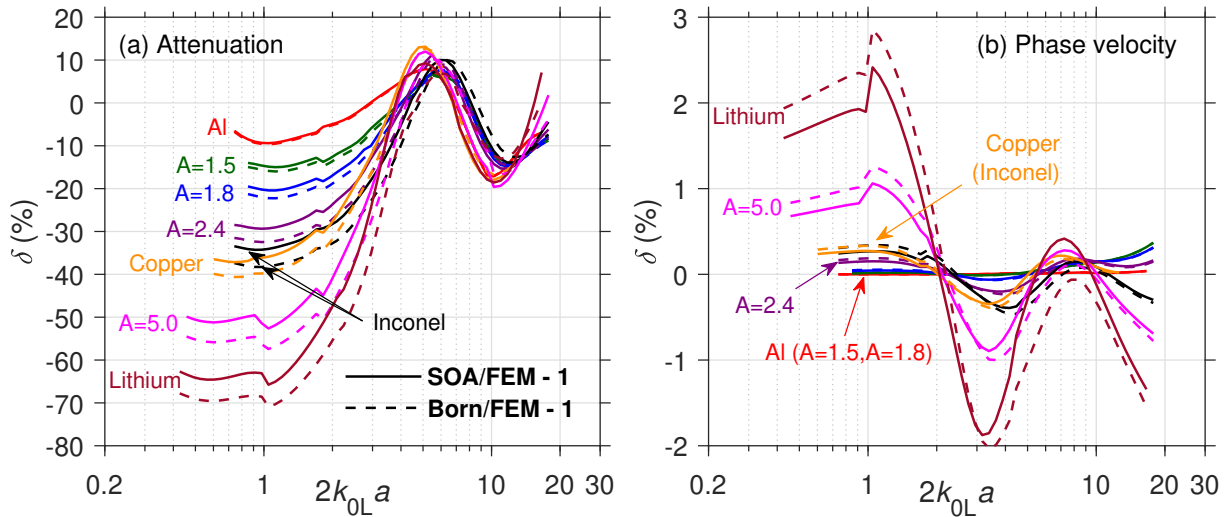


Figure 5.5: Relative difference of (a) attenuation and (b) phase velocity between theoretical (SOA and Born) and numerical (FEM) results versus normalised frequency for longitudinal waves in equiaxed polycrystals. All theoretical and FEM results are taken from Figure 5.1. Their relative differences, with the FEM results as reference, are shown in percentage.

The differences in attenuation and phase velocity between the theoretical and FE models are relatively large at very low frequencies around $2k_{0L}a = 1$. These large differences are somewhat unexpected since it was previously believed that multiple scattering is small in the low-frequency range and can thus be appropriately accounted for by the theoretical models. However, it is now evident that large multiple scattering may also arise at low frequencies, especially for materials of very strong inhomogeneity such as lithium. In comparison to very low frequencies, the middle-frequency range exhibits mostly smaller differences that vary with frequency, and surprisingly, the attenuation differences for the shown materials are nearly overlapped between about $2k_{0L}a = 5$ and $2k_{0L}a = 12$ in panel (a). At very high frequencies, the differences tend to grow substantially with frequency since multiple scattering is increasing. It would be scientifically valuable to actually see this further increase by obtaining higher frequency FE results, but this has currently been limited by the available computational power.

Overall evaluation

The relative differences shown in Figure 5.5 exhibit an overall dependence on material inhomogeneity. In order to assess this dependence, the RMS of each curve in Figure 5.5

is calculated. This parameter, more widely known as the normalised root-mean-square deviation (NRMSD), measures the aggregated relative difference between the theoretical and FE results over the whole frequency range. The NRMSD values for individual curves in Figure 5.5 are provided in Table 5.1 under the label ‘Without SBCs’. This label means that the theoretical calculations have not considered the effect of symmetry boundary conditions (SBCs), which are used in the FE simulations to emulate infinitely-wide models such that plane waves can be initiated. It was demonstrated previously in §4.4 that SBCs can double the sizes of symmetry boundary grains and make these grains larger on average than the grains located within the body of the models. Since this doubling effect is not taken into account in the measurement of the TPC function from FE material models, the theoretical predictions incorporating this TPC function cannot consider the stronger scattering as caused by those doubled, larger grains. This causes a larger difference between theoretical predictions and FE results in comparison to the more accurate case where the SBCs effect is appropriately considered, whose NRMSD values are provided in Table 5.1 under the label ‘With SBCs’.

Table 5.1: Normalised root-mean-square deviation (NRMSD) of theoretical SOA and Born predictions to numerical FE results for longitudinal waves in equiaxed polycrystals. The material inhomogeneity factor $Q_{L \rightarrow T}$ ($\times 10^{-3}$) of each polycrystalline material is provided in the second column. The NRMSDs (%) are specified in the third to tenth columns. For example, the third column specifies the NRMSD of SOA attenuation α_L^{SOA} to its FE counterpart α_L^{FEM} , i.e., $\text{RMS}(\alpha_L^{\text{SOA}}/\alpha_L^{\text{FEM}} - 1)$.

	$Q_{L \rightarrow T}$	Without SBCs				With SBCs			
		α_L^{SOA}	α_L^{Born}	V_L^{SOA}	V_L^{Born}	α_L^{SOA}	α_L^{Born}	V_L^{SOA}	V_L^{SOA}
Al	0.33	8.31	8.38	0.01	0.01	5.69	5.61	0.01	0.01
A=1.5	1.43	10.41	10.93	0.11	0.11	4.98	5.35	0.11	0.11
A=1.8	2.79	13.23	14.30	0.11	0.11	7.19	8.38	0.10	0.10
A=2.4	5.48	18.45	20.49	0.13	0.15	12.30	14.69	0.11	0.12
Inconel	7.59	21.47	24.36	0.22	0.26	15.57	19.03	0.19	0.25
Copper	7.19	24.28	26.76	0.21	0.24	18.02	21.05	0.18	0.21
A=5.0	12.66	33.95	37.61	0.62	0.74	28.56	32.95	0.58	0.72
Lithium	18.70	42.66	46.95	1.35	1.63	38.78	43.80	1.30	1.60

To better interpret the NRMSD data given in Table 5.1, they are further plotted against material inhomogeneity in Figure 5.6. The factor $Q_{L \rightarrow T}$ has been used to describe material inhomogeneity, but note that $Q_{L \rightarrow L}$ can also be alternatively utilized in this case without

5. Elastic waves in polycrystals with equiaxed grains

affecting the conclusion made from this figure. The lines denote the quadratic fits of the points, and the fitted equations are provided in Table 5.2.

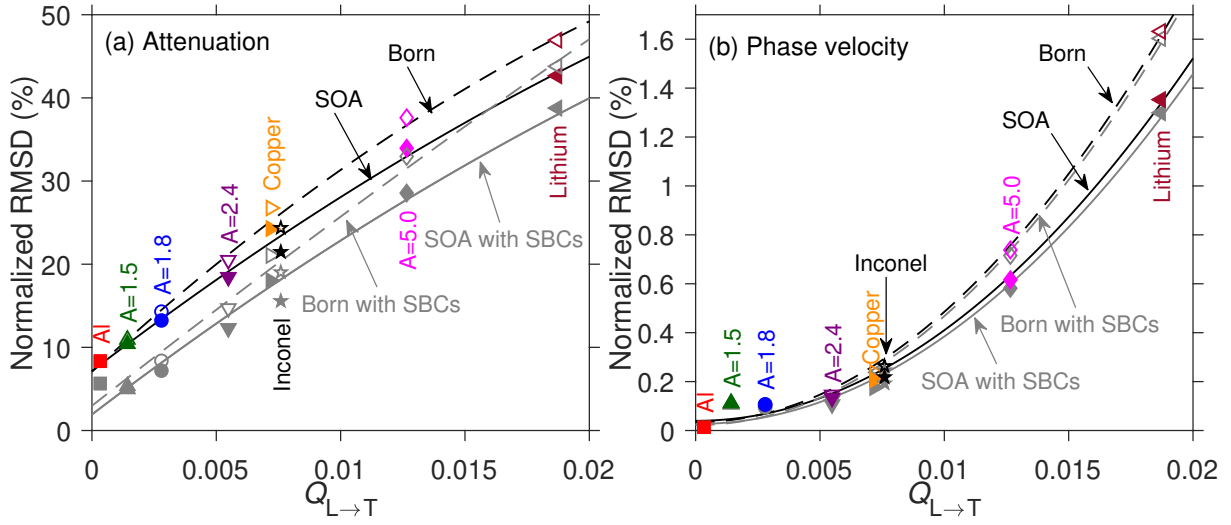


Figure 5.6: Normalised root-mean-square deviation (NRMSD) of the theoretical SOA and Born models to the numerical FE model for longitudinal waves in polycrystalline materials plotted against material inhomogeneity: (a) attenuation and (b) phase velocity. The coloured points are calculated from the data given in Figure 5.1, with the solid and hollow ones representing respectively the NRMSDs of the SOA and Born curves to the FEM points. The grey points are similarly calculated but the SOA and Born curves have considered the effect of symmetry boundary conditions (SBCs). The lines denote the quadratic least-squares fits of the points, and the fitted equations are provided in Table 5.2.

Table 5.2: Normalised root-mean-square deviation (NRMSD) of theoretical SOA and Born predictions to numerical FE results versus material inhomogeneity for longitudinal waves in equiaxed polycrystals: fitted equation. R^2 represents the goodness-of-fit. The fitted equations are plotted in Figure 5.6.

	Fitted equation	R^2
Without SBCs	$\text{RMS}(\alpha_L^{\text{SOA}}/\alpha_L^{\text{FEM}} - 1) \times 100 = -20072.73Q_{L \rightarrow T}^2 + 2291.35Q_{L \rightarrow T} + 7.16$	0.99
	$\text{RMS}(\alpha_L^{\text{Born}}/\alpha_L^{\text{FEM}} - 1) \times 100 = -31979.93Q_{L \rightarrow T}^2 + 2746.44Q_{L \rightarrow T} + 7.07$	0.99
	$\text{RMS}(V_L^{\text{SOA}}/V_L^{\text{FEM}} - 1) \times 100 = 3705.24Q_{L \rightarrow T}^2 + 0.04$	0.99
	$\text{RMS}(V_L^{\text{Born}}/V_L^{\text{FEM}} - 1) \times 100 = 4514.76Q_{L \rightarrow T}^2 + 0.03$	1.00
With SBCs	$\text{RMS}(\alpha_L^{\text{SOA}}/\alpha_L^{\text{FEM}} - 1) \times 100 = -19000.00Q_{L \rightarrow T}^2 + 2281.80Q_{L \rightarrow T} + 1.93$	0.98
	$\text{RMS}(\alpha_L^{\text{Born}}/\alpha_L^{\text{FEM}} - 1) \times 100 = -7002.80Q_{L \rightarrow T}^2 + 2344.12Q_{L \rightarrow T} + 2.97$	0.99
	$\text{RMS}(V_L^{\text{SOA}}/V_L^{\text{FEM}} - 1) \times 100 = 3577.63Q_{L \rightarrow T}^2 + 0.03$	0.99
	$\text{RMS}(V_L^{\text{Born}}/V_L^{\text{FEM}} - 1) \times 100 = 4455.59Q_{L \rightarrow T}^2 + 0.02$	0.99

All goodness-of-fit values in Table 5.2 are very close to 1, meaning that the points can be

described very well by the fitted lines. Therefore, the overall differences in attenuation and phase velocity between the theoretical and FE models are quadratically related to material inhomogeneity. Interestingly, this is consistent with the dependence of attenuation and velocity change at $2k_{0L}a = 1$ on inhomogeneity as demonstrated in §5.2.2, despite that the evaluation here is performed for the whole frequency range.

For attenuation, it is shown in Figure 5.6(a) that the quadratic fits for the case with consideration of the SBCs effect are approximately parallel to the respective counterparts that ignored the SBCs effect. This means that the improvement of accuracy for theoretical predictions made by the consideration of SBCs does not depend on material inhomogeneity, and the improvement is about 5% for all materials. For phase velocity, Figure 5.6(b) shows a negligible improvement of accuracy, which on average is about 0.02%. Since the improvements are not significant as compared to the normalised RMSD values, unless otherwise specified, the SBCs effect is consistently not considered in the theoretical calculations across this thesis.

Evaluation at $2k_{0L}a = 1$

The approximations of the theoretical models are further evaluated at the frequency where the models are most critically challenged. This frequency was identified above as $2k_{0L}a = 1$ in the considered frequency range. At this frequency, the relative differences in attenuation and velocity between the SOA and FE models are analysed in Figure 5.7 as functions of the material inhomogeneity factor $Q_{L \rightarrow T}$. The Born model is also analysed in the figure, but it is evaluated against the SOA model rather than the FE model.

The differences have a quadratic dependence on material inhomogeneity for both attenuation and phase velocity; the fitted quadratic equations are given in Table 5.3. This dependence can also be easily inferred from the same dependence as found for attenuation and velocity in §5.2.2. The quadratic relation is not very obvious for the attenuation difference between the Born and SOA models, and for this reason, the dependence was previously considered to be linear [27] (the inhomogeneity parameter ξ_p^2 therein is equivalent to $Q_{L \rightarrow T}$ as used in this thesis). However, this thesis still treats the dependence as quadratic in order to maintain consistency with that of the velocity difference between

the Born and SOA models.

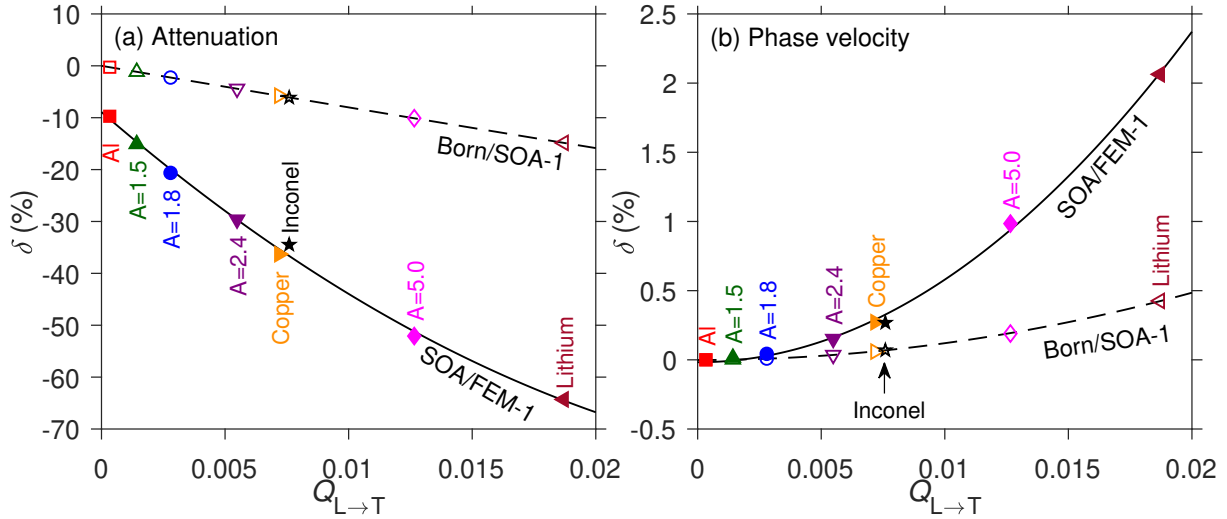


Figure 5.7: Relative difference of (a) attenuation and (b) phase velocity between theoretical and numerical models versus material inhomogeneity for longitudinal waves in polycrystalline materials. The solid points represent the relative differences between the SOA and FE models at the normalised frequency of $2k_{0L}a = 1$, while the hollow points denote those between the theoretical Born and SOA models. The lines represent the quadratic least-squares fits of the points, and the fitted equations are provided in Table 5.3.

Table 5.3: Relative difference of theoretical SOA and Born predictions to numerical FE results versus material inhomogeneity for longitudinal waves in equiaxed polycrystals at $2k_{0L}a = 1$: fitted equation. R^2 represents the goodness-of-fit. The fitted equations are plotted in Figure 5.7.

Fitted equation	R^2
$(\alpha_L^{\text{SOA}}/\alpha_L^{\text{FEM}} - 1) \times 100 = 61131.25Q_{L \rightarrow T}^2 - 4115.27Q_{L \rightarrow T} - 8.92$	0.997
$(\alpha_L^{\text{Born}}/\alpha_L^{\text{SOA}} - 1) \times 100 = 796.09Q_{L \rightarrow T}^2 - 808.64Q_{L \rightarrow T}$	1.000
$(V_L^{\text{SOA}}/V_L^{\text{FEM}} - 1) \times 100 = 5972.40Q_{L \rightarrow T}^2 - 0.02$	0.998
$(V_L^{\text{Born}}/V_L^{\text{SOA}} - 1) \times 100 = 1216.25Q_{L \rightarrow T}^2$	1.000

5.2.4 Quasi-static velocity limit

The quasi-static limit of longitudinal phase velocity is related to the effective elastic constant C_{11} of the polycrystal medium by $V_L = \sqrt{C_{11}/\rho}$. It was demonstrated in §3.7 that this limit can be determined to a high degree of accuracy from 3D FE modelling. Therefore, FE results are well suited to evaluate the suitability of effective medium theories. For this purpose, quasi-static FE velocities are calculated and provided as solid points in Figure 5.8(a) as a function of material inhomogeneity, $Q_{L \rightarrow T}$, for the eight cubic materials

considered. Each point represents the statistically-converged average of 30 realizations of the model N115200 (Table 3.1), and the error bar of each point is smaller than the size of the markers and is thus not shown.

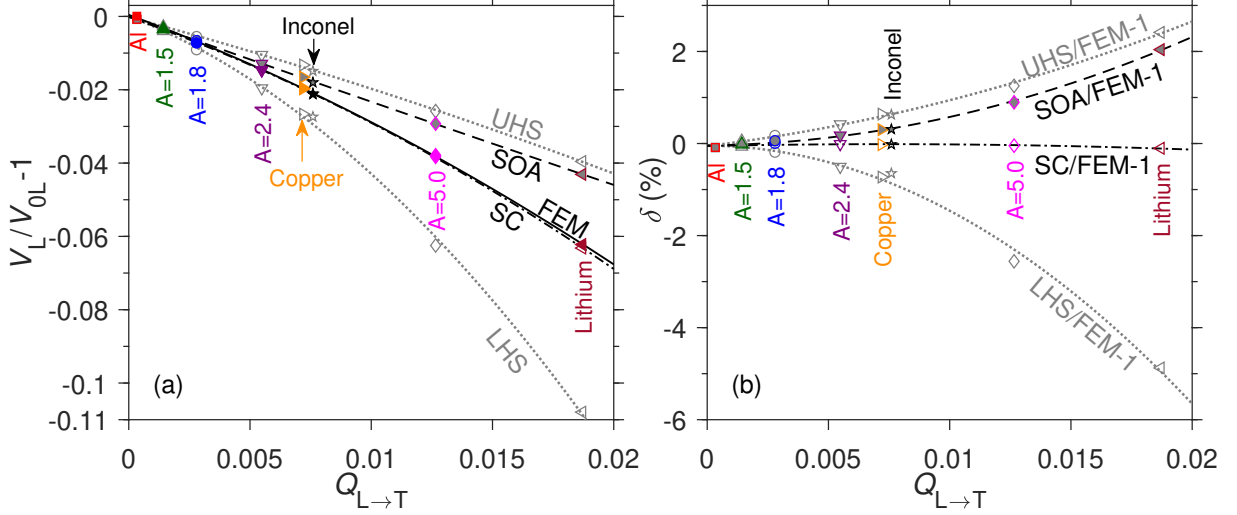


Figure 5.8: (a) Normalised quasi-static velocity versus material inhomogeneity for longitudinal waves in polycrystalline materials comparing theoretical and numerical results; (b) relative difference between theoretical and numerical models versus material inhomogeneity. LHS and UHS represent respectively the lower and upper Hashin-Shtrikman bounds. SC denotes the self-consistent effective theory. SOA corresponds to the Rayleigh asymptote of the SOA model. FEM represents the results obtained from quasi-static FE simulations and each point is the average of 30 realizations. The lines are the quadratic fits of the points. Note that the SC and FEM points are mostly overlapped with each other in (a).

The effective medium theories considered here include the Hashin-Shtrikman (HS) bounds [76–78] and the self-consistent (SC) theory [79]. The lower and upper HS bounds, denoted respectively as LHS and UHS, prescribe the quasi-static velocity range that any predictions or measurements should lie within it. These bounds are calculated with the scripts by Brown [78] and are plotted in Figure 5.8(a) as grey points. The SC theory provides a unique estimation of quasi-static velocity under the condition that the compatibility of stress and strain is fully met throughout the polycrystal. The scripts by Kube and De Jong [79] are used in this study to calculate the SC results as presented in the figure. In addition to these well-known theories, the Rayleigh velocity asymptote of the theoretical SOA model, Equation 2.23, is also examined in this study. Such SOA predictions are shown as shaded points in the figure. The looser first-order bounds, namely the Reuss-Voigt bounds, are not considered here, but it is worth noting that all results shown in

Figure 5.8(a) are normalised to the Voigt velocity, V_{0L} . The deviations of the theoretical predictions to the reference FE results are provided in Figure 5.8(b). Quadratic fits are generated for all datasets shown in the figure.

Consistently for all materials, the FE, SC and SOA points lie well between the LHS and UHS velocity bounds, whose range becomes wider as material inhomogeneity increases. As can be seen from all numerical and theoretical models, the normalised quasi-static velocity, $V_L/V_{0L} - 1$, shows a quadratic relationship with material inhomogeneity. This sole dependence on inhomogeneity is newly found and is simpler than the previously observed that was on both the Poisson's ratio and anisotropy factor [28].

The differences between the theoretical predictions and the FE results also exhibit a quadratic dependence on material inhomogeneity. The HS bounds perform just as well as the SC and SOA estimates for weakly scattering materials, but the latter two estimates are required as inhomogeneity gets larger. The SC theory performs better than the SOA model; the SC results are nearly overlapped with the FE points. This is not surprising since the SC theory takes the full continuity of stress and strain into consideration. However, the SC theory in general needs to be iteratively solved [79], whereas the SOA model has a simple analytical expression that explicitly shows the dependence of quasi-static velocity on material inhomogeneity: $V_L/V_{0L} - 1 \approx -2Q_{L \rightarrow L}^* - 2Q_{L \rightarrow T} \approx -2Q_{L \rightarrow T}$.

5.3 Polycrystal of triclinic crystal symmetry

This section studies equiaxed polycrystals of triclinic symmetry. The aim of this study is to evaluate the suitability of the theoretical SOA and Born models for predicting the longitudinal attenuation and velocity of triclinic polycrystals by comparing with numerical FE simulations. The copper sulfate pentahydrate (CSP) given in Table 3.2 is used for the evaluation. The universal anisotropy factor of this material is close to that of the fictitious material $A=2.4$.

Figure 5.9 shows normalised longitudinal attenuation versus non-dimensional frequency for CSP, with details in the caption. Each FE material model has used 15 realizations to obtain those statistically converged results as shown in the figure. Generally, the

quality of agreement between the theoretical and FE results is remarkable. The overall discrepancy is further quantified by the normalised root-mean-square deviation (NRMSD) over the whole frequency range. With the FE results as reference, the NRMSDs are 9.44% and 11.47% for the SOA and Born models, respectively. Interestingly, these numbers are smaller than those for $A=2.4$, although the two materials have a similar level of anisotropy.

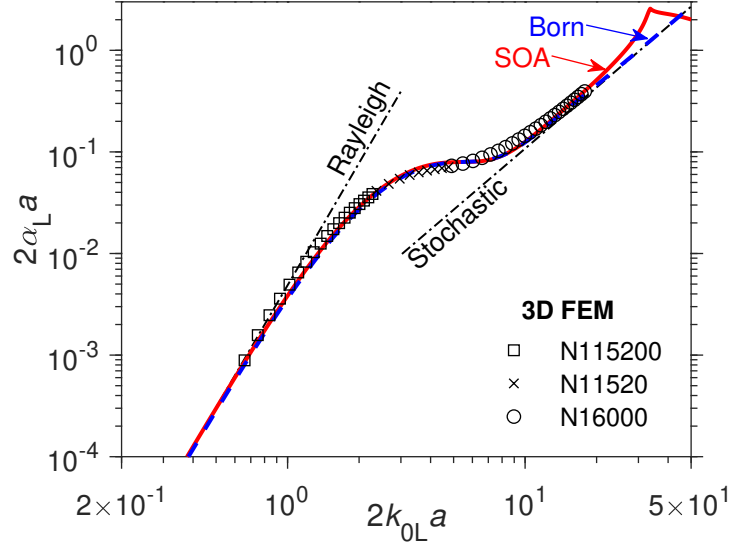


Figure 5.9: Normalised longitudinal attenuation in polycrystalline CSP versus normalised frequency. The points represent the 3D FEM results obtained from the three FE material models. The solid and dash lines denote, respectively, the predictions of the theoretical SOA and Born models with the TPC function measured from FE material models. The dash-dotted lines show the Rayleigh and stochastic asymptotes.

The Born approximation is almost indistinguishable from the SOA model at most frequencies. However, it departs from the SOA model and follows closely with the stochastic asymptote at higher frequencies where forward multiple scattering becomes stronger. This departure is associated with the start of the transition to the geometric region. In comparison, the SOA model predicts a higher level of attenuation and shows the emergence of the geometric regime, due to its partial consideration of forward multiple scattering.

Similarly, phase velocity results are plotted in Figure 5.10 as a function of normalised frequency. The theoretical SOA and Born models are in excellent agreement with the FE results from the Rayleigh to stochastic regimes. The largest discrepancy occurs at $2k_{OL}a \approx 6.34$ with an absolute deviation of 27 m/s, which translates to a relative difference of 0.34% with the FE velocity as reference. The NRMSDs of the SOA and Born predictions to the FE results are 0.12% and 0.10%, respectively. They are similar to those of the

5. Elastic waves in polycrystals with equiaxed grains

material $A=2.4$ but are negligible as compared to the attenuation NRMSDs as observed above.

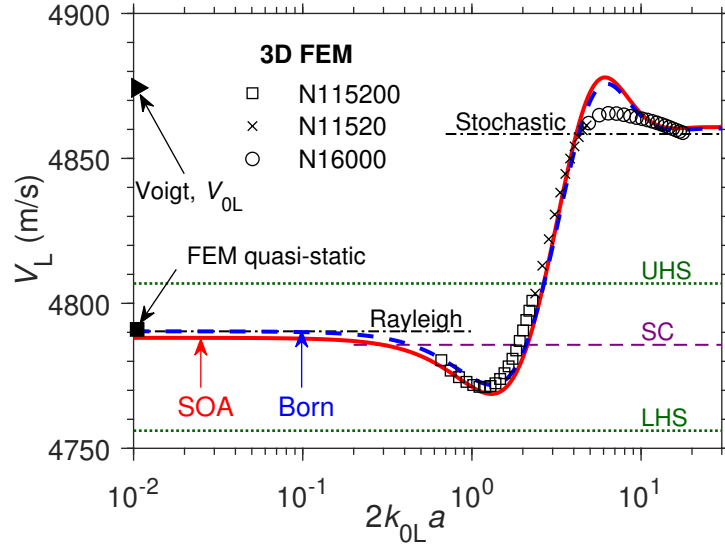


Figure 5.10: Longitudinal phase velocity in polycrystalline CSP versus normalised frequency. The points represent the 3D FEM results obtained from the three FE material models. The solid and dash lines denote, respectively, the predictions of the theoretical SOA and Born models with the TPC function measured from FE material models. The dash-dotted lines show the Rayleigh and stochastic asymptotes. The solid square at $2k_{0L}a = 0.01$ is for the FEM quasi-static velocity, while the solid triangle is for the Voigt velocity, V_{0L} . The other three horizontal lines specify, respectively, the lower and upper Hashin-Shtrikman (LHS and UHS) bounds and the self-consistent (SC) estimate.

The quasi-static limit of phase velocity is also addressed here. The velocity limit obtained from FE simulations is provided as a reference to evaluate the effective medium theories as considered in §5.2.4, including the lower and upper Hashin-Shtrikman (LHS and UHS) bounds, the self-consistent (SC) estimate, and the Rayleigh asymptote of the SOA model. As can be seen from Figure 5.10, the SC and SOA predictions are reasonably close to the FE result, and their relative deviations from the FE point are -0.11% and -0.01%. Therefore, both models are suitable for estimating the quasi-static velocity of polycrystals with generally anisotropic grains. It is observable that phase velocity is constantly between the LHS and UHS bounds in the low-frequency range. In the high-frequency stochastic region, however, phase velocity is even faster than the Voigt velocity, V_{0L} .

5.4 Summary

This chapter studies the propagation and scattering of plane longitudinal waves in untextured polycrystals with equiaxed grains of two extreme crystal symmetries, namely, cubic and triclinic. Theoretical SOA and Born models as well as numerical 3D FE simulations are employed for the study.

For polycrystals of cubic symmetry, eight materials with varying inhomogeneity factors are used to evaluate the change of wave behaviours with inhomogeneity and to establish the range of validity of the theoretical SOA and Born models by comparing to numerical FE simulations. The findings are summarised in the following four aspects:

- 1) Frequency dependence. The theoretical and numerical results show that attenuation has fourth- and second-power dependences on frequency in the Rayleigh and stochastic regimes, while phase velocity is independent of frequency in both regimes. In the transition between these two regimes, attenuation exhibits a hump behaviour and phase velocity is dispersive, owing to the transition of dominant scattering from $L \rightarrow T$ component in the Rayleigh regime to $L \rightarrow L$ in the stochastic regime.
- 2) Inhomogeneity dependence. In the Rayleigh regime, a quadratic relationship to the material inhomogeneity $Q_{L \rightarrow T}$ is found for the attenuation and velocity change results obtained from the SOA and FE models, while the relationship is linear for those predicted from the Born model. In the stochastic regime, the results of all three models show a linear dependence on the inhomogeneity factor $Q_{L \rightarrow L}$ for both attenuation and velocity change. The wavefront fluctuation recorded in the FE simulations intensifies as inhomogeneity increases and the RMS value across the wavefront is quadratically related to $Q_{L \rightarrow T}$ in the Rayleigh regime.
- 3) Approximations of the theoretical models. The FE results are treated as reference for evaluating the approximations of the theoretical SOA and Born models. It is found that the overall approximations, as characterised by the NRMSD over the entire frequency range, of the two theoretical models have a quadratic dependence on material inhomogeneity for both attenuation and velocity change. This quadratic dependence also extends to the theoretical models at a chosen normalised frequency where the models are most

critically challenged. Also, it is demonstrated that the attenuation and velocity predictions of the theoretical models can be improved by about 5% and 0.02% by considering the SBCs effect.

4) Quasi-static velocity limit. The deviation of the quasi-static velocity limit to the Voigt velocity has a quadratic relationship to the material inhomogeneity $Q_{L \rightarrow T}$. This is found from the FE results as well as the predictions of the effective medium theories, including the Hashin-Shtrikman bounds, self-consistent theory, and the Rayleigh asymptote of the SOA model. The discrepancies between the theoretical predictions and the FE results also show a quadratic dependence on material inhomogeneity. The predictions of the self-consistent theory agree the best with the FE results, while the explicit, simpler Rayleigh asymptote of the SOA model performs just as well.

For the polycrystalline CSP of triclinic symmetry, a good agreement for attenuation and phase velocity is found between the SOA and FE models when the accurate TPC function of the FE material system is used in the SOA model; the NRMSD for attenuation is below 10% and it is 0.12% for phase velocity. The Born approximation only differs slightly from the SOA model, but the difference becomes larger as scattering departs the stochastic regime and transits into the geometric region. The quasi-static velocity limits obtained from the SOA model and the self-consistent theory are between the Hashin-Shtrikman bounds and agree very well with the result obtained from 3D FE simulations.

Chapter 6

Elastic waves in polycrystals with elongated grains

6.1 Introduction

This chapter studies the propagation of plane longitudinal waves in polycrystals with statistically elongated grains, investigating the influence of frequency, elastic properties, and grain elongation on scattering-induced attenuation and velocity dispersion.

The average grain shape of the studied materials is ellipsoid-of-rotation and the elongation ratio is 5. This means the average grain radius in the elongated direction is 5 times that of the shortened direction as seen in Figure 3.1(b), and the mean grain geometry is transversely isotropic in a plane normal to the elongated direction. It is important to note that the average grain elongation for practical materials may vary in a wide range. This chapter, however, is not intended to achieve a range of elongation ratios because massive computing resources and times would be needed; theoretical studies addressing this aim can be found in [11, 21, 41–43]. Instead, a representative elongation ratio of 5 is used to establish the fundamental numerical and theoretical approaches that may be applicable to more general cases and to reveal the mechanisms of wave scattering that may be universally true for grains with different aspect ratios. It is also important to emphasise that the elastic properties of the studied materials are transversely isotropic as a result of grain elongation, although the crystallographic axes of the grains within a polycrystal are

uniformly randomly oriented. Therefore, the scattering-induced effective wave parameters exhibit transverse isotropy, and for this reason, the results in this chapter are given for waves propagating in directions that show anisotropy, i.e., the directions lying in the plane that contains both the shortened and elongated directions.

This chapter starts with the study of attenuation in §6.2 by comparing the results of the theoretical and FE models, which is followed by a similar treatment of phase velocity dispersion in §6.3. This chapter is mostly adapted from the manuscript [P3] that has been submitted for possible publication and [P4] with the permission of AIP Publishing.

6.2 Attenuation

6.2.1 Frequency dependence

Figure 6.1 shows normalised attenuation, $2\alpha_L a_x$, versus normalised frequency, $2k_{0L} a_x$, for aluminium, Inconel and CSP. The FEM results are plotted as points in the figure and the SOA predictions are provided as lines. The Rayleigh and stochastic asymptotes derived from the Born approximation of the SOA model are shown as dash-dotted lines. The FEM results are obtained from the FE material models given in Table 3.1 and the average of 15 realizations is used to obtain statistically converged results as presented in the figure. The SOA predictions are obtained by using the TPC function of the FE material models as input, and thus the SOA and FEM results are directly comparable.

It is observable that, in the grain elongated z -direction, the SOA attenuations for Inconel and CSP start to decrease as they enter the geometric regime. The FEM results, however, have not reached such high frequencies to show this phenomenon although their highest normalised frequencies are as large as $2k_{0L} a_z = 42$ and $2k_{0L} a_z = 45$. The results for aluminium do not indicate such a departure from the stochastic regime even at $2k_{0L} a_z = 70$ and it is not predicted by the SOA model even at the highest frequencies of these calculations. As will be discussed later in this chapter, a higher frequency FE simulation may help to reach the SOA predicted transition to the geometric region, but it is currently limited by computation capability.

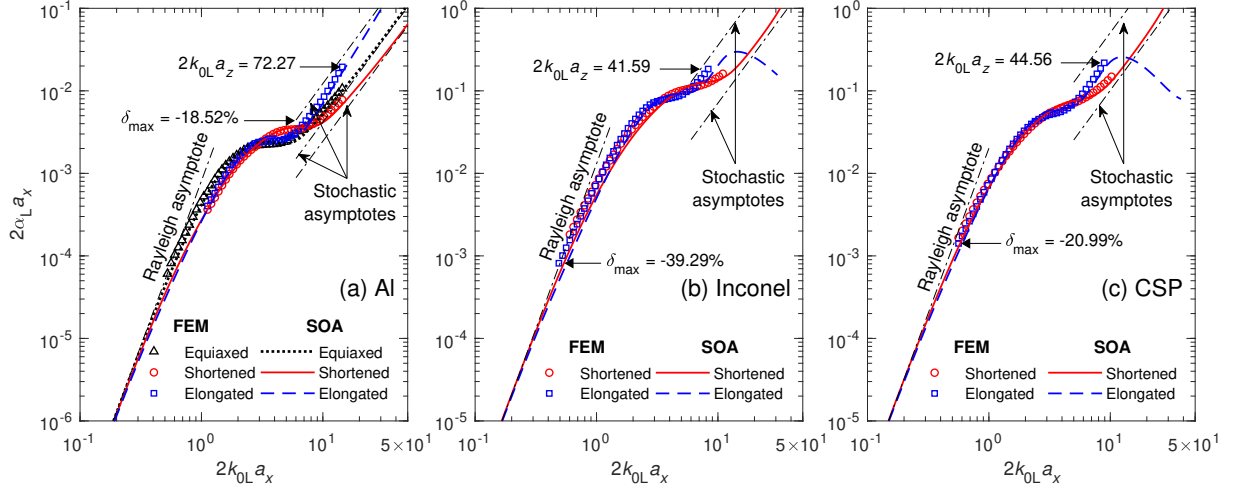


Figure 6.1: Comparison of normalised longitudinal attenuation between the FEM and SOA models for (a) aluminium, (b) Inconel, and (c) CSP. The results are plotted against normalised frequency $2k_{OL} a_x$, where a_x is the mean grain radius in the shortened direction as determined from the slope at the origin of the generalized TPC function (Table 3.3 and Figure 3.3). $\delta_{\max}$ signifies the maximum difference between the SOA and FEM models, and it occurs in the elongated direction for all three materials. The annotation $2k_{OL} a_z$ specifies the maximum normalised frequency of FE modelling for propagation in the elongated direction with the mean grain radius a_z . For clarity of the plots, only a subset of the calculated FEM points is displayed in the figure and the rest of the points between those displayed are skipped.

The case of grains being equiaxed is provided for aluminium to illustrate the similarities and differences between the elongated and equiaxed cases. All results are normalised by the same factor a_x as was conventionally used in the study of elongated grains [21]; this factor corresponds to the mean grain radius in the shortened direction which is determined from the slope at the origin of the generalized TPC function (Table 3.3 and Figure 3.3) by $a_x = 1 / \sum_{i=1}^n (A_i / a_x^i)$. A different factor can be adopted for the normalisation, but it only linearly transforms the data points and curves and does not change the relations between them. Yet, it is important to emphasise that the FE modelling has reached large normalised frequencies for the elongated direction. As annotated in the figure, the frequencies are greater than 40 when they are normalised with the mean grain radius a_z of the elongated direction. While only the shortened and elongated directions are considered in Figure 6.1, the general interest of this chapter is in wave propagation in directions lying in the plane containing both those directions, as will be studied later.

It is clear from the figure that the agreement between the SOA and FEM results is in general remarkable. The overall difference between the SOA and FE models across the

whole frequency range is further quantified by the normalised root-mean-square deviation (NRMSD) with the FEM results as reference; the results for different material cases are shown in Table 6.1. The level of agreement for the polycrystalline aluminium with elongated grains is almost the same as that of the equiaxed case which is also valid for the other two materials, Inconel and CSP, although their equiaxed cases are not shown. The SOA model in the shortened direction is in very good agreement with the FE model in the whole frequency range for all materials, and the agreement decreases slightly in the elongated direction due to the increased wave scattering. The table also shows that the overall difference between the SOA and FE models increases from aluminium through CSP to Inconel, showing a positive correlation with the universal anisotropy factor. For the three materials, the maximum difference between the SOA and FE models is marked as $\delta_{\max}$ in the figure and it occurs in the elongated direction for all three materials. For the studied cases, the largest relative difference, -39.29%, is for Inconel (at the lowest frequency of the FEM results). The discrepancy between the FE and the SOA models is rather modest, considering the approximations involved in both the SOA and FE models. It is important to realise that the difference between the SOA and FE models may also be partially attributed to the effect of symmetry boundary conditions (SBCs), which causes a difference of -20% for equiaxed Inconel as demonstrated in §4.4.

The good agreement between the SOA and FE models indicates that the approximations of the SOA model impose generally only small influences, even for polycrystals with relatively high anisotropy grains, such as Inconel. That the agreement is so good is all the more surprising considering the key approximations of the SOA model, such as the replacement of the polycrystal by a continuously random medium and accounting only partially for the multiple scattering effects; in the formulations, these representations are assumed to be suitable only under conditions of small inhomogeneity perturbations. Another important assumption in the SOA model is the factoring of the two-point correlation function of a polycrystal into the geometric and elastic parts, which has been discussed in §2.2.2. This factorisation has been supported by the direct numerical comparison [49] for the statistically isotropic polycrystals with equiaxed grains; this study further supports (while indirectly) this factorisation for statistically anisotropic elongated polycrystals.

In addition, the good agreement between the SOA and FE models means that both models

Table 6.1: Normalised root-mean-square deviation (NRMSD) of attenuation between the SOA and FE models (with the FE model as reference) for different material systems. The universal anisotropy factor [54] A^U and the elastic scattering factors $Q_{L \rightarrow L, T}$ are also provided in the table.

Material	A^U	$Q_{L \rightarrow L}$	$Q_{L \rightarrow T}$	NRMSD for equiaxed case	NRMSD for elongated case	
					Shortened	Elongated
Aluminium	0.05	7.80×10^{-5}	3.34×10^{-4}	10.15%	6.81%	10.71%
Inconel	1.42	2.26×10^{-3}	7.59×10^{-3}	-	20.22%	24.77%
CSP	0.95	3.23×10^{-3}	7.19×10^{-3}	-	10.47%	11.94%

can be utilized to reveal the mechanisms of wave scattering in polycrystals with elongated grains. The theoretically demonstrated (in §2.2) dependence of attenuation on frequency, grain geometry, and elastic property is analysed below based on the SOA and FEM results shown in Figure 6.1.

a. Frequency dependence. The SOA and the FEM results approach the Rayleigh asymptote at very low frequency and the stochastic asymptote at high frequency. Considering the frequency dependences of the Rayleigh asymptote, Equation 2.18, and the stochastic asymptote, Equation 2.26, it means that attenuation depends on fourth and second powers of frequency in these two frequency ranges respectively. The stochastic regime is not pronounced in the elongated direction for the strongly scattering materials, Inconel and CSP. This was also noted by Stanke and Kino [14] for equiaxed iron and their study showed that the stochastic region becomes shorter as the degree of inhomogeneity increases.

Attenuation shows a smooth transition of frequency dependence from the fourth to the second powers between the Rayleigh and stochastic regimes. A “hump” is noticeable in this transition region. As discussed in §5.2.1 and previous studies [14, 39] for polycrystals with equiaxed grains, this behaviour is a result of the change of the dominant scattering mode, as the dominant longitudinal-to-transverse wave scattering in the Rayleigh regime is replaced by the longitudinal-to-longitudinal scattering in the stochastic regime. This mode transition is a unique feature for the longitudinal waves.

The geometric regime occurs at frequencies above the stochastic regime. This region is manifested in the figure as the decline of attenuation with the increase of frequency for Inconel and CSP in the elongated direction, as shown by the SOA model results (this decline also occurs for aluminium at higher frequencies and was also observed for equiaxed

grains). The geometric region was not reached in the FEM simulations. The decline of the attenuation differs from the observation of Stanke and Kino [14] for equiaxed and Calvet and Margerin [42] for elongated polycrystals, who observed that attenuation is independent of frequency in the geometric regime. This thesis attributes this difference to the difference in the TPC functions.

b. Geometric dependence. In the Rayleigh regime, the attenuation of each material tends to be the same in the shortened and elongated directions, and the equality also applies to the equiaxed case as shown in panel (a) of the figure. This equality occurs because attenuation in the Rayleigh regime depends on the effective volume of the grains, which can be deduced from the Rayleigh asymptote expressed in Equation 2.18. In the high-frequency stochastic regime, grain elongation introduces a clear directional effect on the attenuation as it depends on the correlation length in the direction of wave propagation. These geometric characteristics will be further assessed in §6.2.2.

c. Elastic dependence. As theoretically discussed in §2.3.2 and §2.3.3, the Rayleigh attenuation asymptote is proportional to the mode converted elastic scattering factor $Q_{L \rightarrow T}$ and the stochastic attenuation asymptote is related to $Q_{L \rightarrow L}$. Considering the good agreement of the SOA and FEM results, those dependences will be further evaluated in §6.2.3.

6.2.2 Effect of grain shape

1. Directional ratio

As mentioned above, grain elongation causes the directional dependence of attenuation at high frequencies. Here the ratio of attenuation between the elongated and shortened directions is used as a measure to quantify this. The elastic part of attenuation cancels out after division in the ratio, and thus the effect of the geometric part on attenuation can be observed clearly. The ratios are plotted in Figure 6.2 for the three materials. As with the original attenuation results shown in Figure 6.1, the SOA ratios (lines) agree very well with the FEM ratios (points) across the whole frequency range.

The ratios overlap reasonably well for all materials and for both the FE and SOA models

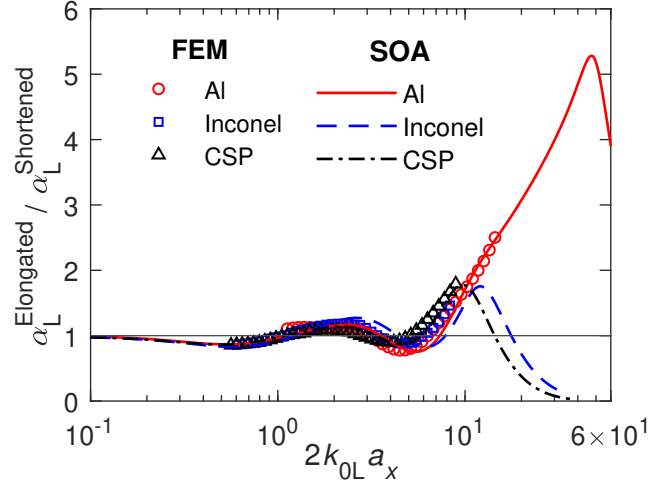


Figure 6.2: Directional ratio of longitudinal attenuation between the elongated and shortened directions. The horizontal reference line shows the ratio of unity. For clarity, only a subset of the original FEM points is displayed in the figure and the remaining points between those displayed are skipped.

except above the stochastic region when the transition to the geometric region begins; here each ratio reaches a separate peak and then begins to decline. This behaviour of a peak followed by decline was also discussed in Rokhlin et al. [26]. The abrupt drop is due to the emergence of the geometric regime in the elongated direction. For Inconel and CSP, the ratio only reaches the value of around 2, which is smaller than the grain elongation ratio of 5. However, the peak occurs much later in frequency for aluminium, which has a relatively weak scattering; the ratio is 5.28 and is a bit greater than the grain elongation ratio. These peaks are observed only for the SOA model, they are not found in the FEM results: for aluminium the peak was not reached and for CSP and Inconel the ratio continues to grow with frequency as in the stochastic regime. We are currently unable to extend the frequency range in the FEM simulations beyond these ranges, and this phenomenon may be further investigated when FE computation capability allows.

In the low-frequency Rayleigh regime, the ratio is almost unity, confirming that attenuation is independent of grain shape and is instead determined by the effective volume of the grains, see Equation 2.18. The Rayleigh-stochastic transition exhibits itself as the non-monotonic variations that are caused by the transition of dominant scattering modes between the two regimes, which was discussed above. It is interesting that consistently for all three materials, the ratio first decreases below one (scattering in a shorter direc-

tion is a bit stronger) when departing from the Rayleigh region. This occurs relatively early in frequency and is supported by the FEM simulations. Importantly, for all studied materials, the directional attenuation ratio is about one until the normalised frequency $2k_{0L}a_x$ increases to five for the SOA and FE models.

2. Wavefield fluctuations

Using CSP as an example material, Figure 6.3 shows the normalised wavefront fluctuation $u_f(x, y; f)$ at different frequencies for both the shortened and elongated directions. To obtain $u_f(x, y; f)$, the z -displacements across all points on the receiving plane $z = d_z$ are recorded as a spatially varied waveform $u = u(x, y; t)$. The spectral amplitude field $u = u(x, y; f)$ is obtained by Fourier transforming the windowed waveform of each point with respect to time. The normalised wavefront fluctuation, as plotted, is then calculated by $u_f(x, y; f) = u(x, y; f) / \langle u(x, y; f) \rangle_{x,y} - 1$, where $\langle \cdot \rangle_{x,y}$ represents the spatial average over all points. The model N11520 is employed to acquire the fluctuations for the normalised frequencies of 0.56, 1.00, and 1.39, while N16000 is used for the frequencies of 5.56 and 8.34.

The fluctuation is surprisingly large for all shown cases, and the magnitude of fluctuation can be nearly 4 times that of the displacement mean (the coherent part of the total field). The directional difference of fluctuation root-mean-square (RMS) between the shortened and elongated directions is consistent with that of attenuation as shown in Figure 6.2: the elongated direction has a smaller fluctuation RMS than the shortened direction at the normalised frequency of $2k_{0L}a_x = 0.56$, and this relation is reversed at higher frequencies. It is also noticeable that the fluctuation RMS intensifies as frequency increases. However, in direct contrast to attenuation as shown in Figure 6.1, fluctuation tends to saturate at high frequencies starting at around $2k_{0L}a_x \leq 5.56$.

3. Polar dependencies

The evident directional difference might be useful for inversely inferring the average shape of the elongated grains. To further elucidate the directional behaviour, the change of attenuation with the propagation direction θ_p is evaluated. θ_p denotes the angle between

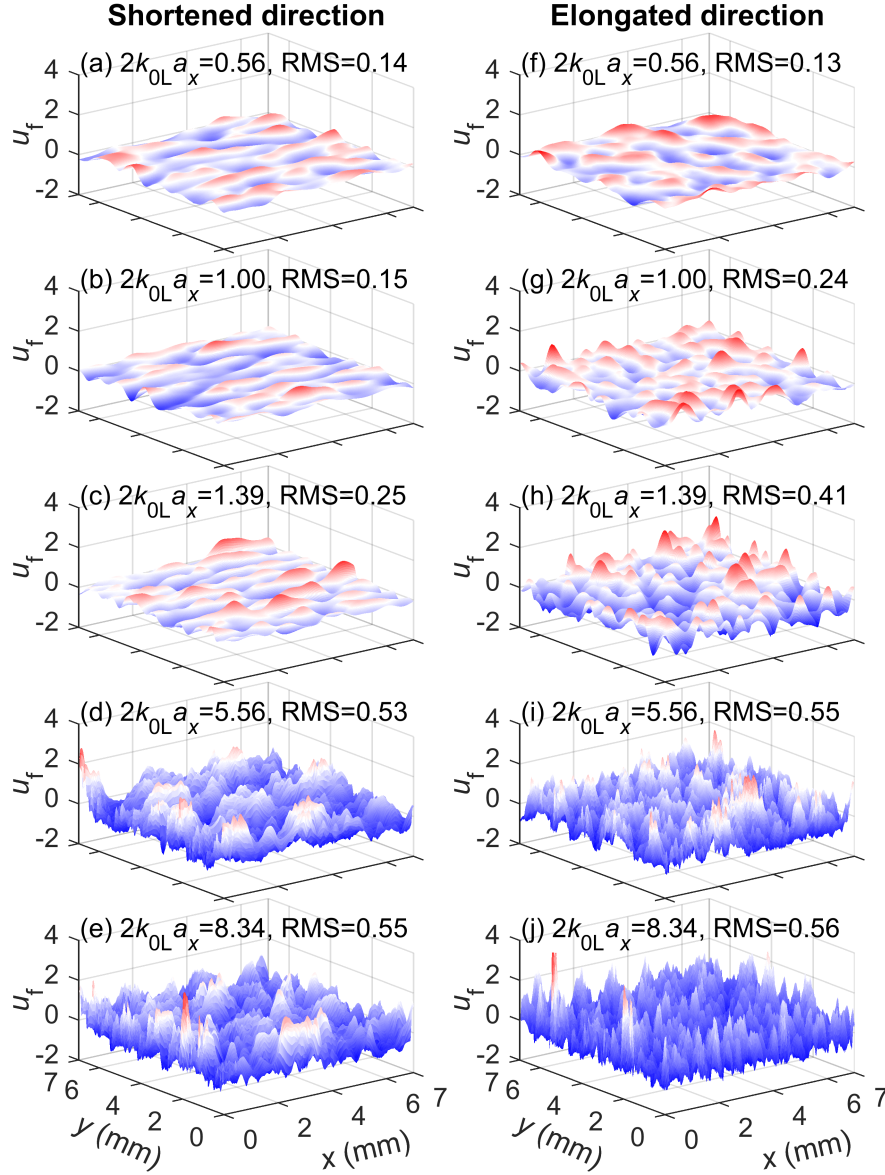


Figure 6.3: Illustration of wavefront fluctuations for the normalised spectral amplitude field $u_f(x, y; f) = u(x, y; f) / \langle u(x, y; f) \rangle_{x,y} - 1$. Panels (a-e) are for shortened and (f-j) for elongated directions at different normalised frequencies. The results are given for the material CSP with elongated grains of elongation ratio 5.

the directions of propagation and grain elongation as illustrated in Figure 2.1 and Figure 3.1(b). Again, CSP is used as the example material for this evaluation and the propagation of waves is simulated in the directions of 0° (elongated direction), 15° , 18.75° , 30° , 45° , 60° , 75° , and 90° (shortened direction). The FEM results together with the predictions of the SOA model are shown in Figure 6.4 versus the normalised frequency for the propagation directions of 0° , 15° , 18.75° , 30° , 45° , and 90° ; the results for 60° and 75° are

not shown as they complicate the figure but they will be used later in Figure 6.5. The FE simulations for different propagation directions have used the same modelling conditions (model dimensions, mesh size, centre frequency, etc.), but their results are given in different frequency ranges in order to have the same level of numerical accuracy.

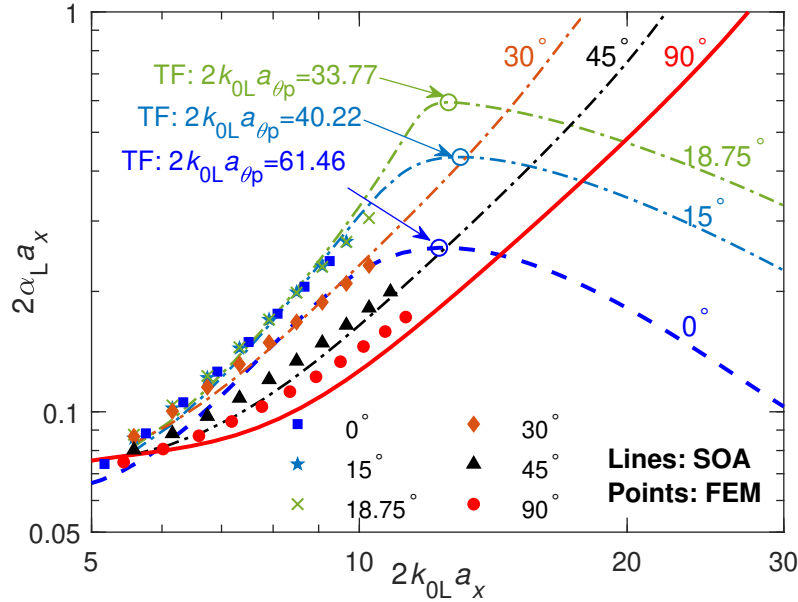


Figure 6.4: Normalised longitudinal attenuation versus normalised frequency in different propagation directions for triclinic CSP. Points are for the FEM results and lines are for the SOA model. The propagation directions θ_p are 0° , 15° , 18.75° , 30° , 45° , and 90° . The FEM points for 0° (squares), 15° (stars), and 18.75° (crosses) are mostly overlapped in the given frequency range. TF denotes the normalised transition frequency, $2k_{0L}a_{\theta_p}$, to the geometric regime, and it corresponds to the peak of the SOA curve. The normalisation factor a_{θ_p} for TF is the mean grain radius in the wave propagation direction θ_p . For clarity, only a subset of the original FEM points is displayed in the figure and the remaining points between those displayed are skipped.

The agreement between the FEM and SOA results is generally good for all plotted directions. The largest difference occurs in the elongated direction (0°) because the FEM result continues to grow while the SOA model is transiting into the geometric regime where attenuation decreases. As the angle deviates from the elongated direction, the mean grain radius in the propagation direction decreases, and therefore in the stochastic region, the level of attenuation should also decrease as follows from the Born approximation [11, 21, 41–43] and the stochastic limit of the SOA model (Equation 2.26). This is valid for the angles of 30° , 45° , and 90° closer to the shortened direction which is supported by both the FEM and SOA models. However, it is not the case as attenuation

approaches the transition to the geometric region which is observed for the angles in the vicinity of the elongated direction. At those angles (0° , 15° , and 18.75°), the FEM results are nearly overlapped while the SOA attenuation for 0° is even smaller than those for 15° and 18.75° since it is deeper into transition to the geometric region. The SOA model results in Figure 6.4 are in general reminiscent of those in Figure 6 of Yang et al. [41] that were obtained for ellipsoidal scatterers in the scalar approximation; however, near-zero propagating angles were not investigated in that work.

It is shown in Figure 6.4 that at the angles 0° , 15° , and 18.75° , the SOA attenuation transitions into the geometric regime at different $2k_{0L}a_{\theta_p}$ (as indicated in the figure by the TF points, open circles) and roughly the same nondimensional frequency $2k_{0L}a_x$. The transition occurs later in frequency for 30° , 45° , and 90° , whose transitions are not shown in the figure. The normalisation factor a_{θ_p} is the mean grain radius in the wave propagation direction θ_p as determined from the slope at the origin of the generalized TPC function (Table 3.3 and Figure 3.3). The FEM results do not exhibit the transition to the geometric region; the current computation capacity does not allow further increase in frequency.

The directional dependence is further evaluated in Figure 6.5 by polar plotting the normalised attenuation against propagation direction θ_p for the normalised frequencies of 5.56 and 8.34. The FEM results are mirrored about the shortened and elongated axes to obtain all FEM points as plotted in the figure. The SOA and Born approximation results are also provided in the figure as solid and dash lines, respectively. The Born approximation model is included here because prior studies are mostly based on this model [11, 41].

The panels (c-d) of Figure 6.5 show for comparison the stochastic asymptote (dash-dotted line) that has the same elliptical shape as the mean elongated grain with the aspect ratio of 5. This is consistent with the accepted view [21, 42, 43] that the stochastic asymptote follows the same shape as the statistical geometry of the grains. The difference with the FEM results indicates again that the stochastic regime did not develop for the CSP material.

Consistent with Figure 6.4, the SOA and Born approximation models in general match very well with the FE model. The SOA model exhibits a more complicated behaviour at, and near, the elongation direction, 0° . The relative differences between the SOA and FE

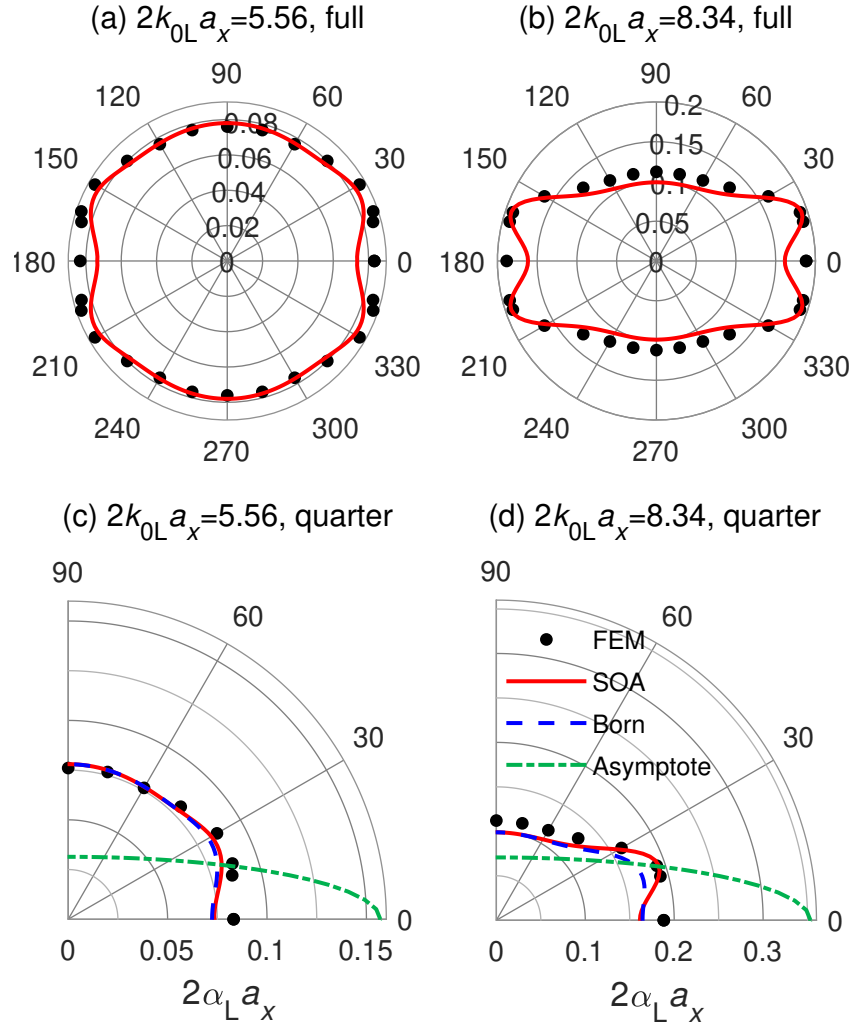


Figure 6.5: Polar plot of normalised longitudinal attenuation (r -axis) versus wave propagation direction (θ -axis) for CSP at the normalised frequencies $2k_{0L}a_x$ of (a) 5.56 and (b) 8.34. (c-d) show the respective quarter plots of (a-b) with the Born approximation and asymptote curves added. Points are for the FEM results and solid lines are for the SOA predictions; dash and dash-dotted lines represent respectively the Born approximation and the stochastic asymptotes that are of elliptical shape. All panels use the same legend as shown in (d).

models are given in Table 6.2 for the plotted frequencies and simulated angles. The largest deviations from the FEM are at a near-zero angle. As shown in Figure 6.4, at the higher frequency of 8.34 the largest attenuation is found in both the SOA and FE models in the vicinity of the propagation direction 18.75° . The complexity of the behaviour arises because different propagation angles are associated with different scattering regimes of the SOA model involving the stochastic, stochastic-geometric transition, and geometric regimes. For example, in the elongated direction (0°) that has the largest difference between the SOA and FE models, the SOA model is already transiting into the geometric

region while the FEM result is still increasing with frequency as shown in Figure 6.4. The Born approximation does not exhibit this nonmonotonic behaviour with angle since it does not follow the transition into the geometric region as was shown in Figure 2.2.

Table 6.2: Relative difference of longitudinal attenuation between the SOA and FE models for polycrystalline CSP with elongated grains.

$2k_{0L}a_x$	$\delta = \alpha_L^{\text{SOA}}/\alpha_L^{\text{FEM}} - 1$ (%)							
	0°	15°	18.75°	30°	45°	60°	75°	90°
5.56	-11.60	-7.05	-6.52	-3.74	-2.62	0.61	1.18	2.58
8.34	-14.25	-1.02	1.05	-2.08	-8.44	-10.18	-11.33	-11.69

6.2.3 Effect of elastic scattering factors

The dependence of attenuation on the elastic properties of the grains is evaluated here. The FEM and SOA results of all three materials given in Figure 6.1 are replotted in Figure 6.6(a) and (c) for the shortened and elongated directions, respectively. The curves for the CSP and Inconel are nearly overlapped, this is because their $Q_{L \rightarrow T}$ and $Q_{L \rightarrow L}$ factors are relatively close (Table 6.1). The attenuation for aluminium is obviously much smaller. By comparing the results of the three materials, the impact of elastic properties on attenuation can be intuitively evaluated. However, the evaluation is made more quantitative in panels (b) and (d) by normalizing the attenuation by the elastic factors that affect the attenuation of the low-frequency Rayleigh and high-frequency stochastic regimes.

In the low-frequency Rayleigh regime, the attenuation results are divided by the elastic factor $Q_{L \rightarrow T}V_{0L}^3/V_{0T}^3$. This factor is chosen based on Equation 2.18 and the factor Q_{LL}^* in the equation is neglected because it is small compared to the chosen factor. Panels (b) and (d) show that after division the results for different materials are nearly overlapped for both the SOA and FE models and for both the shortened and elongated directions. The overlapping means that the proportionality of attenuation to the chosen elastic factor holds for the Rayleigh regime. The studied materials have similar velocity ratios as their Poisson's ratios are close, and thus the factor being divided can be substituted by $Q_{L \rightarrow T}$ with small changes for the overlapping. As a result, the mode-converted elastic scattering

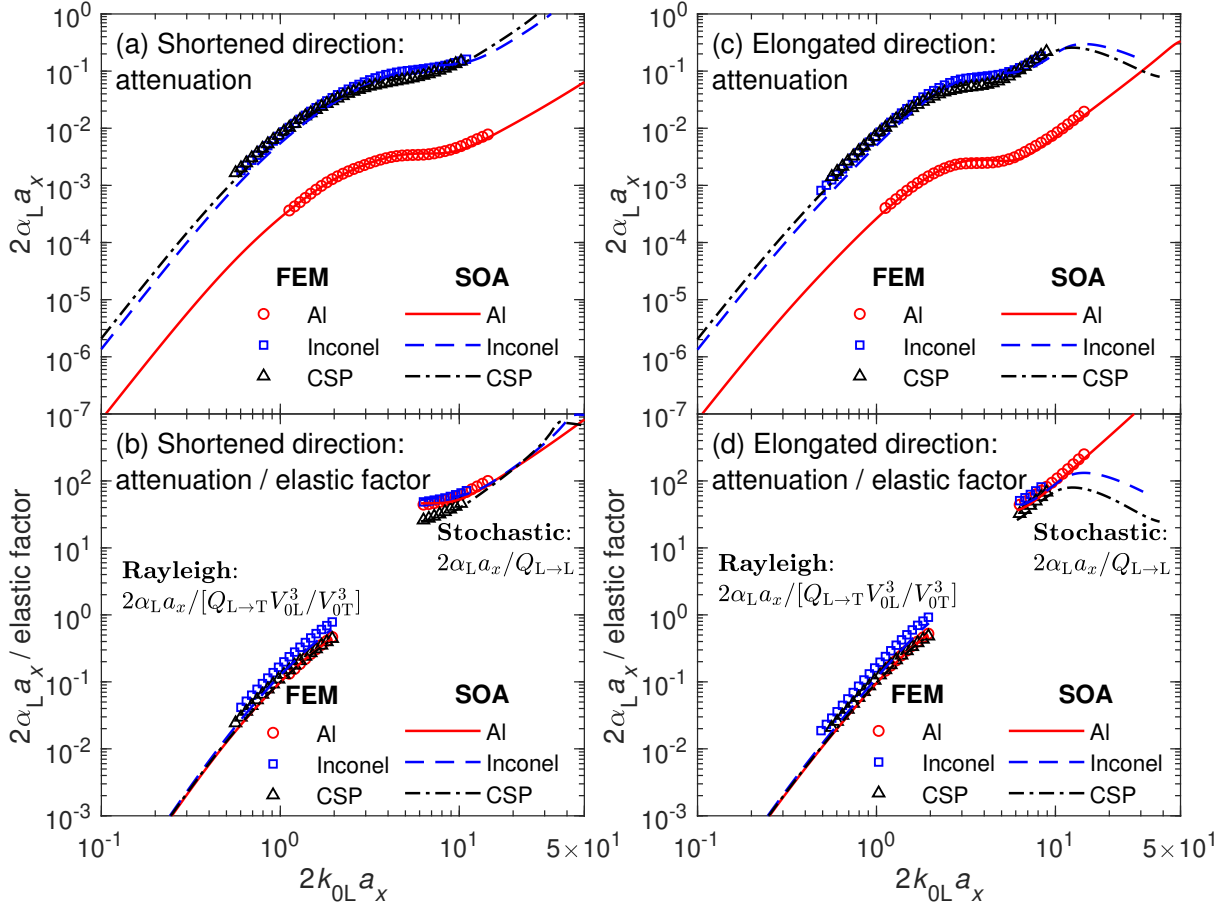


Figure 6.6: Comparison of normalised longitudinal attenuation between the three polycrystalline material systems in the (a) shortened and (c) elongated directions. (b) and (d) show the respective results of (a) and (c) divided by the elastic factors. The elastic factor being divided is $Q_{L \rightarrow T} V_{0L}^3 / V_{0T}^3$ for the low-frequency range ($2k_{0L}a_x \leq 2$), while the factor is $Q_{L \rightarrow L}$ for the high-frequency range ($2k_{0L}a_x \geq 6$). For clarity, only a subset of the original FEM points is displayed in the figure and the remaining points between those displayed are skipped.

factor, $Q_{L \rightarrow T}$, is usually used to describe the degree of inhomogeneity of polycrystals in the long-wavelength scattering range [26].

In the high-frequency stochastic regime, the attenuation results are divided by the elastic scattering factor $Q_{L \rightarrow L}$, which is similarly chosen based on Equation 2.26. It is clear from panels (b) and (d) that the FEM points and SOA curves overlap among different materials. In panel (b), the results for CSP slightly deviate from those of the other two materials below the normalised frequency of 15, which is because CSP reaches the stochastic regime later than the other two materials. The overall good overlapping of the three materials suggests that the attenuation in the stochastic regime is elastically determined by the factor $Q_{L \rightarrow L}$. This conclusion is important because it means that the

level of inhomogeneity of polycrystals can be solely quantified by the elastic scattering factor $Q_{L \rightarrow L}$ in the short wavelength scattering range [26].

The scaling results show that the two scattering factors are needed to normalise the level of inhomogeneity for the Rayleigh and stochastic regimes. These two factors are sufficient to describe the elastic properties of the grains in the whole frequency range. For the transverse incident wave, the attenuation scaling can be achieved by a single elastic scattering parameter [46]. A similar attenuation scaling was performed by Stanke and Kino [14] by using a single inhomogeneity factor ε^2 in the stochastic regime (for longitudinal waves, the factor they used is the same as the elastic scattering factor $Q_{L \rightarrow L}$).

6.3 Phase velocity dispersion

6.3.1 Comparison of theoretical and numerical models

The velocity results of the SOA and FE models are compared in Figure 6.7 for aluminium, Inconel, and CSP. The y -axis of each panel represents the normalised variation in phase velocity V_L from the Voigt velocity, $V_L/V_{0L} - 1$. The leftmost solid points in each panel represent quasi-static velocities obtained from FE simulations and details for these results will be provided in §6.3.5. Although these points correspond to $2k_{0L}a_x \rightarrow 0$, they are plotted at $2k_{0L}a_x \approx 0.1$ to fit the scales of the plots. Small discontinuities can be found as one looks along sequential FEM points, which is clearer for those of aluminium shown in panel (a). These discontinuities occur at the interfaces of neighbouring FE material models (Table 3.1) that are used in this work to cover different frequency ranges, as was explained in §3.5. The discontinuities arise because neighbouring models have slightly different levels of numerical error that is related to frequency and mesh size. The numerical error has been minimised by using a Courant number C as close as possible to unity ($C = 0.98$ in this work) but has not been fully eliminated. The FEM points are provided in slightly different frequency ranges for the shortened x and elongated z directions to achieve the same level of numerical accuracy.

The quality of agreement between the SOA and FE models is excellent. The overall difference between the two models for the phase velocities across the entire frequency

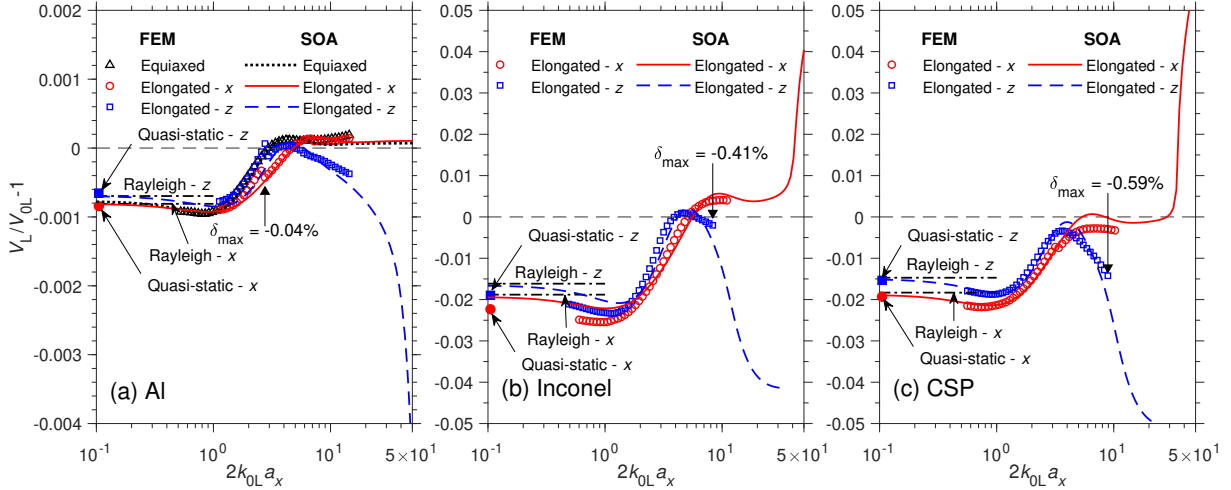


Figure 6.7: The FEM and SOA simulations of the normalised longitudinal phase velocity $V_L/V_{0L} - 1$ against nondimensional frequency $2k_{0L}a_x$ for polycrystalline (a) aluminium, (b) Inconel, and (c) CSP. The results are for the shortened x and elongated z directions of the grains; for aluminium, the results are also given for the equiaxed case. The leftmost points (solid points) correspond to the FEM quasi-static velocities. The dash-dotted lines denote the Rayleigh velocity asymptotes. The largest discrepancy between the SOA and FE models, δ_{max} , occurs in the elongated direction for all materials. For clarity of the plots, only a subset of the calculated FEM points is displayed in the figure and the rest of the points between those displayed are skipped.

range is further quantified by the normalised root-mean-square deviation (NRMSD), with the FEM velocity as reference. The results are given in Table 6.3 for the studied materials (equiaxed aluminium is also included for comparison). The table shows that: 1) the level of agreement for the elongated case is about the same as that of the equiaxed case; 2) for all materials the SOA model has a very good agreement with the FE model in the shortened direction, and the agreement decreases in the elongated direction due to the increased scattering; 3) the overall discrepancy between the two models is smallest for aluminium and largest for Inconel, suggesting that the discrepancy increases with the universal anisotropy factor. In general, the observations for velocity NRMSD between the SOA and the FE models are similar to those for attenuation discussed in §6.2.1, however, the velocity NRMSD is about two orders of magnitude smaller. The point-by-point difference between the SOA and FE models is annotated as δ_{max} in the figure, showing the largest value in the elongated direction for all materials. The maximum discrepancy of -0.59% is found for CSP in the grain elongation direction at the highest normalised frequency of $2k_{0L}a_z = 44.56$. The discrepancy may also be partially attributed

to the SBCs effect, which may cause a discrepancy of -0.2% between the SOA and FE models for equiaxed Inconel as discussed in §4.4. Although scattering is weak at low frequencies, a noticeable difference between the SOA and FE models is observed for Inconel in Figure 6.7(b) for the quasi-static velocity. This difference may be attributed to the approximations involved in both the SOA and FE models.

Table 6.3: Normalised root-mean-square deviation (NRMSD) of phase velocity between the SOA and FE models (with the FE model as reference) for different material systems. Universal anisotropy factor [54] A^U and elastic scattering factors $Q_{L \rightarrow L,T}$ can be found in Tables 3.2 and 6.1 for the three materials.

Material	RMSD for equiaxed case	RMSD for elongated case	
		Shortened	Elongated
Aluminium	0.006%	0.007%	0.014%
Inconel	-	0.225%	0.243%
CSP	-	0.178%	0.183%

The excellent agreement of phase velocity between the SOA and FE models indicates that the SOA model is suitable for accurate velocity estimation.

6.3.2 Frequency dependence

Phase velocity is in general dispersive across the entire frequency range but also exhibits nondispersive behaviours at low and high frequencies. The nondispersive low- and high-frequency regions are first discussed below. They are followed by the discussion of the overall variation of the scattering induced phase velocity dispersion within a frequency range that is usually found in experimental studies.

1. Low-frequency region

In the low-frequency Rayleigh regime, the phase velocity dispersion is small and is well approximated by the quasi-static limit and a reasonable agreement between the theoretical SOA and numerical FE results is observed in Figure 6.7. With the decrease of frequency, the velocity extends asymptotically to the quasi-static velocity limit, which is significantly below the Voigt average; see further discussions in §6.3.5. The FE and the

Born approximations of the phase velocity for the CSP polycrystal are shown in Figure 6.8; which also presents the contributions of the $L \rightarrow L$ and $L \rightarrow T$ scattering components in addition to the total Born velocity. The figure demonstrates that the longitudinal phase velocity is dominated by the $L \rightarrow T$ scattering component in the Rayleigh region, which is consistent with that of attenuation as discussed in §6.2.3.

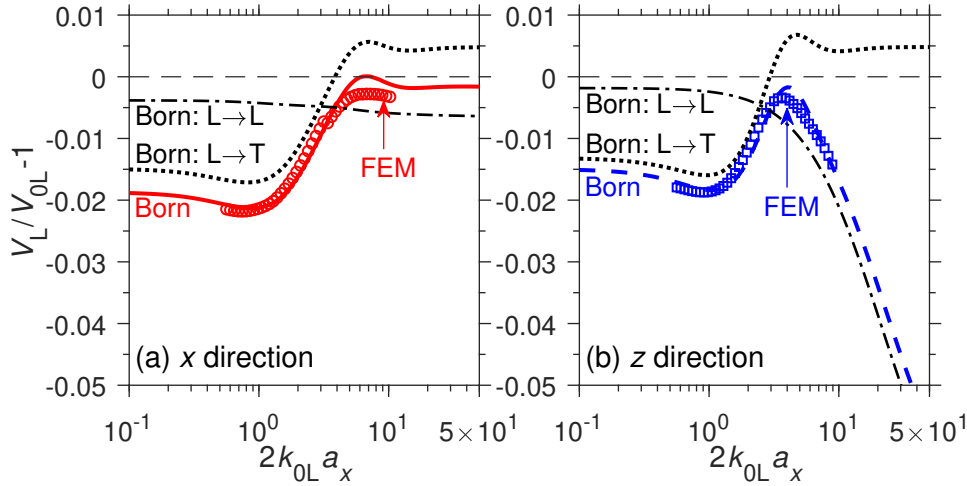


Figure 6.8: Total normalised phase velocity and its $L \rightarrow L$ and $L \rightarrow T$ components in the Born approximation for the CSP in the shortened x and elongated z directions of the grains. The $L \rightarrow L$ and $L \rightarrow T$ components $V_L/V_{0L} - 1 \approx -(\Delta_{L \rightarrow L} + \Delta_{L \rightarrow T})$ are approximately presented by $-\Delta_{L \rightarrow L}$ and $-\Delta_{L \rightarrow T}$ terms, Equation 2.13. The generalized TPC function as provided in Table 3.3 and Figure 3.3 is used for the calculations. The points represent the FEM results.

2. High-frequency region

It is observable from both panels of Figure 6.8 that in the high-frequency stochastic regime the $L \rightarrow T$ velocity components are weakly dispersive and behave similarly on frequency for both propagation directions; interestingly they virtually travel faster than the Voigt velocity V_{0L} . This phenomenon is not well understood especially that the transverse wave is much slower than the longitudinal. Figure 6.7 and Figure 6.8 show that the total velocity in the shortened grain direction is also weakly dispersive in the high-frequency stochastic regime. For aluminium, this region is much longer in frequency than those for Inconel and CSP, which have much higher material inhomogeneity (for equiaxed polycrystals the non-pronouncement of the stochastic regime was indicated in [14]).

In contrast to the propagation in the shortened direction, the total phase velocity in the

elongated direction dramatically decreases with frequency even for the weakly scattering aluminium. It is obvious from Figure 6.8 that this directional difference is caused by the $L \rightarrow L$ scattering velocity component, rather than by the $L \rightarrow T$ component. The dominant $L \rightarrow L$ component in Figure 6.8(b) decreases rapidly with frequency in the high-frequency range, leading to a similar decrease for the total phase velocity. The average grain radius in the elongated direction is significantly longer than the average wavelength of the waves (their ratio is represented by $2k_{0L}a_z$, where $a_z = 5a_x$). The velocity decrease may be associated with the bending of refracted waves; due to longer propagation paths, the phase delays may be sufficient to cause a decrease of effective mean phase velocity. Importantly the velocity decrease phenomenon is supported by the FE results, Figure 6.7 and Figure 6.8. It is observable from Figure 6.7(c) that the FE velocity deviates at the highest frequency points from the SOA velocity, but interestingly, the Born velocity agrees better with the FE velocity at those points, Figure 6.8(b). The high-frequency behaviour of the phase velocity merits further investigation by extending the FE simulations to a higher frequency; however, this is currently limited by computational capacity and by very high scattering-induced attenuation.

3. Comment on a relation of phase velocity dispersion with experiment

Here the theoretical SOA and numerical FE results in Figure 6.7 are used to estimate the range of velocity dispersion. The accuracy of the FE method in measuring frequency-dependent phase velocity is estimated to be around 0.03% (accurate to about three significant digits); the estimation is performed in the worst scenario by using Equation 4.6 for the highest-frequency FE point of the CSP polycrystal in Figure 6.7.

As mentioned in §1.2.2, the author is not aware of any published experimental studies that focus on or account for the dispersion of phase velocity in polycrystals with elongated grains. For polycrystalline copper with equiaxed grains, however, a recent work [28] compared the experimental measurements by Ledbetter [80] with the results of the FE and SOA models. Based on Ledbetter [80], three-to-four significant digits in absolute velocity can be measured in laboratory conditions on well-prepared polycrystalline samples (i.e. comparable to the above-mentioned FE accuracy). The effects of finite transducer size and

beam profile can be accounted for by a diffraction correction [81,82] and thus the measured apparent phase velocity may accurately represent the plane-wave phase velocity [81, 82]. This further enables the direct comparison of actual experiments with theoretical and numerical modelling. In addition, it is useful to note that both phase and group velocities can be measured in real experiments which are not equal but are related in the dispersive frequency range [81].

In most experimental studies, the velocity measurements are done in a relatively narrow frequency range to observe measurable dispersion that can be attributed to microstructure. However, often such measurements are compared with static measurements or low-frequency vibration measurements; see for example the intensive experimental study by Seiner et al. [83], where the ultrasonic velocity was also investigated and compared for different material processing. In such cases of comparison, the scattering induced dispersion needs to be considered for significantly different frequency ranges or different microstructures due to material processing. Therefore, it is practically important to have simple estimates of the range of the phase velocity dispersion.

Between static, vibration, and ultrasonic measurements, the range of the $2ka$ parameter is about 0-10. Due to grain scattering, it is very difficult to receive an ultrasonic wave at a meaningful distance above that frequency limit and to make ultrasonic velocity measurements in polycrystals with a sufficient signal-to-noise ratio. For all material cases shown in Figure 6.7, phase velocity in the normalised frequency range 0-10 is approximately between the Rayleigh asymptote (quasi-static velocity) and the Voigt velocity ($V_L/V_{0L} - 1 = 0$). The phase velocity change is about 0.1% for aluminium and is about 2% for Inconel and CSP (it is about 3% for Inconel in the shortened direction). The quasi-static velocity limit, Equations 2.19 and 2.20, is a good approximation for the lower velocity bound. As mentioned above a slight velocity decrease in the low-frequency regime can be neglected for this estimation. The significant dispersion change starts at about $2k_{0L}a_x \approx 1$ for the shortened and elongated propagation directions. As follows from Figure 6.7, for both the SOA and FE models, this dispersion frequency range continues until the emergence of the stochastic range at $2k_{0L}a_x \approx 5$ in the shortened direction and $2k_{0L}a_z \approx 15$ in the elongated direction, where the phase velocity reaches a peak that is close to the Voigt velocity. In the elongation propagation direction, it is already on the high end of the

assumed practical frequency range.

In the Rayleigh regime, the phase velocity is smaller in the shortened direction than in the elongated direction, while at the end of the transition regime this reverses and the velocity in the shortened direction is slightly above that in the elongated direction. As a result, in the range of $2k_{0L}a_x = 1 - 5$, the change of the phase velocity with frequency is larger in the shortened propagation direction than that in the elongated direction.

6.3.3 Elastic dependence

This section studies the scaling of the relative directional phase velocity difference $\xi_V = (V_L^z - V_L^x)/V_L^x$ by the elastic scattering factors. Similarly to the attenuation study in §6.2.3, the scaling is performed by dividing the relative directional difference by $Q_{L \rightarrow T} V_{0L}^3/V_{0T}^3$ in the low-frequency range ($2k_{0L}a_x \leq 2$) and by $Q_{L \rightarrow L}$ in the high-frequency range ($2k_{0L}a_x \geq 6$). The results are plotted in Figure 6.9. After the scaling, both the FE and the SOA directional velocity differences are almost overlapped for different materials studied. It is important to emphasise that the elastic scattering factors are approximately proportional to the relative directional velocity difference ξ_V rather than the directional ratio V_L^z/V_L^x .

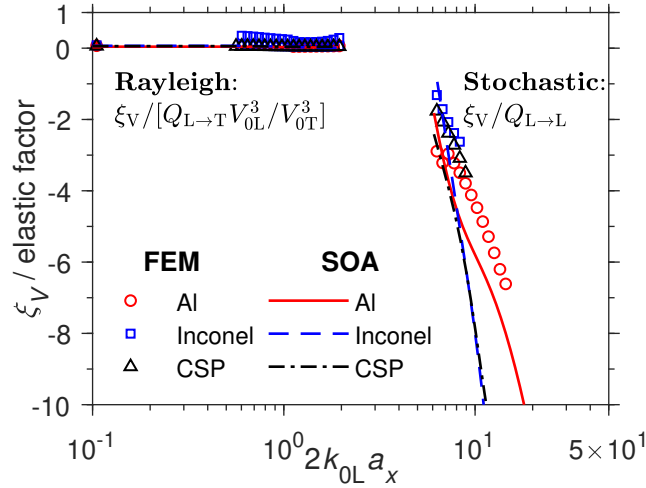


Figure 6.9: The scaled relative longitudinal directional phase velocity difference $\xi_V = (V_L^z - V_L^x)/V_L^x$ versus nondimensional frequency $2k_{0L}a_x$. ξ_V is scaled by the elastic factor $Q_{L \rightarrow T} V_{0L}^3/V_{0T}^3$ in the low-frequency range, and by the scattering factor $Q_{L \rightarrow L}$ in the high-frequency range. For clarity, only a subset of the calculated FEM points is displayed and the rest of the points between those displayed are skipped.

The velocity ratio V_{0L}^3/V_{0T}^3 of the Voigt reference medium depends on the Poisson's ratio

only and is weakly varying for most structural materials. For this reason, it is sufficient in the Rayleigh regime to use only the $Q_{L \rightarrow T}$ factor for velocity scaling. Thus, it concludes that the anisotropy of wave velocity in polycrystals with elongated grains is governed by the degrees of inhomogeneity $Q_{L \rightarrow T}$ and $Q_{L \rightarrow L}$ in the Rayleigh and stochastic regimes, respectively. These are identical to the elastic dependences of attenuation for equiaxed polycrystals as discussed in §5.2.2 and for elongated polycrystals as discussed in [26] and in §6.2.3. As indicated in [26], if different material systems have nearly the same elastic scattering factors $Q_{L \rightarrow T}$ and $Q_{L \rightarrow L}$, they have very similar scattering behaviour in all frequency ranges including the Rayleigh-to-stochastic transition.

6.3.4 Geometric dependence

1. Dependence on propagation direction

The directional dependence of phase velocity is studied here by evaluating the change of phase velocity with the propagation direction θ_p . Similarly to the attenuation study in §6.2.2, the FE results and the predictions of the SOA model are plotted in Figure 6.10 for the directions of 0° , 15° , 18.75° , 30° , 45° , and 90° . The results in the figure are limited to the high-frequency range, while the low-frequency results will be presented in §6.3.5.

The figure shows a generally good agreement between the FE and SOA models for all directions, especially for the three directions closer to the shortened direction (90°) where scattering is relatively smaller than in the other three directions. The two models start to deviate when the transition into the geometric regime begins at the normalised frequency of about 6-8. The largest deviation is about 0.8%.

The mean grain radius in the wave propagation direction decreases as θ_p deviates from the elongated direction (0°). This leads to a decrease of scattering level, which is manifested in two aspects in the figure as θ_p deviates from 0° : phase velocity becomes faster; and the transition point into the geometric regime occurs later in frequency, which is observable from the SOA curves.

The directional dependence is further evaluated in Figure 6.11 by polar plotting the normalised phase velocity against propagation direction θ_p for the normalised frequencies of

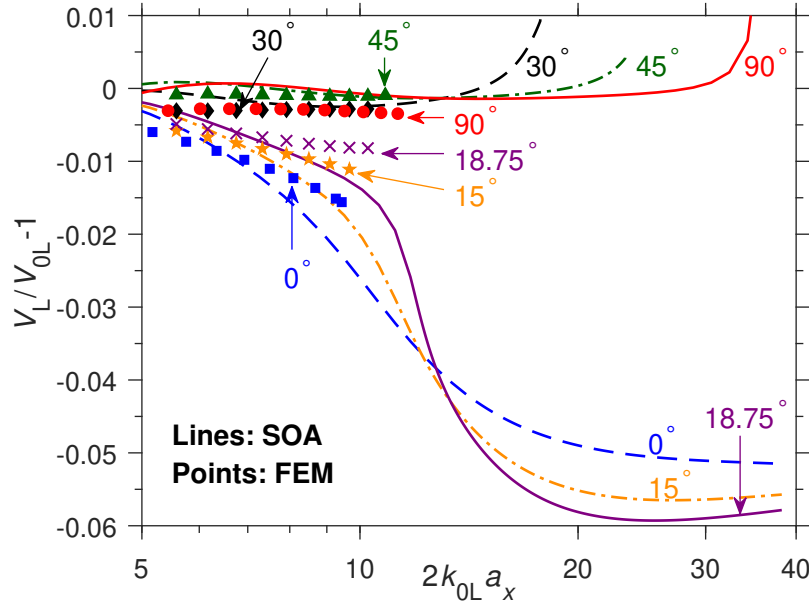


Figure 6.10: Normalised longitudinal phase velocity versus normalised frequency in different propagation directions for triclinic CSP. Points are for the FEM results and lines are for the SOA. The propagation directions θ_p are 0° , 15° , 18.75° , 30° , 45° , and 90° . The FEM points for 30° (diamonds), 45° (triangles), and 90° (circles) are mostly overlapped in the given frequency range. For clarity, only a subset of the original FEM points is displayed in the figure and the remaining points between those displayed are skipped.

5.56 and 8.34. The r -axis of each panel represents the normalised phase velocity $V_L/V_{0L} - 1$ and the θ -axis denotes the propagation direction θ_p . The FEM points are provided for all simulated directions. The SOA and Born approximation results are provided as solid and dash lines in the figure.

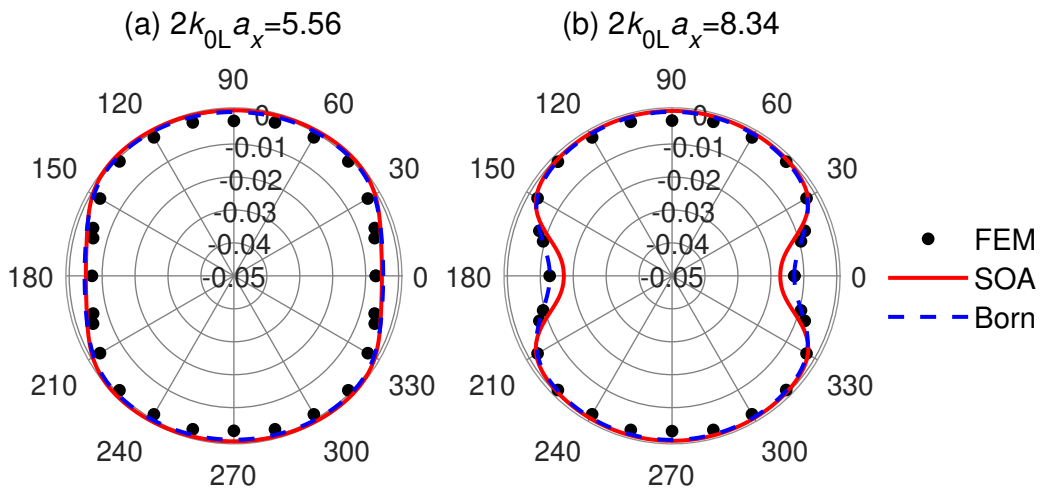


Figure 6.11: Polar plot of normalised longitudinal phase velocity (r -axis) versus wave propagation direction (θ -axis) for CSP at the normalised frequencies of (a) 5.56 and (b) 8.34. The results are given for polycrystalline CSP with elongated grains.

The agreement between the FE and theoretical models is generally very good in all directions. In directions nearer the shortened direction ($90^\circ/270^\circ$), the two theoretical models both provide slightly larger velocities than the FE model. Closer to the elongated direction ($0^\circ/180^\circ$), the FE model matches better with the Born approximation than with the SOA model. This is because the SOA model predicts the transition to the geometric regime; however, at the highest FE frequencies achieved in this study, the FE velocity does not follow this transition and coincides with the Born approximation.

The absolute value of normalised phase velocity in Figure 6.11 increases as the propagation direction changes from the shortened direction ($90^\circ/270^\circ$) to the elongated direction ($0^\circ/180^\circ$), which is observable from both the numerical FE and theoretical SOA models. This means that the scattering-induced variation of phase velocity (characterised by the normalised phase velocity $V_L/V_{0L} - 1$) increases with the mean grain size in the direction of propagation and this determines the level of scattering. This indicates that the phase velocity dispersion in the high-frequency range carries information about the average geometry of the grains. The absolute difference of FEM phase velocity between the shortened and elongation directions are 19.19 and 48.73 m/s at the normalised frequencies of 5.56 and 8.34, respectively.

2. Dependence on grain aspect ratio

The above evaluation of directional dependence has used a representative aspect ratio of $R = 5$. Since in practical materials grain aspect ratio may vary in a wide range, it would be important to see how directional dependence changes with R , which is the ratio of average grain radius between the axial z and transverse x directions and is called aspect ratio rather than elongation ratio in order to consider pancake-shaped grains.

In Figure 6.12(a), the relative directional ratio of phase velocity, $V_L^z/V_L^x - 1$, is plotted against the normalised frequency for CSP with four aspect ratios of 0.1, 0.2, 5, and 10. The predictions of the SOA and the Born approximation models are provided for all cases, while the FEM points are only provided for $R = 5$. In the low-frequency Rayleigh range, the directional ratio has a flat part observable for all cases. This is because phase velocity is nondispersive as explained in §6.3.2. The flat parts appear on the opposite

sides of $V_L^z/V_L^x - 1 = 0$ for $R < 1$ and $R > 1$. They collectively indicate that phase velocity is larger for a longer mean grain radius in the direction of propagation. Beyond the nondispersive Rayleigh regime, the directional ratio exhibits a complicated behaviour. A non-monotonic variation is visible in the Rayleigh-stochastic transition range, and it occurs relatively early in frequency for the two cases with $R > 1$. This variation ends at the frequency where the ratio starts to decrease (for $R > 1$) or increase (for $R < 1$) continuously. The continuous decrease or increase at high frequencies may be caused by the dominant $L \rightarrow L$ scattering component as discussed in §6.3.2.

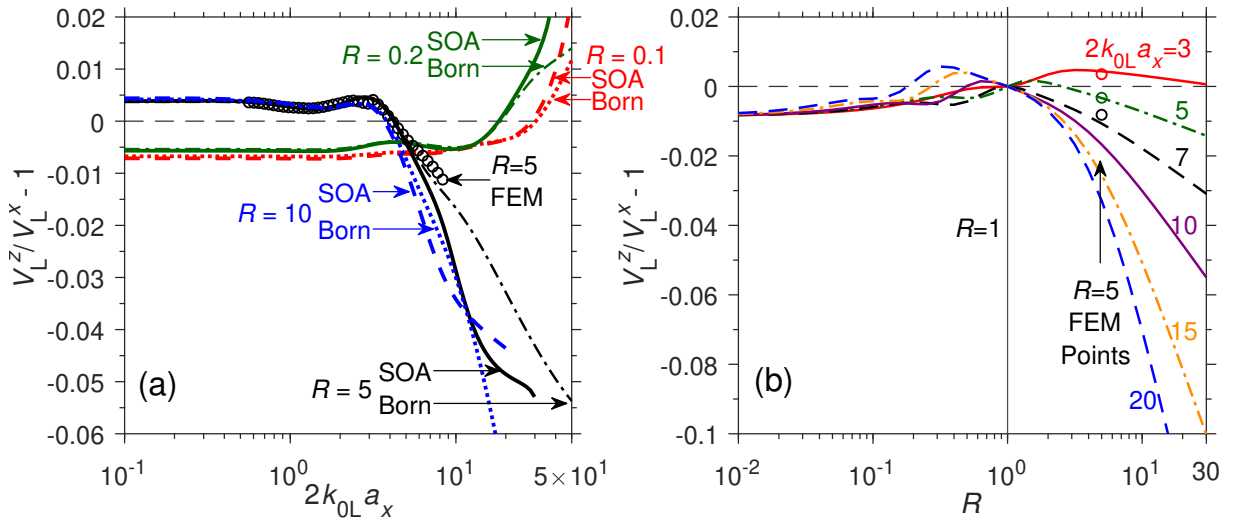


Figure 6.12: Directional velocity ratio versus (a) normalised frequency $2k_{0L}a_x$ and (b) aspect ratio R for polycrystalline CSP. The curves in (a) are obtained from the SOA and Born approximation models, while those in (b) are obtained solely from the Born approximation. The TPC functions used for the calculations are obtained by scaling the generalized equiaxed TPC function with the aspect ratio of R . The y -axis of both panels represents the relative difference of phase velocity between the axial z and transverse x directions.

In Figure 6.12(b), the change of directional velocity ratio with the grain aspect ratio is further evaluated. The normalised frequencies of 3, 5, 7, 10, 15, and 20 are chosen for the evaluation. The lowest frequency corresponds to the peak ratio in Figure 6.12(a) for $R = 5$, so the chosen frequencies are mostly in the high-frequency range. A similar discussion will be given for the low-frequency Rayleigh range (the quasi-static limit) in §6.3.5. The simpler Born approximation, instead of the SOA model, is used to obtain the curves in Figure 6.12(b) because it is computationally efficient and its prediction is very close to that of the SOA model as can be seen in panel (a). As the aspect ratio approaches zero, the directional velocity ratio tends to be independent of the aspect ratio

and it converges to the same value for all frequencies. This converged value is below zero, which is consistent with the above finding that the shorter axial direction has a slower phase velocity than the longer transverse direction. On the right side of the plot, the directional velocity ratio exhibits a continuous decrease with the aspect ratio in the shown range. This may be due to the dominant $L \rightarrow L$ scattering component that tends to have larger phase delays in the elongated z direction as a wave propagates through longer grains. It is noted that a nonpropagative case ($V_L^z/V_L^x - 1 = -1$) will not happen because each curve in the figure will eventually reach a flat part (with the directional ratio being greater than -1) as the aspect ratio further increases.

6.3.5 Quasi-static velocity limit

This section studies the effect of grain elongation on velocity at the quasi-static limit. To the author's knowledge, limited attention has been received to study the quasi-static limit with the consideration of grain shape. While Kocks et al. [5] have included tables showing simulated results for the combined effect of macro-texture and grain shape on elastic moduli, it is difficult to conclude the grain shape effect. This section aims to evaluate the effect of grain elongation on the quasi-static velocity limit.

In addition to the analytical quasi-static limit obtained in Equation 2.19, the FE method outlined in §3.7 is also employed to calculate the quasi-static limit. It is worth noting again that the chosen FE method naturally meets the continuity of stress and strain at grain boundaries and thus delivers a very accurate calculation of quasi-static velocity.

The quasi-static velocities obtained from the FE and SOA models have already been provided in Figure 6.7, but they are more elaborately summarised in Table 6.4 for all three polycrystalline materials. As indicated from the relative difference δ , the SOA results are mostly indistinguishable from the FEM results. The SOA model gives a generally higher quasi-static velocity but the maximum difference between the SOA and FE models for the studied cases is as small as 0.36%, which can be treated as negligible. And, quasi-static velocity shows an identical trend to attenuation and dynamic phase velocity in that the increase of anisotropy (characterised by the universal anisotropy factor as shown in Table 3.2) directly causes the increase of difference between the SOA and FE models.

Table 6.4: Longitudinal quasi-static velocities for polycrystalline aluminium, Inconel, and CSP with elongated grains. The ‘FEM’ columns represent longitudinal quasi-static velocities, V_L (m/s), obtained from FE simulations; each FEM result is the average of 30 realizations. The ‘SOA’ columns correspond to the low-frequency Rayleigh velocity limits obtained from the SOA model, Equation 2.19. $\delta = V_L^{\text{SOA}}/V_L^{\text{FEM}} - 1$ indicates the relative difference of velocity between the SOA and FEM results. $\xi_V = V_L^z/V_L^x - 1$ signifies the directional ratio of FEM velocity between the elongated z and shortened x directions.

Material	Shortened x direction			Elongated z direction			ξ_V (%)	$\frac{\xi_V}{Q_{L \rightarrow T} V_{0L}^3/V_{0T}^3}$
	FEM	SOA	δ (%)	FEM	SOA	δ (%)		
Aluminium	6312.2	6312.4	0.003	6313.4	6313.1	-0.005	0.019	0.069
Inconel	5890.8	5911.6	0.353	5911.1	5927.6	0.280	0.344	0.079
CSP	4780.2	4784.7	0.094	4799.5	4802.3	0.060	0.403	0.059

The emergence of the grain shape effect is clearly visible in the table, which is manifested as the directional difference between the elongated and shortened directions. To further evaluate this effect, the normalised quasi-static velocity is plotted versus propagation direction in Figure 6.13(a). In the figure, FE results are only provided for the elongated and shortened directions, but the excellent agreement between the FE and SOA models means that the FE results should be close to the SOA curves in all directions. In the figure, all SOA curves are approximately elliptical and their major axes overlap with the grain elongation direction, revealing a positive correlation between quasi-static velocity and grain geometry.

The directional difference is further quantified in the table by the ratio ξ_V as used in the above sections. It is clear from the table that this ratio can differ significantly from one material to another, but it tends to deliver the same value when it is divided by the elastic factor $Q_{L \rightarrow T} V_{0L}^3/V_{0T}^3$. This is an important finding that the grain shape effect is also positively correlated with the elastic inhomogeneity perturbation of polycrystals.

In addition, the analytical expression in Equation 2.19 is used to evaluate the directional ratio of quasi-static velocity between the axial z and transverse x directions versus the grain aspect ratio, Figure 6.13(b). Both the pancake-shaped ($R < 1$) and needle-shaped (elongated, $R > 1$) cases are shown in the figure. For this reason, $V_L^z/V_L^x - 1$ is used to denote the velocity ratio in Figure 6.13(b), where the ellipsoid axes z and x are defined in Figure 2.1. The FE results are provided as points in the figure, corresponding to

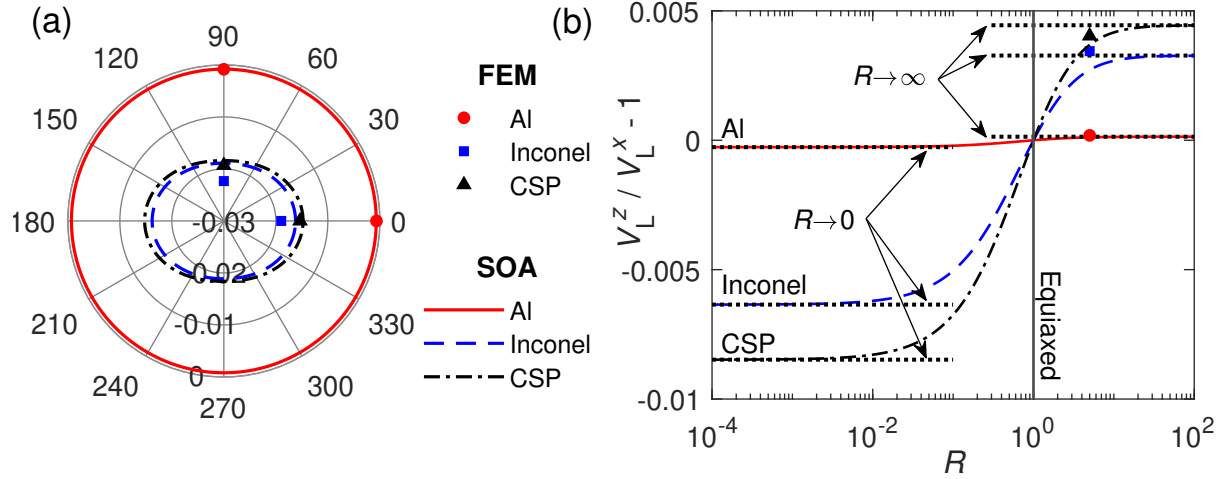


Figure 6.13: Longitudinal quasi-static velocity for polycrystals with statistically ellipsoid-of-rotation grains: (a) normalised velocity (r -axis) versus wave propagation direction (θ -axis); (b) directional ratio of velocity between the axial z and transverse x directions against the grain aspect ratio $R = a_z/a_x$. In (a), the r -axis represents the quasi-static velocity as normalised by the Voigt average: $V_L/V_{0L} - 1$. In (b), the axial z and transverse x directions correspond to the elongated and shortened directions for $R > 1$.

the elongation ratio of $R = 5$. This work is not intended to extend the quasi-static FE simulations to other elongation ratios because it has a very large demand on computational costs, this may be pursued in future work.

The figure shows a general increase in the directional velocity ratio as the grain aspect ratio gets larger. Obviously, the directional difference vanishes for the equiaxed case of $R = 1$, given by Equation 2.22. The velocity ratio reaches its lower bound as R approaches zero ($R \rightarrow 0$), Equation 2.24, which is shown by dotted lines. Similarly, the quasi-static velocity ratio reaches its upper bound as grain elongation increases ($R \rightarrow \infty$), Equation 2.25. These bounds are further listed in Table 6.5, showing a generally larger directional difference for the case of $R \rightarrow 0$ than for $R \rightarrow \infty$. For the latter case, the absolute quasi-static velocity differences between the elongated axial and shortened transverse directions are respectively 0.9, 19.3, and 21.3 m/s for aluminium, Inconel, and CSP.

It has been revealed from Equations 2.24 and 2.25 that the phase velocities for $R \rightarrow 0$ and $R \rightarrow \infty$ are the same along the long axes of the grains (x direction for the former and z direction for the latter). This equality is shown in the third and fifth columns of Table 6.5. It is noted that the equality is only valid for this extreme case, meaning that phase velocity differs between a $R < 1$ case and a $R > 1$ case even though they have the

same grain radius in the long axes of the grains.

Table 6.5: Upper and lower bounds of longitudinal quasi-static velocity for polycrystals with statistically ellipsoid-of-rotation grains. V_L^z and V_L^x represent respectively the quasi-static velocities in the axial z and transverse x directions of the grains. Lower and upper bounds are calculated with Equations 2.24 and 2.25, respectively.

Material	Lower bound at $R \rightarrow 0$			Upper bound at $R \rightarrow \infty$		
	V_L^z (m/s)	V_L^x (m/s)	$V_L^z/V_L^x - 1$	V_L^z (m/s)	V_L^x (m/s)	$V_L^z/V_L^x - 1$
Aluminium	6312	6313	-0.0003	6313	6312	0.0001
Inconel	5892	5930	-0.0064	5930	5911	0.0033
CSP	4764	4805	-0.0085	4805	4784	0.0044

6.4 Summary

The theoretical SOA and 3D FE models are employed in this chapter to study the scattering-induced attenuation and phase velocity dispersion of plane longitudinal waves in polycrystals with statistically elongated grains. The study uses three polycrystalline materials, aluminium, Inconel, and CSP, that have a grain elongation ratio of 5. Based on the comparative studies of the SOA and FE models, the following conclusions are reached:

1) Quantitative agreement has been found between the two models. The difference between the SOA and FE models is quantified by the NRMSD. In general, the NRMSD is positively correlated with the universal anisotropy factor A^U and the mean grain radius in the direction of propagation, showing a direct relation to the level of scattering. The NRMSD for the elongated direction is larger than that for the shortened direction for all studied materials. In the elongated direction, attenuation NRMSD increases from about 11% for aluminium through 12% for CSP to 25% for Inconel, while velocity NRMSD is smaller than 0.3% for all cases. The largest point-by-point difference of attenuation between the SOA and FE models is -39% as observed for Inconel, while that of phase velocity is around -0.6% as found for CSP in the elongated direction.

2) In general, the attenuation of longitudinal waves mostly exhibits anisotropy as a result of grain elongation. The attenuation is independent of grain elongation and is proportional to the effective volume of the grains and the fourth-degree of frequency in the Rayleigh

regime. It shows a complex dependence on grain elongation and frequency in the Rayleigh-stochastic transition. As scattering enters the stochastic regime, attenuation exhibits an angular dependence and is proportional to the frequency squared; for the strongly scattering materials Inconel and CSP, the stochastic regime is not pronounced in the elongated direction. As a result of grain elongation, the onset of the geometric regime varies with the propagation direction and the angular dependence of attenuation becomes complicated. The relative directional difference of phase velocity also shows anisotropy due to grain elongation. This grain elongation effect varies from one scattering regime to another. In the Rayleigh regime, the phase velocity is larger in the direction of grain elongation. This relation is reversed in the stochastic regime, where the velocity is slower in the elongated direction than in the shortened direction.

3) In addition to the dependences on grain elongation and frequency, the attenuation and phase velocity also show reliance on the elastic properties of the polycrystals. This manifests itself mostly through the two elastic scattering factors, $Q_{L \rightarrow T}$ and $Q_{L \rightarrow L}$, that are combinations of crystallite elastic constants. The attenuation and the directional difference of phase velocity are proportional to $Q_{L \rightarrow T}$ in the Rayleigh regime and to $Q_{L \rightarrow L}$ in the stochastic regime. Therefore, the effect of different material systems on attenuation and phase velocity can be scaled by those factors.

4) The analytical and numerical analyses show that the phase velocity at the quasi-static limit follows a similar pattern as found for phase velocity in the low-frequency Rayleigh regime. Namely, the quasi-static velocity is angle-dependent in elongated polycrystals, and its directional change is related to the grain aspect ratio and the elastic scattering factor $Q_{L \rightarrow T}$. The analytical analysis shows that the quasi-static velocity is lower and upper bounded as the grain aspect ratio decreases and increases, respectively.

Chapter 7

Representing spatial autocorrelation by a single exponential

7.1 Introduction

Previous chapters have demonstrated that the calculation of scattering-induced attenuation and velocity dispersion relies on the statistical description of microstructure by the TPC function. For a numerically generated polycrystal as used in 3D FE simulations, its TPC data can be accurately measured from its material volume. This leads to a fairly accurate calculation of attenuation and velocity by incorporating the mathematical representation of the measured TPC data into a theoretical model [28, 39]. Importantly, it has been found that an exponential series is needed for a closer representation of the TPC data than was considered in the earlier work [14, 17] which used a single exponential.

For an experimental sample, however, determining its accurate TPC data is very expensive, because it requires a substantial number of statistical tests to be performed on a lot of micrographs of sample cross-sections [51]. Thus, it is usually desirable to use a limited number of cross-sections and tests, which results in less accurate TPC data. The challenge then is to choose a simple representation of the TPC that can be depended on to work optimally from a small sample set. This chapter sets out to do that, retaining the traditional single exponential function for simplicity, but pursuing the optimal choice of its parameter. This is achieved by choosing several candidate parameters for the single

7. Representing spatial autocorrelation by a single exponential

exponential function and then evaluating their goodness of representation by comparing their attenuation and velocity predictions with those of the accurate TPC function.

For practical applications, it is important to ensure that a selected parameter can be directly measured from cross-sectional micrographs. Thus, an essential first step is to study the measurable statistics that can characterise the spatial autocorrelation of a polycrystal that determines the level of scattering occurring in the medium. Such a study is performed in the following §7.2 by revisiting the TPC function and analysing the other two probability functions, namely, the distributions of line intercept and free path. The latter two functions are better known in materials science and are more widely used in engineering applications. This study provides measurement approaches for these functions and also demonstrates their relations. Additionally, a key investigation is conducted to evaluate the statistical convergence of measurement.

Then, five potential parameters are identified in §7.3 for the single exponential function to replace the actual TPC function. Four parameters are the characteristic lengths of the actual TPC function, with the mean line intercept relating to its slope at the origin, the correlation length being its integral, the effective radius relating to its triple integral, and the best-fit radius being the coefficient of its best fit to the single exponential. The other parameter selected for the study is the equivalent spherical radius that can only be determined by stereological methods.

Lastly, the goodness of representation of the selected parameters is evaluated in §7.4. The single exponential function using these parameters is incorporated into theoretical models for attenuation and velocity calculation. The calculation results are compared with those obtained from the accurate TPC function, leading to the choice of an optimal parameter for the single exponential function.

The purpose of this study is to achieve a reasonably good estimation of attenuation and velocity for experimental applications in which case microstructural statistics are rapidly determined from a limited number of tests on a few cross-sectional micrographs. Achieving this goal, however, requires accurate reference data to be provided for demonstration and evaluation. For this reason, numerical polycrystal samples, rather than actual experimental ones, are used for the study. This is because the microstructure of a numerical

sample can be fully controlled and accurately measured, and the associated scattering parameters can be precisely calculated from FE simulations. Various numerical samples with equiaxed grains of different grain uniformities are generated for the study. This study is being prepared for publication [P6].

7.2 Spatial probability functions

This section studies the three probability functions for the description of spatial autocorrelation for polycrystals, including the TPC function and the distributions of line intercept and free path, which can all be directly measured from cross-sectional micrographs. Initially, the TPC function is revisited. This is followed by the discussions of the line intercept and free path distributions and their relations to the TPC function. Lastly, the statistical convergence of probability function measurement is discussed.

7.2.1 Two-point correlation function revisited

The TPC function has been extensively discussed in previous chapters. It is expressed as $w(r)$ for equiaxed polycrystals, describing the probability that two points separated by a distance r are in the same grain [14, 17, 51]. This function reflects the geometric statistics of grains, and in particular, the statistical variation of material property across grains. Consequently, this function is related to how propagating waves are scattered by (or interact with) grains.

The measurement of $w(r)$ is straightforward for a numerical sample. This is achieved by dropping a substantial number of random point pairs, each being separated by a distance r , into the 3D volume of the sample, and the probability $w(r)$ is then obtained by comparing the number of pairs occurring in the same grain with the total number of test pairs [28, 39].

For an experimental sample, however, the access of measurement is generally limited to its surface, meaning that measurement can only be performed in a 2D way as illustrated in Figure 7.1(a). In this case, volumetric statistics are usually acquired from multiple cross-sections of the sample that are successively exposed for measurement via serial sectioning.

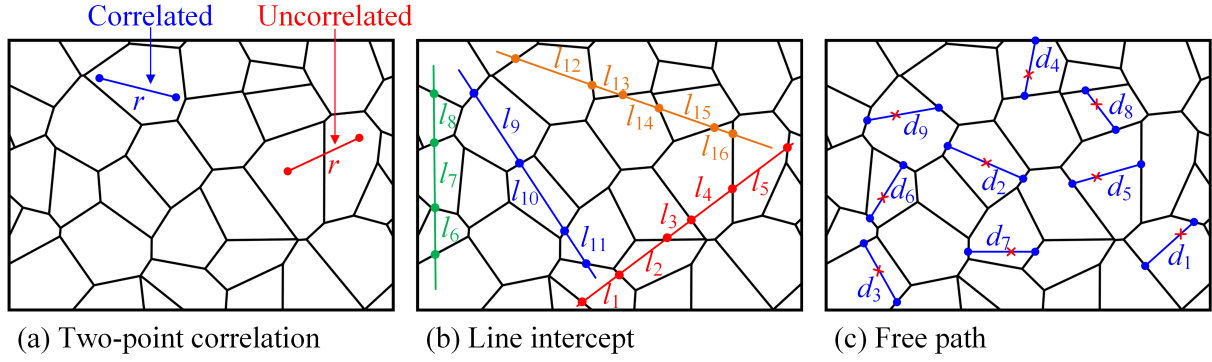


Figure 7.1: Illustration of (a) two-point correlation, (b) line intercept, and (c) free path statistics. In (a), two points are correlated when they fall into the same grain; the probability of two points separated by a distance r being in the same grain is represented by the correlation function $w(r)$. In (b), line intercepts, l_i , denote the lengths of the random test line segments intercepted by grain boundaries. In (c), a free path, d_i , represents the length of a random line that passes through a random test point and is intercepted by grain boundaries.

To emulate this 2D practical procedure, 1000 random cross-sections perpendicular to the z -direction are chosen from the FE material model N11520, Table 3.1. For a given distance r , 1000 random tests are performed on each cross-section. This leads to the TPC data shown as circular points in Figure 7.2. These points are mostly indistinguishable from the triangular ones that are measured directly from the 3D volume of the model by using the same number, 1000×1000 , of tests for each distance r . The normalised root-mean-square deviation (NRMSD) between these two datasets amounts to 0.17%, with the 3D case as reference. Due to this small mismatch, the two datasets are fitted into the same exponential series, $w(r) = \sum_i A_i e^{-r/a_i}$, shown as the solid line in the figure. The coefficients, A_i and a_i , are provided in Table 3.3. In order to maintain consistency with actual practical scenarios, TPC statistics used hereafter are measured from 2D cross-sections, unless otherwise stated.

7.2.2 Probability distribution of line intercept

The microstructure of a polycrystal can also be described by the probability distribution of line intercept. As illustrated in Figure 7.1(b), a line intercept l_i (also called chord length, see e.g., [50, 84, 85]) represents the length of a line segment intercepted by grain boundaries. The mean value of line intercept is being widely used in metallography as

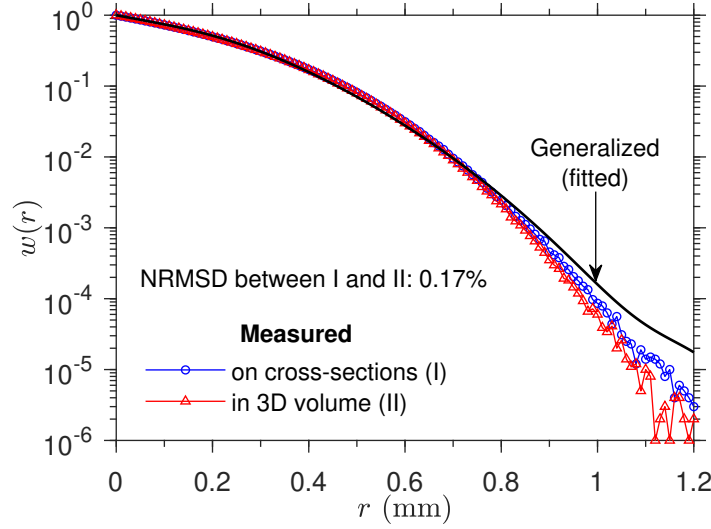


Figure 7.2: Two-point correlation, $w(r)$, for the material model N11520. The circular points are measured from 1000 random cross-sections that are perpendicular to the z -direction of the model, and 1000 random tests are performed on each cross-section to determine each correlation probability $w(r)$. Each triangular point is determined by using the same number, 1000×1000 , of random tests in the 3D volume of the model. The solid line represents the multi-term exponential fit, $w(r) = \sum_i A_i e^{-r/a_i}$, of the points, with coefficients A_i and a_i being given in Table 3.3.

a measure to quantify the average grain size of a polycrystal. For this reason, there are standard approaches (see e.g., [86]) dedicated to the measurement of line intercept statistics from cross-sectional micrographs. Mimicking the approach provided in [86] leads to one of the two methods used here for measuring the line intercepts of a numerical sample. This method is achieved by first selecting multiple random parallel cross-sections from the sample and then dropping a significant number of random test lines onto each cross-section to determine the probability distribution of line intercept. By contrast, the second method simply performs a significant number of random tests in the 3D volume of the sample. These two methods are similar to those used above for TPC measurement.

The probability densities of line intercept, $p_l(x)$, obtained with the two methods are given in Figure 7.3 for the material model N11520. The first method selects 1000 random cross-sections perpendicular to the z -direction of the model and uses 1000 random test lines (the length of each line translates to at least 10 intercepts) on each cross-section. The second method performs the same number, 1000×1000 , of random tests in the 3D volume of the model. It is important to note that, as demonstrated in Figure 7.1(b), the line heads penetrated into the grains are not accounted for in both cases of measurement,

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which is to avoid the scoring of such penetrated heads as half intercepts as used in [86]. Figure 7.3 shows very consistent results between the two methods, demonstrating again the effectiveness of measuring 3D volumetric statistics from 2D cross-sections when a significant number of cross-sections and tests are utilized for measurement.

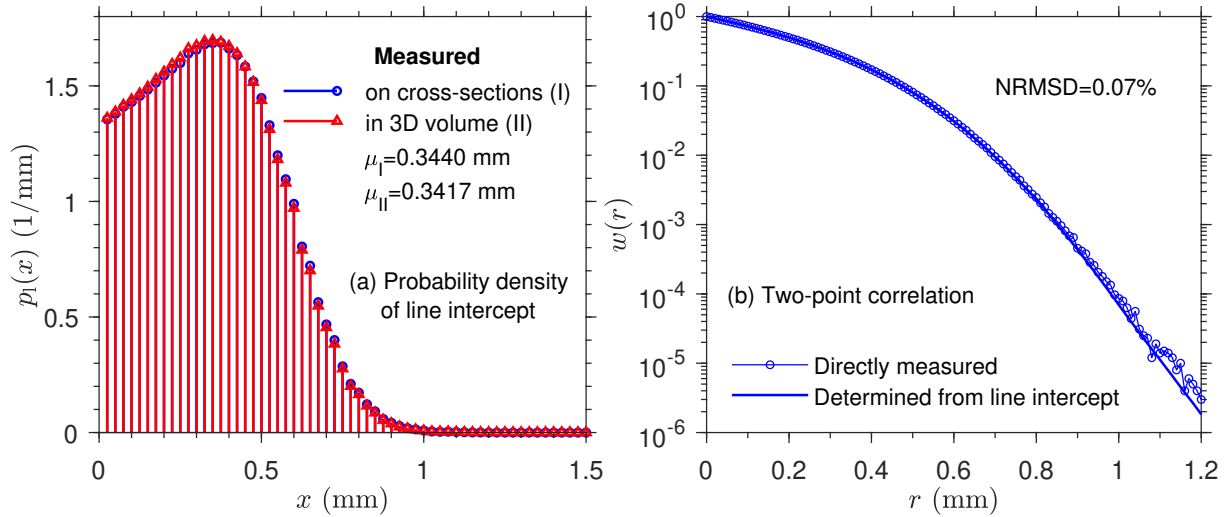


Figure 7.3: (a) Probability density of line intercept for the model N11520; (b) Comparison of the two-point correlation function determined from line intercept distribution with the directly measured one. In (a), case I is measured with 1000 random cross-sections perpendicular to the z -direction and 1000 random test lines per cross-section, while case II is determined by performing 1000×1000 random tests in the 3D volume of the model. In (b), the line with points is taken from Figure 7.2 and the solid line is calculated from case I of panel (a) by using Equation 7.2; the statistics of both lines are determined from random cross-sections.

The distribution of line intercept is directly related to the TPC function. The relation, first reported by Stanke [50] and later mathematically proved by Man et al. [51] under general conditions, is expressed as

$$w(r) = \int_r^\infty \frac{x-r}{\bar{l}} p_l(x) dx, \quad (7.1)$$

where $\bar{l}$ is the mean value of line intercept. For discrete measurements, the relation can be rewritten as [51]

$$w(r) = \sum_{i, l_i \geq r}^N (l_i - r) / \sum_{i=1}^N l_i, \quad (7.2)$$

where l_i is the i -th intercept and N is the total number of intercepts. Applying this

relation to the cross-sectional line intercept data given in Figure 7.3(a) leads to the solid TPC curve shown in panel (b) of the same figure. It is illustrated in the figure that this TPC curve agrees very well with that measured directly from the FE material model, amounting to an NRMSD of 0.07%. To the author's knowledge, this excellent agreement is the first justification of the Man et al. [51] result with actual measurements. This result is of great practical importance because it allows the TPC to be determined by post-processing line intercept statistics measured with standard protocols in materials science.

In addition, it was proven by Man et al. [51] that the mean line intercept, $\bar{l}$, is equal to the negative of the reciprocal of the slope at the origin of the TPC function

$$\bar{l} = -1/w'(r = 0), \quad (7.3)$$

where the prime symbol represents the derivative of w with respect to r . The mean line intercept $\bar{l}$ of the model N11520 is calculated by using the statistics given in Figure 7.3, while the value for $-1/w'(r = 0)$ is numerically estimated from the discrete TPC points given in Figure 7.2. The results are provided in Table 7.1 and they show very small differences, -0.81% and -0.12%, for the cross-sectional and 3D volumetric methods, respectively. In addition to the numerical estimation, the latter parameter can also be analytically obtained from the fitted TPC function by $-1/w'(r = 0) = 1/\sum_i (A_i/a_i)$, and the result only differs from the other values after the second significant digit. The mean line intercept is widely employed in experiments to characterise the mean length scale of grains [50, 51], and to maintain consistency with other parameters used below, it is denoted a_1 hereafter and therefore $a_1 = \bar{l} = -1/w'(r = 0)$.

7.2.3 Probability distribution of free path

Free path is a geometrical attribute defined with respect to randomly chosen points. As shown in Figure 7.1(c), the free path of a given point is the length of the line segment passing through this point and extending to the boundaries of the grain in which the point falls [50]. Unlike line intercepts that are consecutively connected through random

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Table 7.1: Mean line intercept and the slope at the origin of the TPC function for the model N11520. $\bar{l}$ denotes the mean line intercept and the values in the table are obtained from the distributions in Figure 7.3(a). $-1/w'(r=0)$ represents the negative of the reciprocal of the slope at the origin of the TPC function, $w(r)$; it is either numerically estimated from the discrete TPC points in Figure 7.2 or analytically calculated from the fitted curve by $-1/w'(r=0) = 1/\sum_i (A_i/a_i)$. Unit: mm.

	$\bar{l}$	$-1/w'(r=0)$	
		From discrete points	From fitted curve
Measured on cross-sections	0.3440	0.3412	0.3458
Measured in 3D volume	0.3417	0.3413	

lines, free paths are uncorrelated. As a result, free paths are likely to be longer than line intercepts on average, which will be shown below [50].

Similarly to line intercept, two methods are used here for determining the probability distribution of free path. The first method drops random points on multiple cross-sections that are randomly chosen beforehand, and then draws randomly oriented in-plane lines passing through these test points, and eventually measures the lengths, d_i , of the line segments intersected by grain boundaries. In comparison, the second method randomly distributes the locations of the test points and the orientations of the associated test lines across the volume of the sample.

Figure 7.4 shows the probability densities of free path, $p_d(x)$, of the model N11520 as measured with the two methods. The cross-sectional method uses 1000 cross-sections with each using 10000 test points, while the second method directly utilizes the same number, 1000×10000 , of tests in the 3D volume. As shown in the figure, the two methods have an excellent agreement with each other. This proves again the possibility of acquiring volumetric statistics from cross-sectional images.

The probability density of free path is related to that of line intercept by [50] $p_d(x) = p_l(x)x/\bar{l}$. This relation has been verified by using the statistics given in Figures 7.3 and 7.4. Substituting this relation into Equation 7.1 leads to the relationship between the probability density of free path and the TPC function [14]

$$w(r) = \int_r^\infty \frac{x-r}{x} p_d(x) dx, \quad (7.4)$$

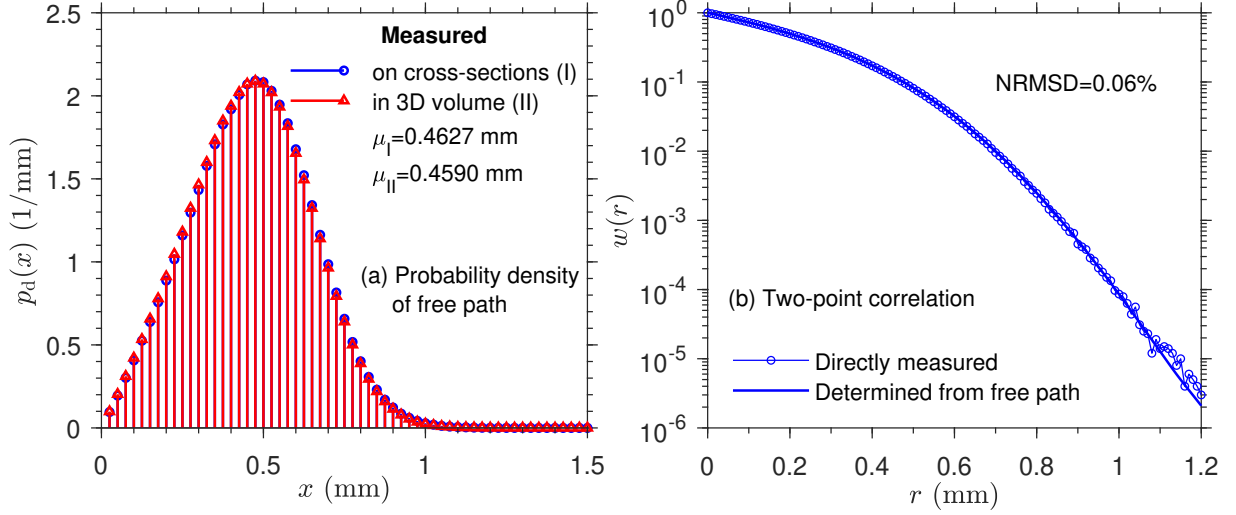


Figure 7.4: (a) Probability density of free path for the model N11520; (b) Comparison of the two-point correlation function determined from free path distribution with the directly measured one. In (a), case I is measured with 1000 random cross-sections perpendicular to the z -direction and 10000 random tests per cross-section, while case II is determined by performing 1000×10000 random tests in the 3D volume of the model. In (b), the line with points is taken from Figure 7.2 and the solid line is calculated from case I of panel (a) by using Equation 7.5; the statistics of both lines are determined from random cross-sections.

which can be written in the discrete form as

$$w(r) = \frac{1}{N} \sum_{i, d_i \geq r}^N \frac{d_i - r}{d_i}, \quad (7.5)$$

where N is the total number of free paths. With the use of this relation, the TPC function calculated from the free path distribution, case I in Figure 7.4(a), is provided in panel (b) of the same figure. The resulting curve agrees very well with the directly measured TPC points, amounting to an NRMSD of 0.06%. This is an important verification of this relation since neither rigorous mathematical proof nor actual justification has been reported previously for this relation.

The mean values of free path in Figure 7.4(a) are larger than those of line intercept shown in Figure 7.3(a). This confirms the earlier postulation that free path is likely to visit a longer grain dimension than line intercept. The half of mean free path is equal to the integral of the TPC function [50]

$$\bar{d}/2 = \int_0^\infty w(r) dr, \quad (7.6)$$

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which is demonstrated here by using the free path and TPC statistics given above. The half of mean free path obtained from Figure 7.4(a) and the integral of the discrete TPC data in Figure 7.2 are provided in Table 7.2, which show very small differences, -0.17% and -0.04%, for the cross-sectional and 3D volumetric methods. The integral of the TPC can also be calculated from the fitted TPC function by $\int_0^\infty w(r) dr = \sum_i A_i a_i$ and the resulting value, provided in Table 7.2, differs very slightly from those obtained from discrete data points.

The integral of the TPC function is commonly known as the correlation length, representing the characteristic length over which a significant correlation exists between values of the medium [87]. This parameter is related to the level of wave scattering in the high-frequency stochastic regime and will be denoted a_{CL} hereafter, i.e., $a_{CL} = \int_0^\infty w(r) dr = \bar{d}/2$.

Table 7.2: Half of mean free path and the integral of the TPC function for the model N11520. $\bar{d}$ denotes the mean free path and the values in the table are obtained from the distributions in Figure 7.4(a). $\int_0^\infty w(r) dr$ represents the integral of the two-point correlation, $w(r)$; it is either numerically estimated from the discrete TPC points in Figure 7.2 or analytically calculated from the fitted curve by $\int_0^\infty w(r) dr = \sum_i A_i a_i$. Unit: mm.

	$\bar{d}/2$	$\int_0^\infty w(r) dr$	
		From discrete points	From fitted curve
Measured on cross-sections	0.2313	0.2309	0.2309
Measured in 3D volume	0.2295	0.2294	

7.2.4 Statistical convergence

The above-converged statistics are measured by combining a significant number of cross-sections with a substantial number of tests for each cross-section. For actual experiments, it is straightforward to perform the same large number of tests on each cross-sectional micrograph with the use of computer programs [51, 86]. However, a major difficulty for actual experiments is to acquire a similar number of parallel cross-sectional micrographs from the volume of a sample, because it requires a considerable effort for serial-sectioning, surface preparation, and micrograph capturing. Therefore, in order to minimise the effort

of acquiring cross-sectional micrographs, it is desirable to investigate how many cross-sections and tests are required to achieve measurement convergence.

Without loss of generality, the mean free path is used here as a measure to evaluate the convergence of measurement. For the model N11520, its mean free path, $\bar{d}$, is progressively calculated as the number of cross-sections increases. The cross-sections are randomly chosen from the model and are all perpendicular to the z -direction. For the completeness of the evaluation, three sets of measurements are performed by utilizing different numbers of tests for each cross-section. The results for the mean free path are plotted against the number of cross-sections in Figure 7.5(a) for individual measurements.

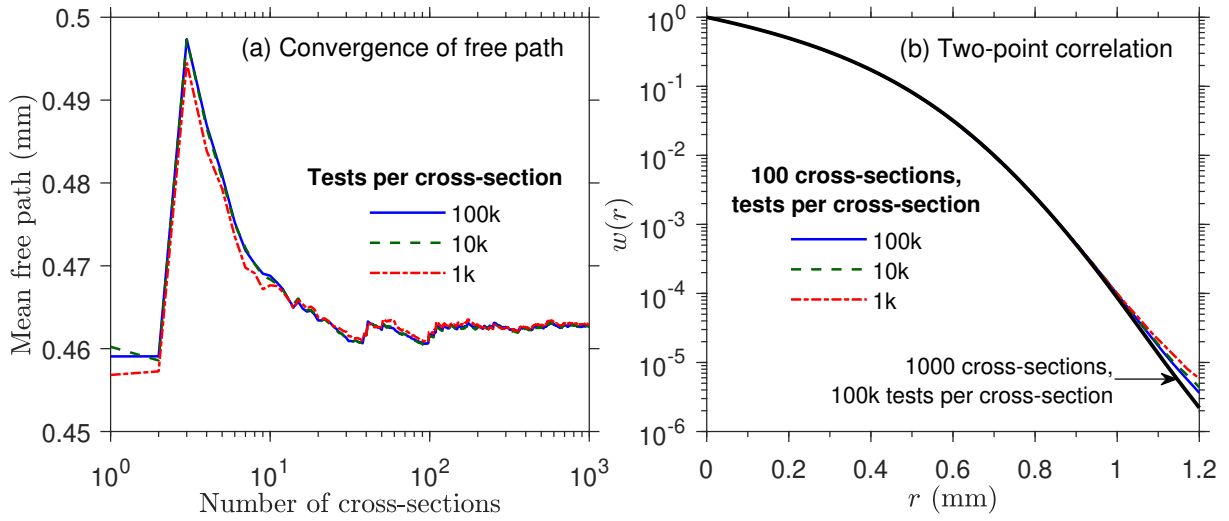


Figure 7.5: Convergence of mean free path: (a) mean free path versus the number of cross-sections, (b) two-point correlation function obtained from free path distribution. The solid, dash, and dash-dotted lines in (a) use respectively 100k, 10k and 1k tests on each cross-section. The thick solid line in (b) is obtained with the largest number, $1000 \times 100k$, of free paths, while the rest lines are derived from 100 cross-sections with 100k, 10k and 1k tests per cross-section.

A clear observation from the figure is that the curves for the three measurements are nearly overlapped, meaning that the number of tests per cross-section is not a determining factor for convergence as long as it is not too small. All three sets of measurements start to converge as the number of cross-sections approach 100. At this number, the free path statistics of the three measurements are converted to the TPC curves shown in Figure 7.5(b) by using Equation 7.5. The three curves are mostly indistinguishable compared to the one obtained using 1000 cross-sections and 100k tests per cross-section. This indicates that the use of 100 cross-sections is sufficient to deliver converged free path statistics that

would enable a fairly accurate calculation of attenuation and velocity for the sample.

It is useful to note that the evaluation here is performed for the specific numerical sample, N11520, that has a cross-section of 12×12 mm in dimensions and 24×24 in average grain numbers. For a larger sample with more grains on each cross-section, it may be sufficient to use less than 100 cross-sections to achieve the same level of convergence.

7.3 Potential parameters for the single exponential

It has been shown above that the microstructure of a polycrystal can be statistically described by the three probability distributions. As a result of their relations, measuring any of these distributions eventually leads to the determination of the TPC function that enables the calculation of attenuation and velocity. For this calculation, the measured TPC of a polycrystal usually needs to be mathematically represented by an exponential series as used in the prior work [28] and this thesis. In many circumstances, however, TPC statistics are not accurately measured due to the lack of a sufficient number of cross-sectional micrographs. In this case, the necessity of representing the measured TPC by an exponential series would not be crucial, and instead, it would be adequate to utilize a single exponential, $w_S(r) = e^{-r/a}$, to characterise the spatial variability of the sample. Note that the subscript ‘S’ is used here to distinguish this single exponential from the actual TPC function, $w(r)$, as measured from the sample. Also, such a simple representation is usually desirable in industrial applications for estimating the material properties of a sample by a simple inverse determination of its mean grain radius, a , from ultrasonic measurements.

The choice of the mean grain radius, a , is a vital step for the single exponential to deliver a satisfactory calculation of attenuation and velocity. In most prior studies on ultrasonic scattering, the mean line intercept a_1 was used as the parameter a . However, it will be shown below that this selection is far from optimal. To assess the selection of a , five lineal parameters are identified here for the mean grain radius and their goodness in representing attenuation and velocity will be evaluated in §7.4. The first parameter is the mean line intercept, a_1 , which has been used in several important studies [14, 50, 51]. However,

despite its relation to the actual TPC function by $a_1 = -1/w'(r=0)$, this parameter is not evidently related to scattering-induced attenuation and velocity dispersion. By contrast, the second parameter, the effective radius, as suggested by Weaver [17] is a well-recognized key parameter determining the level of attenuation in the low-frequency Rayleigh regime, see e.g., [21,26] and Equation 2.18 of this thesis. This effective radius is denoted as a_{ER} in this thesis and is related to the actual TPC function by

$$a_{\text{ER}} = \sqrt[3]{\frac{V_{\text{eff}}^{\text{g}}}{8\pi}} = \sqrt[3]{\frac{\int w(r) \text{d}r^3}{8\pi}}, \quad (7.7)$$

where $V_{\text{eff}}^{\text{g}} = \int w(r) \text{d}r^3$ is the effective volume of the grains. The third parameter is the correlation length, $a_{\text{CL}} = \int_0^\infty w(r) \text{d}r = \bar{d}/2$, which is well understood to be the key microstructural quantity controlling the degree of attenuation in the high-frequency stochastic regime, as can be seen from Equation 2.26 of this thesis. The fourth parameter is the best-fit radius, a_{BF} , which is the coefficient of the single exponential, $w_{\text{S}}(r) = e^{-r/a_{\text{BF}}}$, that best fits the actual TPC. Although a variety of algorithms are suitable for the fitting, this thesis uses an unweighted least-squares approach to determine the best-fit radius a_{BF} . In contrast to the first four parameters, the fifth parameter is not directly related to the actual TPC function. This parameter is the equivalent spherical radius R and is defined as the average of the equivalent spherical radii of the grains, i.e.

$$R = \langle R_i \rangle_i = \left\langle \sqrt[3]{\frac{3v_i}{4\pi}} \right\rangle_i, \quad (7.8)$$

where $R_i = \sqrt[3]{3v_i/(4\pi)}$ is the radius of the sphere that has the same volume, v_i , as that of the grain i . Determining this parameter can be easily achieved for a numerical sample but is not as trivial for practical experimental samples. This is because the 3D volumes of individual grains cannot be simply determined from 2D cross-sectional measurements, and instead, complex stereological methods are required for the determination [88]. Also, it is useful to note that in most cases the mean equivalent circular radius of a cross-section is smaller than the mean equivalent spherical radius of the corresponding 3D sample. All five parameters are summarised in Table 7.3.

Three polycrystalline microstructures with the same number of grains per unit volume

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Table 7.3: Five potential parameters defined for the mean grain radius a of the single exponential $w_S(r) = e^{-r/a}$.

	Notation	Relation to the actual TPC $w(r)$
Mean line intercept	a_l	$-1/w'(r = 0)$
Effective radius	a_{ER}	$\sqrt[3]{\int w(r)dr^3/(8\pi)}$
Correlation length	a_{CL}	$\int_0^\infty w(r) dr$
Best-fit radius	a_{BF}	$e^{-r/a_{BF}}$ best fits $w(r)$
Equivalent spherical radius	R	-

but different grain uniformities, as illustrated in Figure 7.6(a), are generated to evaluate the five selected parameters. The three microstructures are generated respectively by the Laguerre, Poisson Voronoi, and centroidal Voronoi tessellations [52, 89, 90]. The Poisson Voronoi tessellation (PVT) has been used throughout this thesis to create polycrystalline models. This method utilizes a Poisson point process to drop random seeds into model space and then generates seamless, non-overlapping grains under the conditions that each grain encloses a seed and all points in a grain are closer to its own seed than to any other. As would be expected from the central limit theorem, the equivalent spherical radii of the grains are normally distributed, as can be seen from Figure 7.6(b). In comparison to the PVT, the seeds of the Laguerre tessellation are weighted in order to create more complex microstructures [89, 90]. This method is used to generate the type of microstructure as commonly found in applications [13] in which case the equivalent spherical radii of the grains follow the lognormal distribution, as shown in Figure 7.6(b). The centroidal Voronoi tessellation (CVT) iteratively changes the locations of its seeds in order to achieve a uniform distribution of grains. The equivalent spherical radii of the generated grains follow a much narrower normal distribution than that of the PVT.

The TPC statistics of the three microstructures are plotted in Figure 7.6(c) as connected points. These statistics are measured with the cross-sectional approach by randomly choosing 1000 z -direction cross-sections from each model and performing 1000 random tests on each cross-section to determine every single TPC point. As can be seen from the shown statistics, the likelihood of having a long autocorrelation distance becomes smaller as grain uniformity increases. The thick lines in the figure are the mathematical fits of the

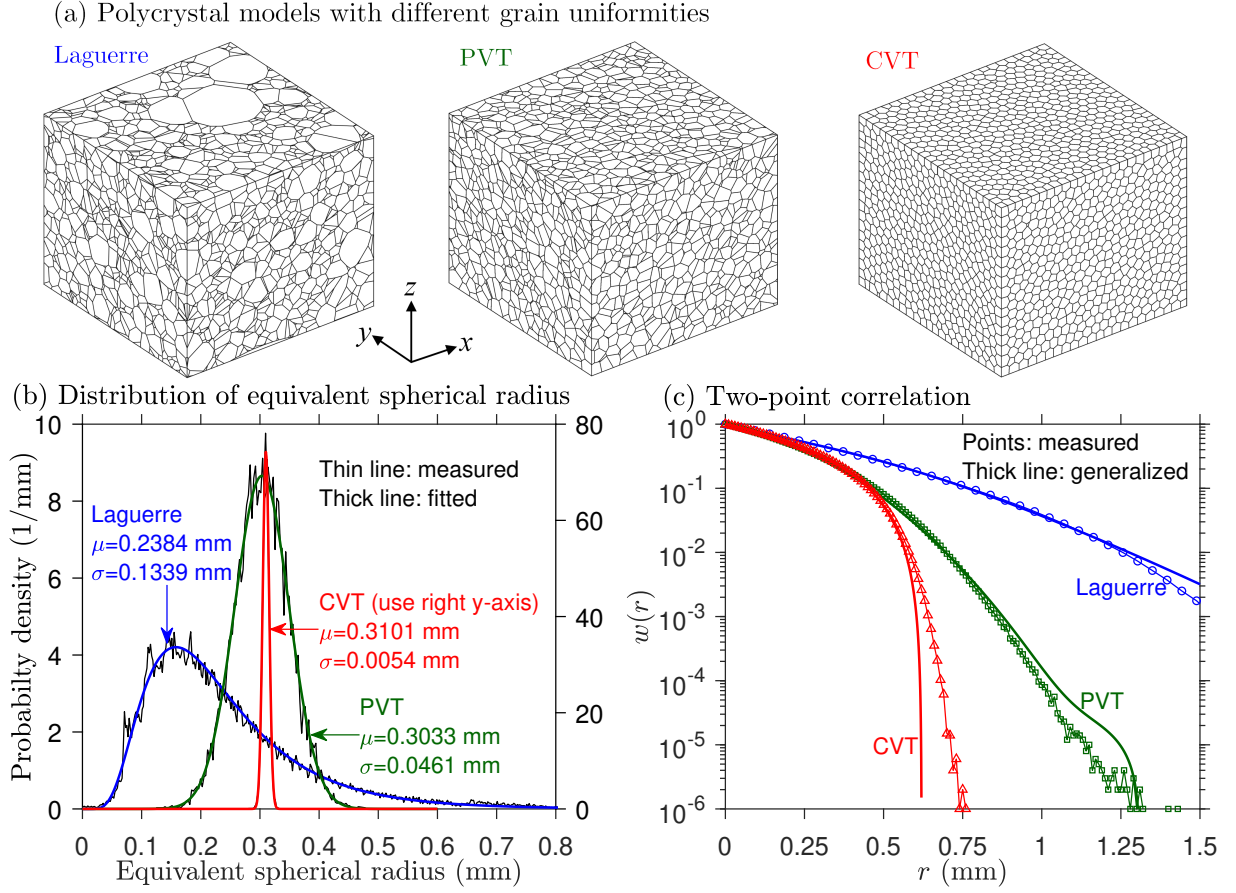


Figure 7.6: Three polycrystalline microstructures of different grain uniformities: (a) illustration of grain structure, (b) probability density of the equivalent spherical radii of the grains, and (c) two-point correlation statistics. The three microstructures are generated by the Laguerre, Poisson Voronoi (PVT), and centroidal Voronoi (CVT) tessellations. Each microstructural model has 11520 grains and has the dimensions of $12 \times 12 \times 10$ mm in the three coordinate directions. The data points of the Laguerre case in (b) are fitted to the lognormal distribution, while the other two cases are fitted to the normal distribution.

TPC points and the fitted expressions are provided in Table 7.4. Similarly to the PVT case that has been fitted earlier in §3.6, the Laguerre case is fitted to the same multi-term exponential form, $w(r) = \sum_{i=1}^8 A_i e^{-r/a_i}$. Obtaining the same fit is difficult for the CVT case, so it uses an alternative function [50,91,92]

$$w(r) = \begin{cases} 1 - 3r/(4R) + r^3/(16R^3), & 0 \leq r \leq 2R \\ 0, & r > 2R \end{cases}, \quad (7.9)$$

where R is the equivalent spherical radius of the grains, as defined above. The figure shows a very good agreement between the fitted functions and the measured TPC statistics.

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Following the prior work [28], the fitted functions are called the generalized TPC functions below.

Table 7.4: Generalized two-point correlation functions for the three polycrystalline microstructures of different grain uniformities.

Laguerre	$w(r) = \sum_{i=1}^8 A_i e^{-r/a_i}$								
	i	1	2	3	4	5	6	7	8
	A_i	-2713.43	-35.09	4017.09	-3579.02	474.15	377.42	428.05	1031.83
	a_i (mm)	0.1329	0.1443	0.1352	0.1446	0.1437	0.1449	0.1442	0.1509
PVT	$w(r) = \sum_{i=1}^8 A_i e^{-r/a_i}$, A_i and a_i are given in Table 3.3								
CVT	$w(r) = \begin{cases} 1 - 3r/(4R) + r^3/(16R^3), & 0 \leq r \leq 2R \\ 0, & r > 2R \end{cases}$, $R = 0.3101$ mm								

The five lineal parameters are calculated and provided in Table 7.5 for the three polycrystalline microstructures. The mean line intercept a_l , effective radius a_{ER} , and correlation length a_{CL} of each microstructure are analytically calculated from the respective generalized TPC function by using the relations given in Table 7.6. Since the generalized TPC functions match very well with the measured points in Figure 7.6(c), the analytical results only differ slightly from those numerically calculated from discrete TPC points. The best-fit radius a_{BF} of each microstructure is obtained by fitting to the measured TPC points, while the equivalent spherical radius is the mean value of the respective distribution in Figure 7.6(b).

Table 7.5: Differently defined mean grain radii (mm) for the three polycrystalline microstructures of different grain uniformities.

	Laguerre	PVT	CVT
Mean line intercept, a_l	0.4323	0.3458	0.4134
Effective radius, a_{ER}	0.3034	0.1793	0.1706
Correlation length, a_{CL}	0.3474	0.2309	0.2326
Best-fit radius, a_{BF}	0.3611	0.2431	0.2449
Equivalent spherical radius, R	0.2384	0.3033	0.3101

The single exponentials with the five differently defined mean grain radii are compared to the measured and generalized TPC functions in Figure 7.7. Overall, the single exponentials better describe an actual (measured or generalized) TPC when the grains of a

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Table 7.6: Relations of the mean line intercept, effective radius, and correlation length to the generalized TPC functions. Refer to Table 7.4 for the generalized TPC functions of the Laguerre, PVT and CVT cases.

	Laguerre and PVT	CVT
Mean line intercept, a_1	$1/\sum_i^8 (A_i/a_i)$	$4R/3$
Effective radius, a_{ER}	$\sqrt[3]{\sum_i^8 A_i a_i^3}$	$R/\sqrt[3]{6}$
Correlation length, a_{CL}	$\sum_i^8 A_i a_i$	$3R/4$

polycrystal are less uniform. The best and worst representations are achieved, respectively, for the Laguerre and CVT microstructures, which form the two extreme cases of this work. The three microstructures represent the typical scenarios where a single exponential can describe the actual TPC to the best, modest, and worst extents, respectively. Therefore, they are suitable for evaluating the goodness of the lineal parameters in delivering attenuation and velocity predictions in the next step.

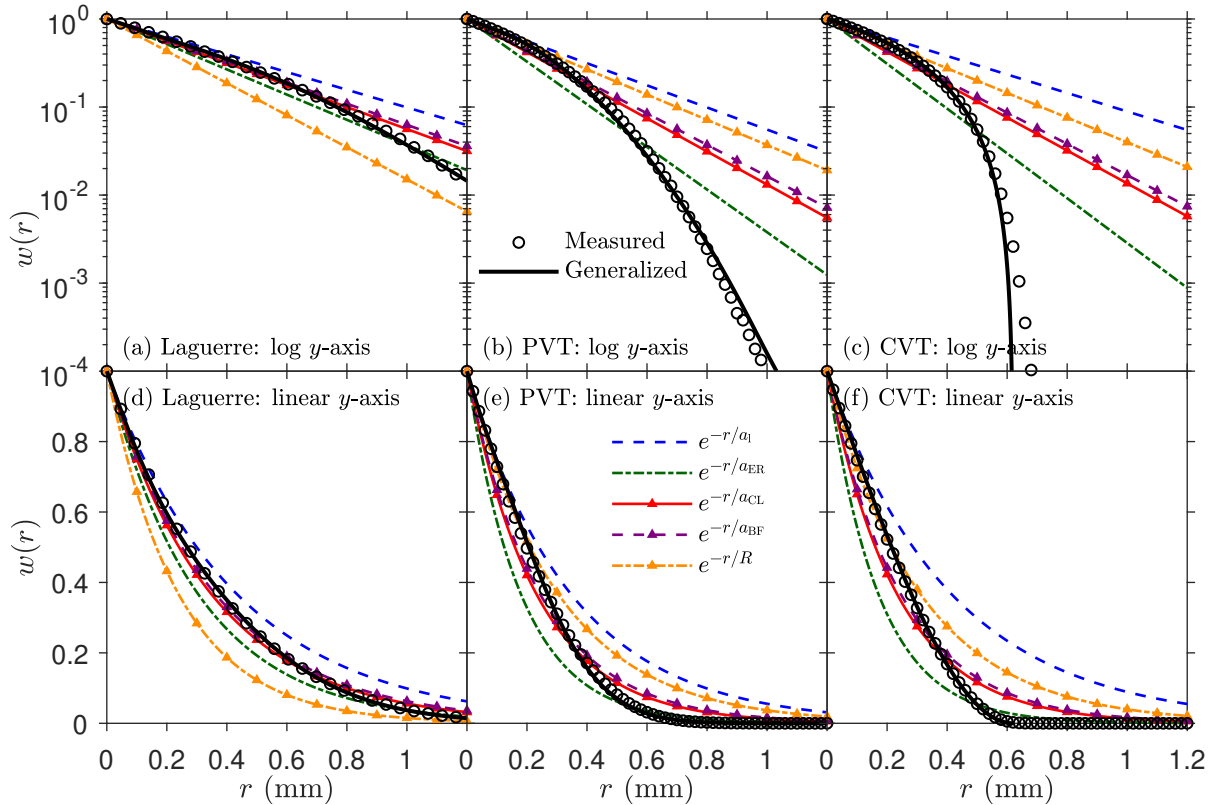


Figure 7.7: Comparison of the single exponentials $e^{-r/a}$ with differently defined mean grain radii a to the measured and generalized TPC functions for the Laguerre, PVT and CVT microstructures. Refer to Table 7.5 for the values of the five lineal parameters: a_1 , a_{ER} , a_{CL} , a_{BF} , and R .

For all three microstructure cases, the exponential e^{-r/a_1} , whose slope at $r = 0$ is the same as that of the actual TPC, defines the upper bound of the five single exponentials. Consistently for all microstructures, the exponential $e^{-r/a_{BF}}$ lies slightly above $e^{-r/a_{CL}}$, while $e^{-r/a_{ER}}$ rests further below the latter. It is useful to emphasise that the integral (namely, the correlation length) of $e^{-r/a_{CL}}$ and the triple integral (i.e., the effective grain volume) of $e^{-r/a_{ER}}$ are equal to the respective integrals of the actual TPC. The exponential $e^{-r/R}$ varies across different microstructures: it defines the lower bound for the Laguerre case but lies just below the topmost e^{-r/a_1} for the PVT and CVT cases.

7.4 Optimal parameter for the single exponential

This section proceeds to choose an optimal mean grain radius a from the above-identified lineal parameters in order for the single exponential $w_S(r) = e^{-r/a}$ to deliver the best calculation of attenuation and phase velocity.

With the use of the single exponential, the theoretically calculated attenuation and velocity are plotted in Figure 7.8 in comparison with the more accurate theoretical predictions from the generalized TPC functions and the results of 3D FE simulations. The results are given for plane longitudinal waves in equiaxed CSP, whose material properties are provided in Table 3.2. The normalised frequency, $2k_{0L}a$, is used for the x -axis of each panel and the normalisation factor a corresponds to the mean line intercept a_1 . The y -axis of each left panel represents the normalised longitudinal attenuation, $2\alpha_L a$, while that of each right panel denotes the normalised variation in phase velocity V_L from the Voigt velocity V_{0L} . The FE simulation of each microstructure employs three models, N115200, N11520 and N16000, with different dimensions and numbers of grains to minimise numerical errors. The model parameters are given in Table 3.1, and the three different microstructures of the model N11520 are illustrated in Figure 7.6(a). A combination of 15 realizations is used for each modelling case to obtain converged results; the average is shown as points in the figure while the standard deviation is not provided since the corresponding error bar is smaller than the size of the point markers. For the Laguerre and PVT microstructures, the SOA model is utilized for theoretical predictions. For the CVT microstructure, however, the convergence of numerical integration in the SOA model is

made difficult by its generalized TPC function, Equation 7.9, and therefore the simpler Born approximation is used for this case.

The theoretical predictions from the generalized TPC functions agree very well with the FEM results, and the NRMSDs between them amount to 7.20%, 9.06%, and 10.40% in attenuation and 0.08%, 0.12%, and 0.09% in phase velocity for the three microstructures. As a result of the good agreement, these theoretical predictions will be used below as reference to choose the optimal parameter for the single exponential. Note that an oscillatory behaviour is observable from the theoretical curve in the high-frequency range of the CVT case, inset in Figure 7.8(e). This behaviour was also observed in FE results by Rzyzy et al. [39] and was attributed to the resonance of waves within the uniform grains; however, this oscillation does not appear in the FE results of this work, the reason for which will be investigated in future work.

It is observable from Figure 7.8 that the single exponential delivers different attenuation and phase velocity for each microstructure when using different lineal parameters as the mean grain radius a . It is important to emphasise that these theoretical curves will be overlapped if they are differently normalised by using their respective lineal parameters as the normalisation factor a in the figure. For phase velocity, the use of a larger a simply results in the transition of scattering into a more strongly scattering regime at a lower frequency. This influence is more evident in the middle-frequency dispersive region and is negligible in the nondispersive Rayleigh and stochastic regimes due to the independence of phase velocity on grain size, as can be seen from Equations 2.23 and 2.30. Nonetheless, the various phase velocity curves for each microstructure only differ slightly from each other and it may be difficult to detect such differences in actual experiments; therefore, phase velocity is not utilized below to evaluate the goodness of the lineal parameters.

In contrast to phase velocity, attenuation can differ substantially with the use of different lineal parameters in the single exponential. In the shown frequency ranges in Figure 7.8, this difference is most significant in the low-frequency Rayleigh regime. This is because the longitudinal attenuation in this regime has a cubic dependence on the mean grain radius a . This dependence is described by the Rayleigh attenuation asymptote, Equation

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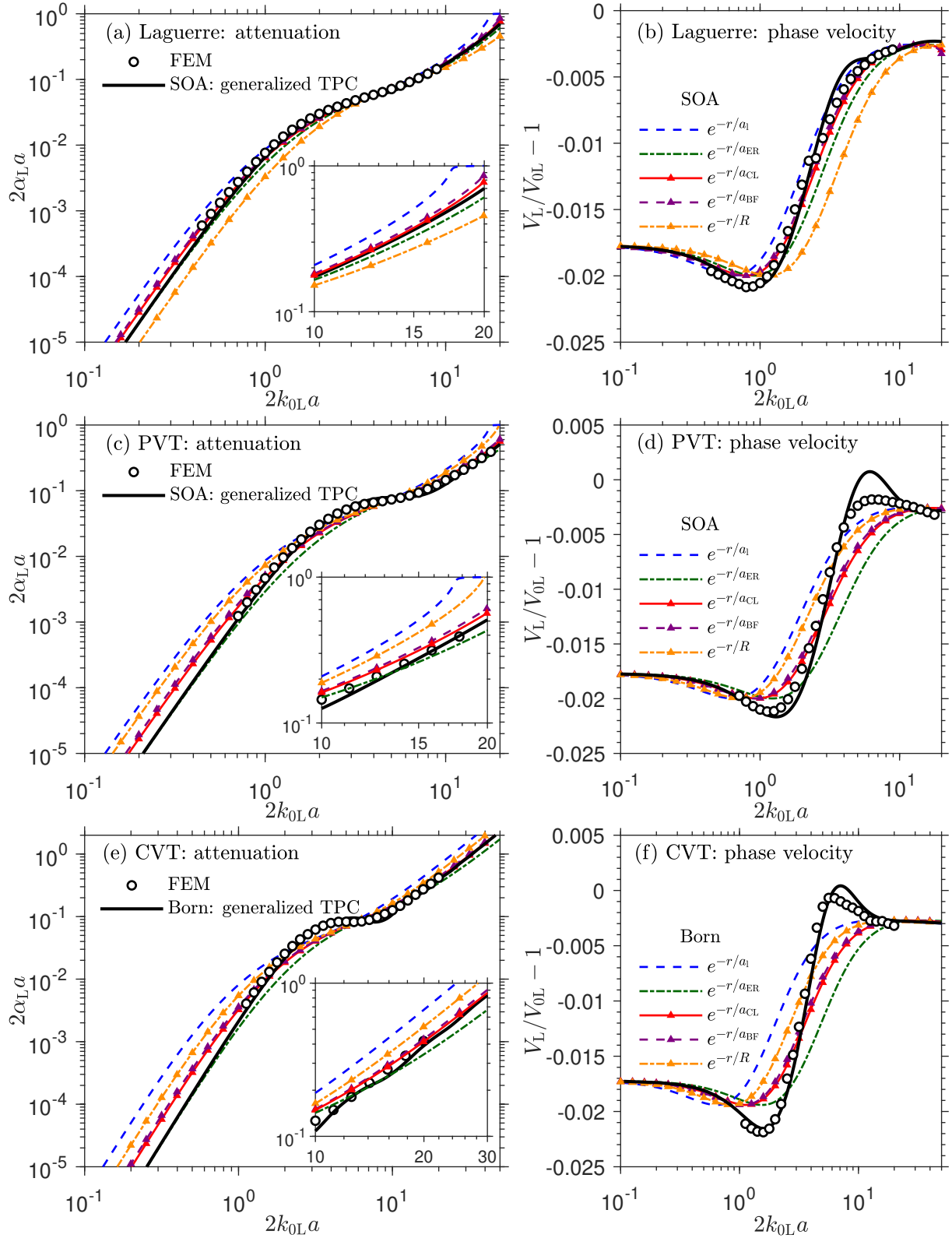


Figure 7.8: Normalised attenuation (a, c, e) and phase velocity (b, d, f) versus normalised frequency for longitudinal waves in equiaxed polycrystalline CSP with the Laguerre, PVT and CVT microstructures, comparing different theoretical predictions with numerical FEM results. The mean line intercept a_1 of each microstructure is used as the normalisation factor a . The left and right panels use the same legends.

2.18, which is rewritten below as

$$\alpha_L^R = \frac{1}{2\pi} k_{0L}^4 V_{\text{eff}}^g \left(Q_{LL}^* + \frac{V_{0L}^3}{V_{0T}^3} Q_{L \rightarrow T} \right), \quad (7.10)$$

where the effective volume of the grains is given by $V_{\text{eff}}^g = 8\pi a^3$ for a single exponential $w_S(r) = e^{-r/a}$. For a given material and a given frequency, the Rayleigh attenuation asymptote is solely determined by V_{eff}^g because the rest parameters in the equation are constant. The effective grain volumes of individual single exponentials are provided in Table 7.7 for all three microstructures alongside those of the generalized TPC functions. A frequency that falls into the Rayleigh regime is chosen for each microstructure, and at the chosen frequency, the theoretically predicted attenuation is given in the table for the various TPC functions. With the predictions from the generalized TPC functions as reference, it is found that a single exponential produces a more accurate attenuation if its effective grain volume is closer to that of the respective generalized TPC. The exponential $e^{-r/a_{\text{ER}}}$ delivers the most accurate prediction because its effective volume is exactly the same as that of the generalized TPC. The predictions of the exponentials $e^{-r/a_{\text{CL}}}$ and $e^{-r/a_{\text{BF}}}$ may be acceptable in practice, but those of e^{-r/a_1} and $e^{-r/R}$ deviate too much from the respective reference value, especially for the PVT and CVT microstructures.

The attenuation predictions from the single exponentials also differ greatly from the reference curves in the high-frequency stochastic regime. In this regime, the attenuation asymptote is given by Equation 2.26, which is repeated below as

$$\alpha_L^S = k_{0L}^2 a_{\text{eff}} Q_{L \rightarrow T}, \quad (7.11)$$

where the correlation length of the grains is given by $a_{\text{eff}} = a$ for a single exponential $w_S(r) = e^{-r/a}$. The correlation lengths of the various TPC functions are summarised in Table 7.7 and attenuation predictions are also provided in the table for each microstructure at a chosen frequency that roughly falls into the stochastic regime. Unsurprisingly, the exponential $e^{-r/a_{\text{CL}}}$ performs the best in this regime because it has the same correlation length as that of the generalized, reference TPC. The exponentials $e^{-r/a_{\text{ER}}}$ and $e^{-r/a_{\text{BF}}}$ may be treated as satisfactory in this regard, while e^{-r/a_1} and $e^{-r/R}$ are less appealing.

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Table 7.7: Longitudinal waves in equiaxed polycrystalline CSP with the Laguerre, PVT and CVT microstructures, comparing generalized TPC functions with single exponentials of differently defined mean grain radii. Two normalised frequencies, $2k_{0L}a$, are chosen from the Rayleigh and stochastic regimes for each microstructure, and the respective characteristic parameters (effective grain volume V_{eff}^g and correlation length a_{eff}) and normalised attenuation values are given for the chosen frequencies. The attenuation results are extracted from the theoretical curves shown in Figure 7.8, and the results of the single exponentials are given as relative deviations to those of the respective generalized TPC functions. The last column provides the normalised root-mean-square deviation (NRMSD) in theoretical attenuation from single exponentials to their respective generalized TPC functions over the frequency ranges shown in Figure 7.8.

	TPC	Rayleigh, at $2k_{0L}a = 0.3$		Stochastic, at $2k_{0L}a = 18$		NRMSD
		V_{eff}^g (mm ³)	$2\alpha_{La}$	a_{CL} (mm)	$2\alpha_{La}$	
Laguerre	Generalized	0.7021	9.6380×10^{-5}	0.3474	0.5402	-
	e^{-r/a_I}	+189.10%	+148.49%	+24.43%	+82.81%	42.83%
	$e^{-r/a_{ER}}$	+0.00%	-4.41%	-12.65%	-11.75%	10.46%
	$e^{-r/a_{CL}}$	+50.07%	+38.79%	+0.00%	+6.25%	8.91%
	$e^{-r/a_{BF}}$	+68.50%	+54.13%	+3.94%	+13.34%	12.66%
	$e^{-r/R}$	-51.51%	-51.66%	-31.38%	-30.83%	24.48%
	TPC	Rayleigh, at $2k_{0L}a = 0.3$		Stochastic, at $2k_{0L}a = 18$		NRMSD
		V_{eff}^g (mm ³)	$2\alpha_{La}$	a_{CL} (mm)	$2\alpha_{La}$	
PVT	Generalized	0.1449	4.0593×10^{-5}	0.2309	0.4061	-
	e^{-r/a_I}	+616.83%	+490.28%	+49.74%	+143.13%	107.52%
	$e^{-r/a_{ER}}$	+0.00%	-3.72%	-22.34%	-12.48%	18.81%
	$e^{-r/a_{CL}}$	+113.50%	+97.56%	+0.00%	+10.79%	25.08%
	$e^{-r/a_{BF}}$	+149.01%	+127.99%	+5.26%	+17.58%	30.42%
	$e^{-r/R}$	+384.01%	+317.81%	+31.37%	+65.78%	70.12%
	TPC	Rayleigh, at $2k_{0L}a = 0.3$		Stochastic, at $2k_{0L}a = 22$		NRMSD
		V_{eff}^g (mm ³)	$2\alpha_{La}$	a_{CL} (mm)	$2\alpha_{La}$	
CVT	Generalized	0.1249	1.9611×10^{-5}	0.2326	0.4622	-
	e^{-r/a_I}	+1322.22%	+1055.18%	+77.78%	+74.22%	129.40%
	$e^{-r/a_{ER}}$	+0.00%	-2.67%	-26.62%	-13.91%	22.05%
	$e^{-r/a_{CL}}$	+153.13%	+138.16%	+0.00%	+6.26%	21.05%
	$e^{-r/a_{BF}}$	+195.45%	+175.81%	+5.29%	+10.58%	25.38%
	$e^{-r/R}$	+500.00%	+434.32%	+33.33%	+34.46%	58.34%

Now it is clear that the effective radius a_{ER} and the correlation length a_{CL} are the best choices for the single exponential to deliver a good calculation of attenuation for the low- and high-frequency ranges [50], respectively. However, it is usually desirable to achieve a good quality of calculation for the whole, measurable frequency range. For this purpose, the NRMSDs in attenuation from the single exponentials to their respective generalized

TPC functions are calculated across the shown frequency ranges in Figure 7.8 and the results are provided in Table 7.7. In this case, the best choice varies between a_{ER} and a_{CL} depending on microstructure. Nonetheless, the effective radius, a_{ER} , is selected in this work as the optimal parameter for the single exponential because its attenuation prediction consistently agrees very well with the reference result in individual frequency ranges as well as across the whole frequency range for all microstructures.

7.5 Summary

This chapter attempts to represent the two-point correlation (TPC) of an equiaxed polycrystal by a single exponential function. This is to address the practical need of performing a rapid but fairly accurate calculation of attenuation and velocity based on not-so-accurate TPC data measured from a small sample set. The main work is to choose an optimal parameter for the single exponential such that the spatial variability of the medium can be best described by the exponential function and the attenuation and velocity of the propagating wave can then be best predicted.

This chapter first studies the three measurable probability functions, namely the two-point correlation function and the distributions of line intercept and free path, that can describe the spatial variability of polycrystals. An ideal 3D volumetric approach and a practical cross-sectional approach are utilized to measure these functions. The latter approach is found to be very effective in measuring volumetric statistics when using a significant number of cross-sections and tests, and the convergence study suggests that 100 cross-sections may be sufficient for achieving a satisfactory convergence. Actual measurements are used to demonstrate the important relations between the three functions which allow the TPC function to be determined by measuring either of the other two. Also, the characteristic parameters of the line intercept and free path distributions, i.e., the mean line intercept and the half of mean free path (also known as correlation length), are related to the slope at the origin and the integral of the TPC function, respectively.

Then, this chapter introduces the five potential parameters that can be used as the mean grain radius a in the single exponential, $w_S(r) = e^{-r/a}$. Four parameters are the char-

7. Representing spatial autocorrelation by a single exponential

acteristic lengths of the TPC function, with 1) the mean line intercept a_l relating to its slope at the origin, 2) the correlation length a_{CL} being its integral over r , 3) the effective radius a_{ER} relating to its triple integral over r , and 4) the best-fit radius a_{BF} being the coefficient of its best fit to the single exponential. The fifth parameter is the equivalent spherical radius R which needs to be determined by stereological methods. Three sets of equiaxed polycrystals with the same number of grains per unit volume but different grain uniformities are generated to demonstrate these lineal parameters. The three polycrystalline microstructures represent the typical scenarios where a single exponential can describe the actual TPC to the best, modest, and worst extents, respectively.

Lastly, this chapter evaluates the goodness of the single exponential in delivering attenuation and velocity predictions when using different lineal parameters. Longitudinal attenuation and phase velocity are calculated for the three microstructures by using theoretical models and 3D FE simulations. The theoretical predictions obtained from the actual, generalized TPC function agree very well with the results of the FE simulations, and they are thus used as reference to assess the predictions from the single exponentials. It is found that fairly accurate velocity results can be produced from the single exponential by using any of the five lineal parameters, while attenuation results are very sensitive to the choice of parameter. It is discovered that the effective radius a_{ER} and the correlation length a_{CL} are the best choices for low- and high-frequency ranges, but the former is the best overall choice for the single exponential to deliver an accurate prediction of attenuation in the whole frequency range for all three microstructures.

In conclusion, the effective radius a_{ER} is the optimal parameter selected in this chapter for the single exponential. Practically, this means that the discrete TPC function $w(r)$ needs to be first measured from the cross-sectional micrographs of a sample. The measurement is then used to determine the effective radius by $a_{ER} = \int w(r)dr^3$ via discrete numerical integration. Fairly accurate attenuation and phase velocity results will eventually be obtained by inserting the single exponential $w_S(r) = e^{-r/a_{ER}}$ into a theoretical model for prediction. On the contrary, the a parameter inversely determined from attenuation and phase velocity measurements would most closely represent the effective radius of the grains when using the single exponential $w_S(r) = e^{-r/a}$ as the basis function for inversion.

Chapter 8

Elastic waves in polycrystals can have three modes

8.1 Introduction

It is a common knowledge that one longitudinal and two transverse modes exist in a homogeneous elastic solid while only one longitudinal acoustic mode can be found in a fluid. There is no doubt that the situation would be much more complex for random inhomogeneous media. For a fluid-saturated porous medium for example, it was theoretically predicted by Biot [93, 94] and later experimentally observed by Plona [95] that two bulk longitudinal modes co-exist in the medium, with the fast mode travelling predominantly in the solid and the slow mode propagating primarily in the liquid. A similar finding was experimentally discovered [96] and then theoretically explained [97] for colloidal suspensions in which case two longitudinal modes occur in the high-frequency regime: the velocity of the first mode is between those of the solid and fluid phases, while the second mode is even slower than the fluid and was interpreted as a coupled interfacial Stoneley wave [96, 97]. The occurrence of two longitudinal modes has since been widely found in a variety of random media containing fluids, and particularly, in trabecular bones [98–100]. For random polycrystalline media, prior theoretical studies [23, 26] have disclosed the co-existence of two longitudinal modes at high frequencies that have similar levels of attenuation but greatly differing phase velocities. The same studies have also demonstrated

the occurrence of two transverse modes. The experimental and numerical studies so far, however, have observed only one mode, see e.g. [13, 14, 17, 28, 29, 38, 39], and no evidence has been found for the second mode. This may be because these studies have not reached a high enough frequency where the second mode is prominent.

Although the occurrence of the second mode is still in doubt, the theoretical study of this thesis has discovered a third mode for either longitudinal or transverse waves in polycrystals. The purpose of this chapter is to report this new finding and discuss the possibility of three modes co-existing in actual wave propagation problems. This chapter is first devoted to the study of a simpler scalar case in §8.2. This scalar case is formulated by considering only longitudinal wave scattering and neglecting the contribution of mode-converted scattering in the dispersion equation. Whereas it is an ideal, unphysical case, its study forms the basis for the more complex elastic case as addressed in §8.3 and facilitates the interpretation of the latter. This part of work is in preparation for a short communication [P7].

8.2 Two modes for scalar wave approximation in polycrystals

The dispersion equation for scalar waves in polycrystals is given by Equation 2.1 by considering only the $L \rightarrow L$ term in the total mass operator; i.e., $m_L = m_{L \rightarrow L}$. In the SOA model, the mass operator $m_{L \rightarrow L}$ is provided in Equation 2.2. Two solutions can be found from this equation for the perturbed wave number k , representing two propagation modes of the wave. Example solutions are given in Figure 8.1 as solid lines for polycrystalline iron with equiaxed grains. The polycrystal is statistically isotropic and macroscopically homogeneous, and its microstructure is described by a single-term TPC function; i.e., $w(r) = \exp(-r/a)$, $a = 0.25$ mm. The polycrystal is of cubic single-crystal symmetry with $c_{11} = 219.2$ GPa, $c_{12} = 136.8$ GPa, $c_{44} = 109.2$ GPa, and $\rho = 7860$ kg/m³. The left and right panels show respectively the imaginary and real parts of k , $\alpha_L = \text{Im}k$ and $V_L = \omega/\text{Re}k$, as normalised by the mean grain diameter $2a$ and the Voigt velocity V_{0L} ; they are plotted versus normalised frequency $2k_{0L}a$.

The existence of the two modes can be more explicitly illustrated by the FFA model. The mass operator $m_{L \rightarrow L}$ of this model has a simple expression for equiaxed polycrystals

$$m_{L \rightarrow L} = \frac{-8\pi a^2 k^2 V_{0L}^2 k_{0L}^2 Q_{L \rightarrow L}}{a^2 k^2 - (i + a k_{0L})^2}. \quad (8.1)$$

With the substitution of this mass operator, the dispersion equation can be rewritten as

$$\frac{A_4 k^4 + A_2 k^2 + A_0}{a^2 k^2 - (i + a k_{0L})^2} = 0, \quad (8.2)$$

where

$$\begin{aligned} A_4 &= -a^2 V_{0L}^2, \\ A_2 &= 8\pi a^2 V_{0L}^2 k_{0L}^2 Q_{L \rightarrow L} + (i + a k_{0L})^2 V_{0L}^2 + a^2 \omega^2, \\ A_0 &= -(i + a k_{0L})^2 \omega^2. \end{aligned} \quad (8.3)$$

The numerator of Equation 8.2 is a quadratic function of k^2 , meaning that two pairs of solutions can be obtained for k from the FFA model. The two solutions with positive real and imaginary parts are chosen because they represent forward-propagating wave modes. For polycrystalline iron, the two solutions are provided in Figure 8.1 as dash lines. These solutions agree very well with those of the SOA model at all frequencies for both attenuation and phase velocity. While the FFA solutions are analytically solved, those of the SOA model are numerically obtained by using a variant of the Newton's method. A difficulty arises in this numerical method to find a solution that is close to a pole. This difficulty has resulted in the absence of the second SOA solution in Figure 8.1 in the low-frequency range. This is because the second solution in this range is in close proximity to one of the poles of the dispersion equation, which is estimated to be $k = k_{0L} + i1/a$ from the denominator of Equation 8.2.

It is observable from both the SOA and FFA models that the two solutions are approximately symmetric about $k = k_{0L} + i1/(2a)$. This is exhibited as the vertical symmetry of attenuation about $2\alpha_L a = 1$ as can be clearly seen from the inset of panel (a), and it is also shown as the symmetry of phase velocity about $V_L/V_{0L} - 1 \approx 0$ in panel (b).

A distinctive feature of the first mode is that its phase velocity at the low-frequency

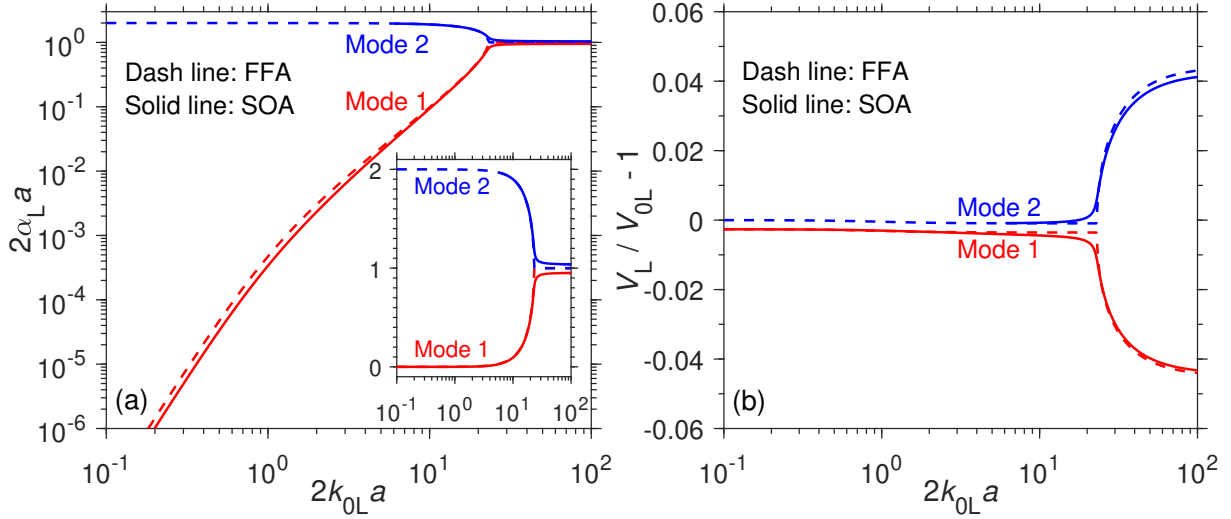


Figure 8.1: Two modes for scalar waves in polycrystalline iron with equiaxed grains: (a) attenuation and (b) phase velocity. For the first mode of the FFA model, its phase velocity has been corrected by adding a constant $V_L^R - V_{0L}$, where V_L^R is the Rayleigh velocity limit; see details in §2.4.

Rayleigh limit, V_L^R , is larger than that of the high-frequency geometric limit, V_L^G . This contradicts the Kramers-Kronig causality relations which require an opposite relationship of $V_L^R < V_L^G$ [101]. It was shown [23] that the causality relations are very well satisfied by the combination of the two modes for scalar waves in two-phase random media. Similarly, it is reasonable to believe that the two scalar modes in random polycrystals also collectively obey the causality relations, owing to their close analogy to those in two-phase random media. This suggests that the two modes may physically co-exist for scalar waves in polycrystals.

Although two modes may co-exist, the amplitude of the second mode is negligible as compared to that of the first mode in the low- to intermediate-frequency range where wave scattering is generally studied in physical experiments and numerical simulations. The dominance of the first mode can be revealed by the spectral function of the mean Green's function, which allows for the identification of the relative amplitudes of propagating modes. The spectral function (SF) is defined as the imaginary part of the mean Green's function [23]

$$\text{SF}(\omega, k) = -\text{Im}(\langle G(\omega, k) \rangle) = -\text{Im}\left(\frac{V_{0L}^2}{\omega^2 - k^2 V_{0L}^2 - m_L}\right), \quad (8.4)$$

where the perturbed wave number k is considered to be on the real axis. The denominator $\omega^2 - k^2 V_{0L}^2 - m_L$ is the dispersion function. By varying the two independent variables ω and k , the SF surface of polycrystalline iron is calculated and plotted in Figure 8.2(a). ω and k are represented, respectively, by the horizontal, $k_{0L} = \omega/V_{0L}$, and vertical, $V_L = \omega/k$, axes in the figure. The SF varies over several orders of magnitude in the plotted range, and thus at each frequency ω , it is normalised by the corresponding maximum value. This enables the visualisation of the two modes and the identification of their amplitude contributions. Normalised SF curves are also provided in panels (b-d) for the normalised frequencies of 1, 100, and 1000.

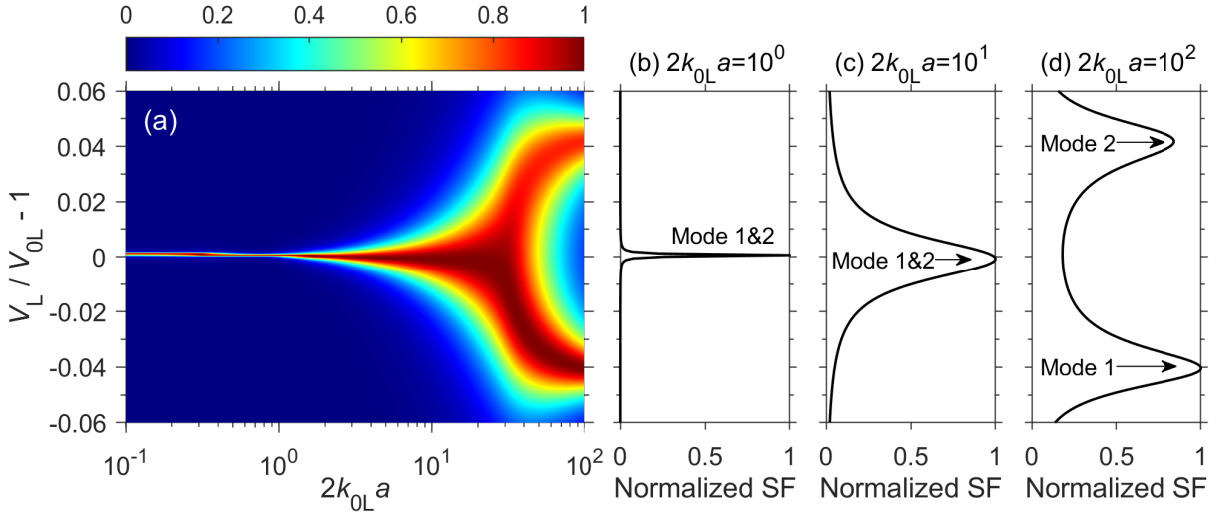


Figure 8.2: Normalised spectral function (SF) for scalar waves in polycrystalline iron with equiaxed grains. (a) shows normalised SF against normalised frequency (horizontal x -axis) and phase velocity (vertical y -axis), while (b-d) provides details for the normalised frequencies of 1, 100, and 1000.

At low frequencies below $2k_{0L}a \approx 20$, the two modes have very similar phase velocities and are thus located at nearly the same positions with respect to the vertical axis. A further calculation of the relative amplitudes of the two modes (by fitting $\sum_{i=1}^2 A_i / \{[(\text{Re}k_i)^2 - (\text{Im}k_i)^2 - k_{0L}^2]^2 + (2\text{Re}k_i\text{Im}k_i)^2\}$ to SF data, where A_i is the amplitude of mode i) reveals that the second mode has a negligible amplitude as compared to the first mode. The amplitude proportion of the second mode becomes larger as frequency further increases, and it gets very close to that of the first mode at the normalised frequency of 100 as shown in panel (d).

8.3 Three modes for elastic waves in polycrystals

8.3.1 Occurrence of three modes

For the propagation of elastic longitudinal waves in equiaxed polycrystals, its dispersion equation involves two mass operators, $m_{L \rightarrow L}$ and $m_{L \rightarrow T}$. In the FFA model, they have closed-form expressions for equiaxed polycrystals

$$m_{L \rightarrow N} = \frac{-8\pi a^2 k^2 V_{0L}^2 k_{0N}^2 Q_{L \rightarrow N}}{a^2 k^2 - (i + a k_{0N})^2}. \quad (8.5)$$

Substituting the total mass operator, $m_L = m_{L \rightarrow L} + m_{L \rightarrow T}$, into the dispersion equation (Equation 2.1) and rearranging the terms leads to

$$\frac{A_6 k^6 + A_4 k^4 + A_2 k^2 + A_0}{[a^2 k^2 - (i + a k_{0L})^2] [a^2 k^2 - (i + a k_{0T})^2]} = 0, \quad (8.6)$$

where

$$\begin{aligned} A_6 &= -a^4 V_{0L}^2, \\ A_4 &= a^2 q_{LL} + a^2 q_{LT} + a^2 p_L V_{0L}^2 + a^2 p_T V_{0L}^2 + a^4 \omega^2, \\ A_2 &= -p_T q_{LL} - p_L q_{LT} - p_L p_T V_{0L}^2 - a^2 p_L \omega^2 - a^2 p_T \omega^2, \\ A_0 &= p_L p_T \omega^2, \end{aligned} \quad (8.7)$$

and

$$\begin{aligned} p_L &= (i + a k_{0L})^2, \\ p_T &= (i + a k_{0T})^2, \\ q_{LL} &= 8\pi a^2 V_{0L}^2 k_{0L}^2 Q_{L \rightarrow L}, \\ q_{LT} &= 8\pi a^2 V_{0L}^2 k_{0T}^2 Q_{L \rightarrow T}. \end{aligned} \quad (8.8)$$

As a cubic function of k^2 , the numerator of Equation 8.6 delivers three pairs of solutions for k . Each pair has a solution with positive real and imaginary parts, representing a forward-propagating wave mode. Altogether, three forward-propagating modes can be found from the FFA model for longitudinal waves in polycrystals.

The three FFA solutions are provided as dash lines in Figure 8.3 for the same polycrystalline iron as used in §8.2. By using the FFA solutions as initial guesses, three SOA solutions are also numerically obtained and plotted as solid lines in the figure. Similarly to the second SOA solution of the scalar case, the second and third SOA solutions have not been found at low frequencies because they are very close to two of the poles of the dispersion equation ($k = k_{0L} + i1/a$ and $k = k_{0T} + i1/a$ as obtained from the denominator of Equation 8.6). The SOA and FFA models in general agree very well with each other across the whole frequency range for all three modes.

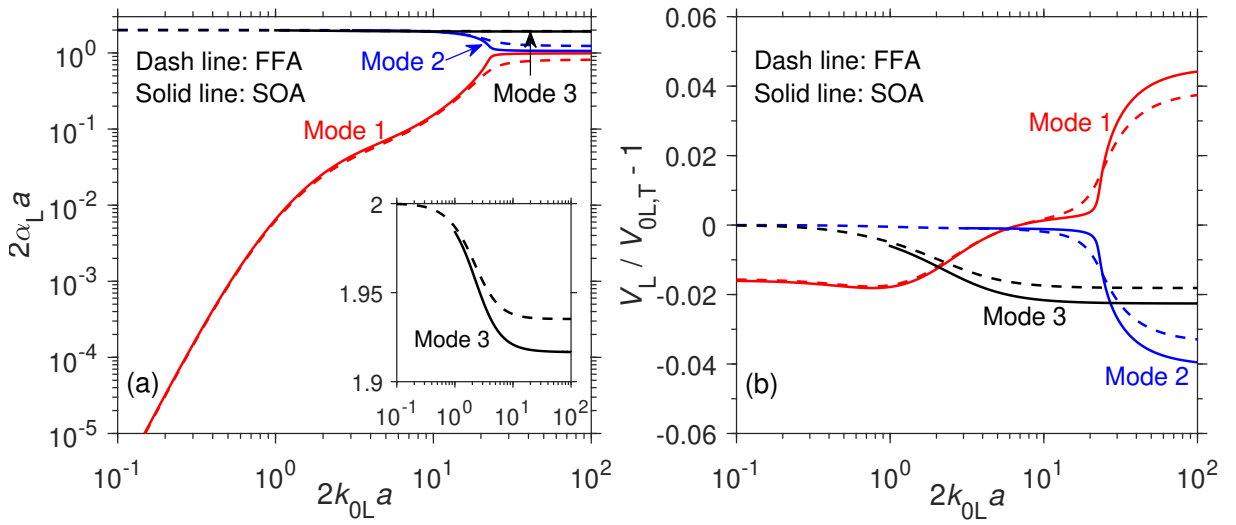


Figure 8.3: Three modes for longitudinal waves in polycrystalline iron with equiaxed grains: (a) attenuation and (b) phase velocity. For the first mode of the FFA model, its phase velocity has been corrected by adding a constant $V_L^R - V_{0L}$, where V_L^R is the Rayleigh velocity limit; see details in §2.4. The first and second modes in (b) are normalised by the longitudinal Voigt velocity V_{0L} , while the third mode is normalised by the transverse Voigt velocity V_{0T} .

Similarly to the scalar case, the first two modes are approximately symmetric about $k = k_{0L} + i1/(2a)$. Their attenuation rises and falls as frequency increases, respectively; they show independences on frequency when the high-frequency geometric regime sets in. Their phase velocities are close to the longitudinal Voigt velocity V_{0L} but the first mode shows a stronger dispersion in the low- to intermediate-frequency range than the second mode. The third mode exhibits a very high attenuation across the whole frequency range, and its phase velocity nearly coincides with the transverse Voigt velocity V_{0T} .

The three modes for transverse waves in equiaxed polycrystals can be similarly obtained from the FFA and SOA models. They are given in Figure 8.4 for polycrystalline iron.

8. Elastic waves in polycrystals can have three modes

The first two modes show an approximate symmetry about $k = k_{0T} + i1/(2a)$. In contrast to the longitudinal case, these two modes have phase velocities close to the transverse Voigt velocity V_{0T} . The third mode has a strong attenuation at all frequencies and has a phase velocity in close proximity to the longitudinal Voigt velocity V_{0L} . Its overall shape in phase velocity is similar to that of the first mode of the longitudinal case.

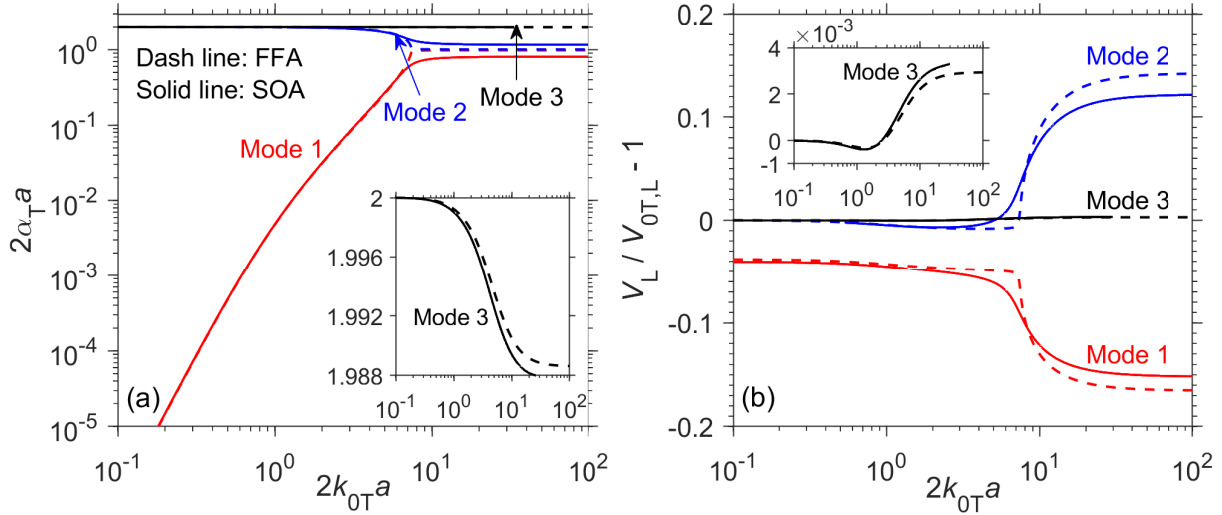


Figure 8.4: Three modes for transverse waves in polycrystalline iron with equiaxed grains: (a) attenuation and (b) phase velocity. For the first mode of the FFA model, its phase velocity has been corrected by adding a constant $V_T^R - V_{0T}$, where V_T^R is the Rayleigh velocity limit; see details in §2.4. The first and second modes in (b) are normalised by the transverse Voigt velocity V_{0T} , while the third mode is normalised by the longitudinal Voigt velocity V_{0L} .

8.3.2 Difficulty in observing the second and third modes

As mentioned in §8.1, only the first mode has been observed in actual experiments and numerical simulations. The lack of evidence for the other two modes may be due to their difficulty in observation, which is manifested in two aspects.

The first aspect is related to the strong attenuation of the second and third modes. These two modes are associated with strongly attenuated signals and high degrees of scattering-induced noises, and their wave signals are thus difficult to be measured within a reasonable level of signal-to-noise ratio. The first mode also involves such a measurement difficulty as frequency increases to a certain level where the coherent signal almost disappears.

The second aspect is due to the small amplitude proportions of the second and third

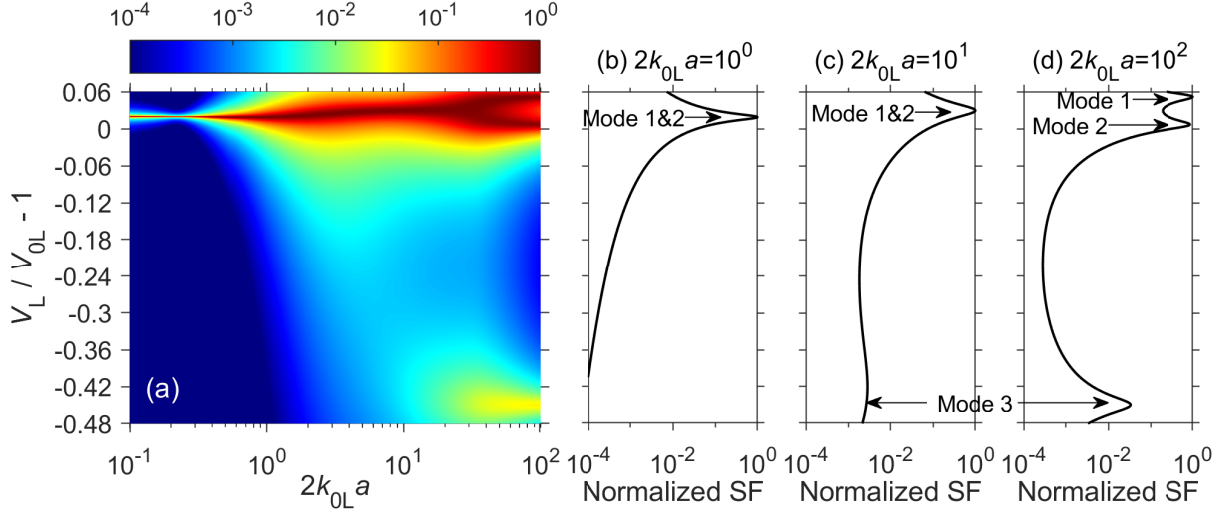


Figure 8.5: Normalised spectral function (SF) for longitudinal waves in polycrystalline iron with equiaxed grains. (a) shows the logarithm of normalised SF against normalised frequency (horizontal x -axis) and phase velocity (vertical y -axis), while (b-d) provides details at the normalised frequencies of 1, 100, and 1000.

modes. Using longitudinal waves as an example, the normalised spectral function (SF) surface of polycrystalline iron is shown in Figure 8.5. At low frequencies below $2k_{OL}a \approx 20$, the second mode co-exists with the first one and they are contained in the same SF peak. However, the amplitude of the second mode is negligible as compared to that of the first mode, which can be inferred from the analysis of amplitude contributions by fitting $\sum_{i=1}^3 A_i / \{[(\text{Re}k_i)^2 - (\text{Im}k_i)^2 - k_{OL}^2]^2 + (2\text{Re}k_i\text{Im}k_i)^2\}$ to SF data. The amplitude proportion of the second mode becomes larger as frequency increases and is comparable to that of the first mode at $2k_{OL}a = 100$. The third mode emerges only at very high frequencies. Its amplitude increases with frequency but is still an order of magnitude smaller than those of the first two modes at the highest frequency of $2k_{OL}a = 100$. Therefore, both the second and third modes have small amplitudes in the low- to intermediate-frequency ranges where actual experiments and numerical simulations are generally performed, and thus they have not been observed so far.

It is also interesting to note that the second and third modes for longitudinal waves (and the first mode for transverse waves) contradict the Kramers-Kronig causality relations by violating the required condition of $V_L^R < V_L^G$. It is speculated that the combination of all three modes may allow the causality relations to be fully satisfied.

8.4 Summary

This chapter reports the theoretical existence of three modes in the dispersion equation for either longitudinal or transverse waves in polycrystals and discusses the possibility of their co-existence in actual problems. The theoretical SOA and FFA models are employed for the study and the spatial autocorrelation of the polycrystals is represented by a single exponential.

The simpler scalar case, rather than the elastic case of interest, is first discussed. This case is formulated by considering only longitudinal wave scattering and neglecting the contribution of mode-converted scattering in the dispersion equation. It is found from the SOA and FFA models that two longitudinal modes occur in the considered scalar medium and their perturbed wave numbers are approximately symmetric about $k = k_{0L} + i1/(2a)$. The first mode evidently contradicts the Kramers-Kronig causality relations, and it is believed that the combination of both modes would naturally avoid this contradiction. It is shown from the spectral function analysis that the amplitude proportion of the second mode is only prominent at very high frequencies.

This chapter then investigates the elastic case. Both the SOA and FFA models reveal that three modes co-exist for either longitudinal or transverse waves in polycrystals. The longitudinal wave case is utilized for further discussions. The first two longitudinal modes are approximately symmetric about $k = k_{0L} + i1/(2a)$, while the third longitudinal mode has a phase velocity in close proximity to the transverse Voigt velocity, V_{0T} . There is a lack of evidence from actual experiments and simulations to support the existence of the last two modes. This is attributed to two possible reasons: the two modes are too strongly attenuated to be detected at a reasonable signal-to-noise ratio, and the amplitude proportions of the two modes are too small at ultrasonic frequencies as found from the spectral function analysis. Also, it is speculated that the three modes may collectively obey the causality relations.

Chapter 9

Conclusions

9.1 Thesis review

Chapter 2 describes the theoretical models for plane elastic wave propagation in polycrystals with statistically equiaxed and elongated grains of arbitrary crystal symmetry. The description is primarily performed for the second-order approximation (SOA) which has a second-order accuracy in material inhomogeneity and accounts for some possibilities of multiple scattering. The SOA model takes the elastic and geometric properties of the polycrystals, represented respectively by the elastic covariance and two-point correlation (TPC) function, as input and outputs scattering-induced attenuation and phase velocity dispersion. Then, the SOA model is simplified by invoking the Born approximation to obtain explicit expressions for attenuation and velocity. The resulting Born model only considers single scattering and it has a good agreement with the SOA model at low frequencies but gradually deviates from the SOA model as frequency increases and transits into the geometric regime. The analytical Rayleigh and stochastic asymptotes are derived from the Born model in order to gain closed-form insights into the wave behaviours. Lastly, this chapter describes the far-field approximation that is more computationally efficient but still maintains a very good accuracy when compared to the SOA model.

Chapter 3 presents the three-dimensional (3D) finite element (FE) method for simulating plane longitudinal waves in polycrystals with statistically equiaxed and elongated grains. The equiaxed grains of a polycrystal are generated with the Voronoi tessellation, while the

elongated grains are formed by stretching the equiaxed grains with the desired elongation ratio. Then, a created polycrystal model is discretized in space and time, and a plane longitudinal wave is initiated by applying uniformly distributed dynamic forces to all nodes on the transmitting surface and by prescribing symmetry boundary conditions (SBCs) to all outer surfaces that are parallel to the wave propagation direction. Coherent waves are monitored on the transmitting surface and its opposite receiving surface, and attenuation and phase velocity are determined by comparing the two coherent signals in the frequency domain. To enable a direct comparison with the theoretical models, the TPC function is directly measured from the FE material models and mathematically fitted into exponential series. Lastly, a modelling approach is provided to calculate the quasi-static limit of phase velocity.

Chapter 4 presents researches into maximising the accuracy of the 3D FE model. First, this chapter evaluates the through-transmission and fitting approaches for the determination of attenuation and phase velocity, and it is found that the two approaches are practically equivalent and can thus be used interchangeably. Then, this chapter performs thorough analytical and numerical studies to estimate the modelling errors and uncertainties as caused by FE approximations and statistical considerations. It is demonstrated that the errors and uncertainties can be well suppressed by using a proper combination of modelling parameters. Finally, an elaborated investigation is presented to assess the influence of SBCs on the theoretical calculation of attenuation and velocity. It shows that the theoretical calculation has a better agreement with the FE model if the SBCs effect is considered in the TPC function and incorporated into the adopted theoretical model.

Chapter 5 uses the theoretical and FE models to study plane longitudinal wave propagation in polycrystals with equiaxed grains of two extreme crystal symmetries, namely, cubic and triclinic. For cubic symmetry, eight materials with varying inhomogeneity factors are employed. The theoretical and FE results show that attenuation has fourth- and second-power dependences on frequency in the Rayleigh and stochastic regimes, while phase velocity is independent of frequency in both regimes. Both attenuation and the deviation of phase velocity to the Voigt velocity exhibit proportionalities to the inhomogeneity factors $Q_{L \rightarrow T}$ and $Q_{L \rightarrow L}$ in the Rayleigh and stochastic regimes, respectively. The difference between the theoretical and FE models has a quadratic relationship to the material

inhomogeneity factors. For triclinic symmetry, polycrystalline CSP is used to demonstrate the good agreement in attenuation and velocity between the SOA and FE models.

Chapter 6 uses the theoretical and FE models to study plane longitudinal wave propagation in polycrystals with statistically elongated grains. A quantitative agreement is found between the theoretical and FE models for all evaluated material cases. For attenuation, the FE simulations support the SOA model prediction that grain shape does not exert any influence on attenuation in the Rayleigh regime, and grain shape effect emerges as frequency increases to the stochastic regime, showing anisotropy in attenuation. This attenuation anisotropy intensifies with the increase of frequency and exhibits a complicated behaviour as frequency transits into the geometric regime. For phase velocity, it is nearly constant on frequency in the Rayleigh regime and exhibits dependence on propagation angle. In the stochastic regime, phase velocity behaves differently depending on propagation direction: it remains nearly constant in the grain shortened direction while decreases with frequency in the grain elongated direction. Also, both attenuation and directional velocity change show proportionalities to the two elastic scattering (inhomogeneity) factors.

Chapter 7 evaluates the possibility of representing the spatial autocorrelation of polycrystals by a single exponential. First, this chapter finds that the TPC function, line intercept distribution, and free path distribution are cross-related and they equally describe the spatial autocorrelation of a polycrystal. These probability functions can be measured with an ideal 3D volumetric approach and a practical cross-sectional approach, and a convergence study suggests that the latter can accurately measure volumetric statistics when a sufficiently large number of cross-sections and tests are used. Then, five lineal parameters are identified for the single exponential function to replace the actual TPC function: four parameters are the characteristic lengths of the TPC function, while the fifth is a parameter that can only be determined by stereological methods. Three sets of polycrystals are generated to demonstrate these lineal parameters, and the polycrystals have statistically equiaxed grains of different grain uniformities and represent three typical scenarios where a single exponential can describe the actual TPC to the best, modest, and worst extents. Finally, this chapter evaluates the goodness of the selected parameters in representing actual microstructure and in calculating attenuation and phase velocity. It is discovered that the effective radius a_{ER} is the best overall choice for the single exponential

to deliver an accurate prediction of attenuation and velocity in the whole frequency range for all three microstructures.

Chapter 8 reports the theoretical existence of three modes in the dispersion equation. Three solutions are found in the far-field approximation and the SOA model, indicating the possibility of three modes co-existing for longitudinal (or transverse) waves in polycrystals. A further study by the spectral function approach reveals that the two non-dominant modes are mostly not pronounced in comparison to the dominant mode, making their detection difficult in actual experimental and numerical studies.

9.2 Key contributions

This thesis has contributed mainly in six aspects.

1) This thesis has developed a theoretical SOA model for elastic wave propagation in polycrystals with statistically elongated grains. In contrast to prior theoretical studies addressing the same problem [11, 21, 24–26, 40–43], this SOA model has maintained the exact second-order accuracy in material inhomogeneity. This thesis has also derived a new representation for phase velocity in the Born approximation of the SOA model. This representation greatly simplifies velocity calculation by analytically evaluating the complex Cauchy integral, which has to certain extent prevented previous studies from calculating phase velocity. In addition, this thesis has derived a closed-form expression for the Rayleigh velocity asymptote and its two extremes with polycrystals having statistically infinitely-thin pancake-shaped and infinitely-long needle-shaped grains.

2) This thesis has advanced a 3D FE method for solving plane elastic wave propagation in the time domain. The first contribution in this regard is the generation of statistically elongated grains by stretching equiaxed ones, enabling the convenient, accurate determination of the TPC function of the elongated grains by scaling that of the equiaxed ones. The second contribution concerns the study of the accuracy of the FE method. This includes studying the difference between the through-transmission and fitting approaches in determining attenuation and phase velocity and establishing their equivalency. It also involves the comprehensive study of FE modelling errors and uncertainties and the offer-

ing of practical approaches to suppress them by using a proper combination of modelling parameters. Additionally, the contribution also encompasses the investigation of the SBCs effect and the proper consideration of this effect in the theoretical calculation of attenuation and velocity.

3) It has long been a great interest to evaluate when the theoretical models break down by their lack of representation of high-order material inhomogeneity terms. Such evaluation is achieved in this thesis by using the results of the high-quality FE modelling as reference data. With the use of eight cubic materials with equiaxed grains and greatly differing inhomogeneities, an increase in difference between the theoretical and FE models has been observed as material inhomogeneity becomes larger, and the difference is shown to have a quadratic relationship with material inhomogeneity.

4) Studying wave propagation in polycrystals with statistically elongated grains is practically important because the grains of most polycrystals in practice tend to be elongated [5, 10, 22, 40]. Prior studies [11, 21, 26, 40–43] were mostly focused on theoretical investigation and lacked quantitative experimental or numerical measurements to assess their theoretical findings. This thesis has made a step change towards studying this problem by using both theoretical predictions and numerical simulations. It is found that the theoretical SOA model has a surprisingly good agreement with the FE model for the studied polycrystals over a wide frequency range. The findings of this thesis are mostly consistent with those already known in the literature, especially the dependence of attenuation [11, 21, 41–43] and phase velocity [42, 43] on frequency and grain elongation. However, this thesis has additionally observed the decrease of phase velocity with frequency in the grain elongated direction in the stochastic regime, and the quantitative relations of attenuation and directional velocity change to the two elastic scattering (inhomogeneity) factors.

5) This thesis has attempted to represent the TPC of equiaxed polycrystals by a single exponential. This is a practical need for performing a rapid but fairly accurate calculation of attenuation and velocity based on not-so-accurate TPC data measured from a small number of cross-sections of a polycrystal sample. It is found that the effective grain radius a_{ER} is an optimal parameter for the single exponential, which can be determined

in experiments from the measured TPC function $w(r)$ by $a_{\text{ER}} = \int w(r)dr^3$ via discrete numerical integration. Also, this thesis has demonstrated the mutual relations between the TPC function, line intercept distribution, and free path distribution. This allows the TPC function to be determined by measuring either of the other two.

6) This thesis has, for the first time, reported the theoretical existence of three modes in the dispersion equation for either longitudinal or transverse waves in polycrystals and discussed the possibility of their co-existence in actual problems.

9.3 Future work

Following this thesis, two studies may be conducted in the future. The first study is to achieve the inverse characterisation of microstructure for polycrystals by using ultrasound. This thesis has established forward understanding and theoretical models to relate ultrasonic behaviours to microstructure and has demonstrated the great potential of using these models for inversion, so inversion is now feasible. As discussed in Chapter 1, such inverse characterisation is practically important because microstructural statistics, such as the size, shape and orientation of the grains, are key parameters determining the macroscopic properties of polycrystals, such as yield strength, fatigue, and creep. Measuring these statistics is desirable to ensure the required properties and structural integrity be met by the polycrystalline materials. This is especially important for safety-critical applications such as aerospace and nuclear.

The second study is to understand how ultrasonic waves interact with more complex polycrystals. This thesis has studied polycrystals with statistically equiaxed and elongated grains, but the materials have been assumed to be homogeneous on the macro scale and isotropic on average. The polycrystals in practice, however, may also exhibit microtexture regions, leading to inhomogeneity on the macro scale, and macrotexture, resulting in anisotropy on average. Thus, it is necessary to study the propagation of ultrasonic waves in such complex materials and establish forward models to describe the wave propagation behaviours in terms of attenuation and dispersion. Also, such forward study will facilitate microstructure characterisation for practical polycrystals of complex microstructure.

Appendix A

Voigt velocities, inner product coefficients, and elastic scattering factors

This appendix provides the expressions for the Voigt velocities, inner product coefficients, and elastic scattering factors of single-phase polycrystals that have untextured, isotropic properties in an ensemble average sense. The crystallographic symmetry of the grains is arbitrary. The elastic constants of the grains are denoted as c_{ij} that are contracted from the fourth-rank elastic tensor c_{ijkl} by using the Voigt convention: $11 \rightarrow 1$, $22 \rightarrow 2$, $33 \rightarrow 3$, $23 \rightarrow 4$, $13 \rightarrow 5$, and $12 \rightarrow 6$; a total of 21 independent constants exist for a triclinic crystal. The mass density of the grains is denoted as ρ .

The homogenised Voigt velocities are expressed as

$$\begin{aligned} V_{0L} &= \sqrt{[3(c_{11} + c_{22} + c_{33}) + 2(c_{23} + c_{13} + c_{12}) + 4(c_{44} + c_{55} + c_{66})]/(15\rho)}, \\ V_{0T} &= \sqrt{[(c_{11} + c_{22} + c_{33}) - (c_{23} + c_{13} + c_{12}) + 3(c_{44} + c_{55} + c_{66})]/(15\rho)}. \end{aligned} \tag{A.1}$$

For the A_{MN} , B_{MN} , and C_{MN} coefficients of the inner product $\text{IP}_{M \rightarrow N}$, the seven independent ones are given in Table A.1. The rest coefficients are related to the independent ones by $C_{LT} = C_{TL} = -C_{TT} = -C_{LL}$, $A_{TL} = A_{LT}$, $B_{TL} = B_{LT}$.

The elastic scattering factors are given by

$$Q_{M \rightarrow N} = \begin{cases} \frac{A_{MM} + B_{MM} + C_{MM}}{4\eta\rho^2 V_{0M}^4} & M = N \\ \frac{A_{MN} + B_{MN}/3 + C_{MN}/5}{4\eta\rho^2 V_{0M}^2 V_{0N}^2} & M \neq N \end{cases}, \quad (\text{A.2})$$

where the factor η takes the values of 1 and 2 for longitudinal ($M = \text{L}$) and transverse ($M = \text{T}$) propagating waves, respectively. The following elastic factors have also been used in this thesis to simplify the notation of the equations

$$Q_{MN}^* = \begin{cases} \frac{A_{MM} + B_{MM}/3 + C_{MM}/5}{4\eta\rho^2 V_{0M}^4} & M = N \\ \frac{A_{MN} + B_{MN} + C_{MN}}{4\eta\rho^2 V_{0M}^2 V_{0N}^2} & M \neq N \end{cases}. \quad (\text{A.3})$$

Care must be taken to differentiate them from the elastic scattering factors as defined in Equation A.2.

Table A.1: The A_{LL} , B_{LL} , C_{LL} , A_{LT} , B_{LT} , A_{TT} , and B_{TT} coefficients of the inner product. Multiplying the individual numbers listed in each column by the corresponding quadratic elastic constants in the first column and then taking the sum of the product leads to the expression for each coefficient. *Continue on next page.*

	A_{LL}	B_{LL}	C_{LL}	A_{LT}	B_{LT}	A_{TT}	B_{TT}
c_{11}^2	8	46	12	2	16	23	-9
$c_{11}c_{12}$	4	18	-24	0	-17	-46	18
$c_{11}c_{13}$	4	18	-24	0	-17	-46	18
$c_{11}c_{22}$	1	-43	-11	-1	-13	1	12
$c_{11}c_{23}$	-26	-42	46	-2	28	44	-42
$c_{11}c_{33}$	1	-43	-11	-1	-13	1	12
$c_{11}c_{44}$	28	-44	-68	0	-54	-42	66
$c_{11}c_{55}$	-32	16	32	-2	21	-27	-39
$c_{11}c_{66}$	-32	16	32	-2	21	-27	-39
c_{12}^2	83	-49	47	5	1	68	-39
$c_{12}c_{13}$	-74	52	-46	-4	2	-44	42
$c_{12}c_{22}$	4	18	-24	0	-17	-46	18
$c_{12}c_{23}$	-74	52	-46	-4	2	-44	42
$c_{12}c_{33}$	-26	-42	46	-2	28	44	-42
$c_{12}c_{44}$	52	-76	68	2	9	42	-66
$c_{12}c_{55}$	52	-76	68	2	9	42	-66
$c_{12}c_{66}$	-68	164	-132	0	-6	12	144
c_{13}^2	83	-49	47	5	1	68	-39
$c_{13}c_{22}$	-26	-42	46	-2	28	44	-42
$c_{13}c_{23}$	-74	52	-46	-4	2	-44	42
$c_{13}c_{33}$	4	18	-24	0	-17	-46	18
$c_{13}c_{44}$	52	-76	68	2	9	42	-66
$c_{13}c_{55}$	-68	164	-132	0	-6	12	144
$c_{13}c_{66}$	52	-76	68	2	9	42	-66
c_{14}^2	240	-150	140	14	0	180	-120
$c_{14}c_{24}$	60	120	-140	4	-90	-180	120
$c_{14}c_{34}$	60	120	-140	4	-90	-180	120
$c_{14}c_{56}$	-240	480	-400	-4	-30	-60	420
c_{15}^2	60	150	40	10	60	165	-15
$c_{15}c_{25}$	60	120	-140	4	-90	-180	120
$c_{15}c_{35}$	-60	240	60	0	60	-150	-90
$c_{15}c_{46}$	-120	120	200	-4	150	30	-210
c_{16}^2	60	150	40	10	60	165	-15
$c_{16}c_{26}$	-60	240	60	0	60	-150	-90
$c_{16}c_{36}$	60	120	-140	4	-90	-180	120
$c_{16}c_{45}$	-120	120	200	-4	150	30	-210
c_{22}^2	8	46	12	2	16	23	-9

Table A.1: *continued.*

	A_{LL}	B_{LL}	C_{LL}	A_{LT}	B_{LT}	A_{TT}	B_{TT}
$c_{22}c_{23}$	4	18	-24	0	-17	-46	18
$c_{22}c_{33}$	1	-43	-11	-1	-13	1	12
$c_{22}c_{44}$	-32	16	32	-2	21	-27	-39
$c_{55}c_{22}$	28	-44	-68	0	-54	-42	66
$c_{66}c_{22}$	-32	16	32	-2	21	-27	-39
c_{23}^2	83	-49	47	5	1	68	-39
$c_{23}c_{33}$	4	18	-24	0	-17	-46	18
$c_{23}c_{44}$	-68	164	-132	0	-6	12	144
$c_{55}c_{23}$	52	-76	68	2	9	42	-66
$c_{66}c_{23}$	52	-76	68	2	9	42	-66
c_{24}^2	60	150	40	10	60	165	-15
$c_{24}c_{34}$	-60	240	60	0	60	-150	-90
$c_{56}c_{24}$	-120	120	200	-4	150	30	-210
c_{25}^2	240	-150	140	14	0	180	-120
$c_{25}c_{35}$	60	120	-140	4	-90	-180	120
$c_{25}c_{46}$	-240	480	-400	-4	-30	-60	420
c_{26}^2	60	150	40	10	60	165	-15
$c_{26}c_{36}$	60	120	-140	4	-90	-180	120
$c_{26}c_{45}$	-120	120	200	-4	150	30	-210
c_{33}^2	8	46	12	2	16	23	-9
$c_{44}c_{33}$	-32	16	32	-2	21	-27	-39
$c_{55}c_{33}$	-32	16	32	-2	21	-27	-39
$c_{66}c_{33}$	28	-44	-68	0	-54	-42	66
c_{34}^2	60	150	40	10	60	165	-15
$c_{56}c_{34}$	-120	120	200	-4	150	30	-210
c_{35}^2	60	150	40	10	60	165	-15
$c_{46}c_{35}$	-120	120	200	-4	150	30	-210
c_{36}^2	240	-150	140	14	0	180	-120
$c_{45}c_{36}$	-240	480	-400	-4	-30	-60	420
c_{44}^2	92	-36	108	8	54	207	-81
$c_{55}c_{44}$	-56	48	-104	-4	-42	-111	93
$c_{66}c_{44}$	-56	48	-104	-4	-42	-111	93
c_{45}^2	240	-120	320	20	150	525	-255
c_{46}^2	240	-120	320	20	150	525	-255
c_{55}^2	92	-36	108	8	54	207	-81
$c_{66}c_{55}$	-56	48	-104	-4	-42	-111	93
c_{56}^2	240	-120	320	20	150	525	-255
c_{66}^2	92	-36	108	8	54	207	-81

Appendix B

Derivation of analytical asymptotes

B.1 Rayleigh attenuation asymptote

The Rayleigh asymptote for attenuation is derived based on the Born approximation. At the low-frequency Rayleigh limit, the wavelength is large compared to the average grain radius. Thus, the TPC function in Equation 2.7 can be simplified to $W_{M \rightarrow N}(k, \omega, \xi, \theta, \varphi) = \sum_{i=1}^n (A_i a_x^i a_y^i a_z^i) / \pi^2$ by neglecting the dimensionless wave number $q_x^2(a_x^i)^2 + q_y^2(a_y^i)^2 + q_z^2(a_z^i)^2$. For the attenuation component $\alpha_{M \rightarrow N}$ in Equation 2.18, the TPC function can now be pulled out of its double integral and the remaining integral can be obtained as $4\pi(A_{MN} + B_{MN}/3 + C_{MN}/5)$, leading to

$$\alpha_{M \rightarrow N} = \frac{\omega^4 \sum_{i=1}^n (A_i a_x^i a_y^i a_z^i) (A_{MN} + B_{MN}/3 + C_{MN}/5)}{\eta \rho^2 V_{0M}^3 V_{0N}^5}. \quad (\text{B.1})$$

By summing up the two components $\alpha_{M \rightarrow M}$ and $\alpha_{M \rightarrow N}$, the total attenuation for wave M in the low-frequency Rayleigh limit can be derived as

$$\alpha_M^R = \frac{1}{2\pi} k_{0M}^4 V_{\text{eff}}^g \left(Q_{MM}^* + \frac{V_{0M}^3}{V_{0N}^3} Q_{M \rightarrow N} \right), \quad (\text{B.2})$$

where $M, N \in \text{L, T}$ and $M \neq N$. $V_{\text{eff}}^g = 8\pi \sum_i A_i a_x^i a_y^i a_z^i$ is the effective grain volume. The mode-converted elastic scattering factor $Q_{M \rightarrow N}$ and the elastic factor Q_{MM}^* are given in Appendix A and they follow the same definition as Rokhlin et al. [26].

B.2 Rayleigh velocity asymptote

The derivation in this section is limited to elongated grains that are axially symmetric about the z -axis of the global coordinate system. In this case, the coefficients of the generalized two-point correlation (TPC) function in Equation 2.7 satisfy $a_x^i = a_y^i$, and an elongation ratio can be defined as $R_i = a_z^i/a_x^i$. In the Born approximation, the functions C_0^i , C_1^i and C_2^i in Equation 2.15 can thus be written in a simpler form as

$$\begin{aligned} C_0^i &= 1 + k_{0M}^2(a_x^i)^2[1 + (R_i^2 - 1)\cos^2\theta_p], \\ C_1^i &= 2k_{0M}k_{0N}(a_x^i)^2[\cos\theta_{ps} + (R_i^2 - 1)\cos\theta\cos\theta_p], \\ C_2^i &= k_{0N}^2(a_x^i)^2[1 + (R_i^2 - 1)\cos^2\theta]. \end{aligned} \quad (\text{B.3})$$

For the function C_0^i , its second term is bounded in the interval $[k_{0M}^2(a_x^i)^2, k_{0M}^2(a_z^i)^2]$ when $R_i \geq 1$ and in the inverted interval when $R_i < 1$. This function can thus be approximated as $C_0^i = 1$, because in the low-frequency Rayleigh regime the dimensionless wave number $k_{0M}a_x^i$ and $k_{0M}a_z^i$ are small. Similarly, the function C_2^i is bounded by $k_{0N}^2(a_x^i)^2$ and $k_{0N}^2(a_z^i)^2$, and thus $C_2^i \ll 1$ at the low-frequency limit. The function C_1^i is not always positive and its bounds can be given as $[-2k_{0M}k_{0N}(a_z^i)^2, 2k_{0M}k_{0N}(a_z^i)^2]$ and $[-2k_{0M}k_{0N}(2(a_x^i)^2 - (a_z^i)^2), -2k_{0M}k_{0N}(a_z^i)^2]$ for $R_i \geq 1$ and $R_i < 1$, respectively. The absolute value of C_1^i is always much smaller than unity in the Rayleigh limit.

Equation 2.14 can now be written as

$$\sum_{i=1}^n \frac{A_i a_x^i a_y^i a_z^i}{\pi^2} \text{P.V.} \int_0^\infty \frac{\xi^4}{(1 - \xi^2)(1 + C_2^i \xi^2)^2} \int_0^\pi \int_0^{2\pi} \frac{\text{IP}_{M \rightarrow N}(\theta, \varphi)}{\left[1 - \frac{C_1^i \xi}{1 + C_2^i \xi^2}\right]^2} \sin\theta d\varphi d\theta d\xi, \quad (\text{B.4})$$

where the factor $[1 - C_1^i \xi / (1 + C_2^i \xi^2)]^2$ can be approximated as unity. This conclusion is reached differently for different signs of the function C_1^i . When $C_1^i > 0$, the factor $C_1^i \xi / (1 + C_2^i \xi^2)$ is a positive function of ξ in the range of $[0, \infty]$. Its maximum occurs at $\xi = 1/\sqrt{C_2^i}$ and the maximum value is $C_1^i / (2\sqrt{C_2^i})$, which is smaller than unity according to the above-mentioned bounds of C_1^i and C_2^i . Thus, the factor $1/(1 - C_1^i \xi / (1 + C_2^i \xi^2))^2$ can be expressed in Taylor series as $\sum_{j=1}^\infty j [C_1^i \xi / (1 + C_2^i \xi^2)]^{j-1}$. By neglecting higher-order terms, the factor becomes unity. Similarly, the same conclusion can be reached for $C_1^i \leq 0$.

As a result, the double integral in Eq B.4 is independent of ξ and can be pull-out from the Cauchy integral, and it can be evaluated.

It is clear that the limit of the integrand $\xi^4 / [(1 - \xi^2)(1 + C_2^i \xi^2)^2]$ is approaching zero as ξ approaches infinity. This allows the Cauchy integral to be solved by the contour integral and residue theorem

$$\text{P.V.} \int_0^\infty \frac{\xi^4 d\xi}{(1 - \xi^2)(1 + C_2^i \xi^2)^2} = \frac{1}{2} \text{P.V.} \int_{-\infty}^\infty \frac{\xi^4 d\xi}{(1 - \xi^2)(1 + C_2^i \xi^2)^2} = \frac{-\pi(3C_2^i + 1)}{4(C_2^i + 1)^2(C_2^i)^{3/2}}. \quad (\text{B.5})$$

The result can be further simplified by taking the first term of its Taylor series (with respect to C_2^i), leading to the integral being given as $-\pi/4/(C_2^i)^{3/2}$. Substituting the result for the triple integral in Equation B.4 into Equation 2.13, the relative change of velocity is obtained as

$$\Delta_{M \rightarrow N} = \frac{1}{8\pi\eta\rho^2 V_{0M}^2 V_{0N}^2} \sum_{i=1}^n A_i R_i \int_0^\pi \int_0^{2\pi} \frac{\text{IP}_{M \rightarrow N}(\theta, \varphi)}{[1 + (R_i^2 - 1) \cos^2 \theta]^{3/2}} \sin \theta d\varphi d\theta. \quad (\text{B.6})$$

Evaluating the inner integration of Equation B.6 over φ and denoting $x = \cos \theta$ leads to

$$\Delta_{M \rightarrow N} = \frac{1}{8\pi\eta\rho^2 V_{0M}^2 V_{0N}^2} \sum_{i=1}^n A_i R_i \int_{-1}^1 \frac{\text{IP}_{M \rightarrow N}(x)}{D(x)} dx, \quad (\text{B.7})$$

where

$$\begin{aligned} \text{IP}_{M \rightarrow N}(x) &= \frac{\pi}{4}(q_0 + q_2 x^2 + q_4 x^4), \\ D(x) &= [1 + (R_i^2 - 1)x^2]^{3/2}, \end{aligned} \quad (\text{B.8})$$

and

$$\begin{aligned} q_0 &= 8A_{MN} + 4B_{MN} [1 - \cos^2 \theta_p] + 3C_{MN} [1 - 2\cos^2 \theta_p + \cos^4 \theta_p], \\ q_2 &= -4B_{MN} [1 - 3\cos^2 \theta_p] - 6C_{MN} [1 - 6\cos^2 \theta_p + 5\cos^4 \theta_p], \\ q_4 &= C_{MN} [3 - 30\cos^2 \theta_p + 35\cos^4 \theta_p]. \end{aligned} \quad (\text{B.9})$$

The single integral in Equation B.7 can be further evaluated and it leads to the final

expression as provided in Equation 2.20, §2.3.2.

B.3 Stochastic velocity asymptote

For polycrystals with equiaxed grains, the relative change of phase velocity $\Delta_{M \rightarrow N}$ is given by Equation 2.13 in the Born approximation. The factor $f_{M \rightarrow N}$ in the equation is expressed as

$$f_{M \rightarrow N}(k_{0M}, \omega, \xi, \theta, \varphi) = \sum_{i=1}^n \frac{\text{IP}_{M \rightarrow N}(\theta, \varphi) A_i a_i^3}{\pi^2 (1 + k_{0M}^2 a_i^2 - 2k_{0M} k_{0N} a_i^2 \cos \theta \xi + k_{0N}^2 a_i^2 \xi^2)^2}, \quad (\text{B.10})$$

where the inner product has the form of $\text{IP}_{M \rightarrow N}(\theta, \varphi) = A_{MN} + B_{MN} \cos^2 \theta + C_{MN} \cos^4 \theta$. It is clear that $f_{M \rightarrow N}$ is independent of angle φ , and the integral over φ in Equation 2.13 results in a constant value of 2π . By performing a variable substitution of $x \rightarrow \cos \theta$, Equation 2.13 can be rewritten as

$$\Delta_{M \rightarrow N} = \frac{-\omega^3}{\pi \eta \rho^2 V_{0M}^2 V_{0N}^5} \sum_{i=1}^n A_i a_i^3 \times \text{P.V.} \int_0^\infty \frac{\xi^4 d\xi}{1 - \xi^2} \int_{-1}^1 \frac{A_{MN} + B_{MN} x^2 + C_{MN} x^4}{(1 + k_{0M}^2 a_i^2 - 2k_{0M} k_{0N} a_i^2 x \xi + k_{0N}^2 a_i^2 \xi^2)^2} dx. \quad (\text{B.11})$$

Pulling x independent terms out of the inner integral leads to

$$\Delta_{M \rightarrow N} = \frac{-\omega^3}{\pi \eta \rho^2 V_{0M}^2 V_{0N}^5} \sum_{i=1}^n A_i a_i^3 \text{P.V.} \int_0^\infty \frac{\xi^4 d\xi}{(1 - \xi^2)(1 + k_{0M}^2 a_i^2 + k_{0N}^2 a_i^2 \xi^2)} \times \int_{-1}^1 \frac{A_{MN} + B_{MN} x^2 + C_{MN} x^4}{[1 - D(\xi)x]^2} dx, \quad (\text{B.12})$$

where $D(\xi) = 2k_{0M} k_{0N} a_i^2 \xi / (1 + k_{0M}^2 a_i^2 + k_{0N}^2 a_i^2 \xi^2)$. The denominator term $1/[1 - D(\xi)x]^2$ in the inner integral has a sharp peak at $x \rightarrow 1$ and $\xi \rightarrow 1$, while the numerator term $A_{MN} + B_{MN} x^2 + C_{MN} x^4$ is a smooth, relatively slowly changing function. Without loss of accuracy, the numerator can be pulled out of the integral and be replaced by its value

at $x = 1$, leading to

$$\Delta_{M \rightarrow N} \approx \frac{-\omega^3(A_{MN} + B_{MN} + C_{MN})}{\pi\eta\rho^2 V_{0M}^2 V_{0N}^5} \sum_{i=1}^n A_i a_i^3 \times \text{P.V.} \int_0^\infty \frac{\xi^4 d\xi}{(1-\xi^2)(1+k_{0M}^2 a_i^2 + k_{0N}^2 a_i^2 \xi^2)} \int_{-1}^1 \frac{1}{[1-D(\xi)x]^2} dx. \quad (\text{B.13})$$

The inner integral can now be evaluated and it results in

$$\Delta_{M \rightarrow N} = \frac{-\omega^3(A_{MN} + B_{MN} + C_{MN})}{\pi\eta\rho^2 V_{0M}^2 V_{0N}^5} \sum_{i=1}^n A_i a_i^3 \times \text{P.V.} \int_0^\infty \frac{\xi^4 d\xi}{(1-\xi^2)(1+k_{0M}^2 a_i^2 + k_{0N}^2 a_i^2 \xi^2)[1-D^2(\xi)]}. \quad (\text{B.14})$$

Substituting $D(\xi)$ into the equation and re-arranging it leads to

$$\Delta_{M \rightarrow N} = \frac{-\omega^3(A_{MN} + B_{MN} + C_{MN})}{\pi\eta\rho^2 V_{0M}^2 V_{0N}^5} \sum_{i=1}^n A_i a_i^3 \times \text{P.V.} \int_0^\infty \frac{\xi^4 d\xi}{(1-\xi^2)[(1+k_{0M}^2 a_i^2)^2 + 2k_{0N}^2 a_i^2(1-k_{0M}^2 a_i^2)\xi^2 + k_{0N}^4 a_i^4 \xi^4]}. \quad (\text{B.15})$$

The Cauchy integral can be explicitly solved by using the contour integration and the residue theorem. Under the conditions of $k_{0M} a_i \gg 1$ and $k_{0N} a_i \gg 1$, the solution is given by

$$\begin{aligned} & \text{P.V.} \int_0^\infty \frac{\xi^4 d\xi}{(1-\xi^2)[(1+k_{0M}^2 a_i^2)^2 + 2k_{0N}^2 a_i^2(1-k_{0M}^2 a_i^2)\xi^2 + k_{0N}^4 a_i^4 \xi^4]} \\ &= \begin{cases} -5\pi/(16k_{0M}^3 a_i^3) & N = M \\ -\pi/[4k_{0N}^3 a_i^3(1-k_{0N}^2/k_{0M}^2)] & N \neq M \end{cases}. \end{aligned} \quad (\text{B.16})$$

Thus, the relative change of phase velocity can be obtained as

$$\Delta_{M \rightarrow N} = \begin{cases} \frac{5(A_{MM} + B_{MM} + C_{MM})}{8\eta\rho^2 V_{0M}^4} & N = M \\ \frac{(A_{MN} + B_{MN} + C_{MN})}{2\eta\rho^2 V_{0M}^2 V_{0N}^2 (1 - V_{0M}^2/V_{0N}^2)} & N \neq M \end{cases}, \quad (\text{B.17})$$

which can be further simplified to the final expression given in Equation 2.29.

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List of Publications

Journal publications

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- [P5] M. Huang, S. I. Rokhlin, and M. J. S. Lowe, “Elastic wave propagation in polycrystals under conditions of strong scattering,” In preparation for submission to *Proc. R. Soc. A - Math. Phys. Eng. Sci.*
- [P6] M. Huang, S. I. Rokhlin, and M. J. S. Lowe, “Elastic waves in polycrystals: representing actual spatial autocorrelation by a single exponential” In preparation for submission to *Proc. R. Soc. A - Math. Phys. Eng. Sci.*

- [P7] M. Huang, S. I. Rokhlin, and M. J. S. Lowe, “Elastic waves in polycrystals can have three modes,” In preparation for submission to *J. Acoust. Soc. Am.*

Conference presentations

- [C1] M. Huang, G. Sha, A. Van Pamel, P. Huthwaite, S. I. Rokhlin, M. J. S. Lowe, “Finite element modelling of wave propagation in polycrystals”, at *Anglo-French Physical Acoustics Conference*, 17-19 Jan 2018, Surrey, UK.
- [C2] M. Huang, G. Sha, A. Van Pamel, P. Huthwaite, S. I. Rokhlin, M. J. S. Lowe, “Effect of grain elongation on wave propagation in polycrystalline materials”, at *45th Annual Review of Progress in Quantitative Nondestructive Evaluation*, 15-19 Jul 2018, Burlington, VT, USA.
- [C3] M. Huang, M. J. S. Lowe, G. Sha, S. I. Rokhlin, “Elastic wave propagation in polycrystals under conditions of strong scattering”, at *46th Annual Review of Progress in Quantitative Nondestructive Evaluation*, 15-18 Jul 2019, Portland, OR, USA.
- [C4] M. Huang, G. Sha, P. Huthwaite, S. I. Rokhlin, M. J. S. Lowe, “Elastic wave propagation in polycrystalline materials with elongated grains”, at *International Congress on Ultrasonics*, 3-6 Sep 2019, Bruges, Belgium.