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Understanding Elastic Wave Propagation Effects in Complex Polycrystalline Materials

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Declaration of Originality

I hereby declare that this thesis is the result of my own work, under the supervision of Professor Michael J.S. Lowe and Professor Bo Lan. All sources of information and data have been referenced and acknowledged accordingly.

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Abstract

The presence of macrozones, also referred to as micro-textured regions, in Ti-64 has been identified as a potential contributor to the onset of cold dwell fatigue, leading to a significant reduction in fatigue life. Previous studies have demonstrated the potential of ultrasonic testing for macrozone characterisation through variations in attenuation, backscatter, and wave velocity. However, due to the hierarchical complexity of the microstructure, several observed wave-microstructure interactions remain poorly understood.

In this work, a finite element polycrystalline modelling framework is developed to systematically investigate ultrasonic wave-macrozone interactions. Using two-dimensional idealised models, key correlations between macrozone characteristics, including size, shape, and crystallographic texture, and ultrasonic responses such as attenuation, backscatter, and wave velocity are identified through controlled parametric studies. These trends are subsequently validated experimentally, demonstrating how such systematic relationships may support the ultrasonic characterisation of macrozones in Ti-64 samples.

A complementary methodology for generating realistic synthetic macrozone models is then introduced, incorporating hierarchical microstructural information obtained from Electron Backscatter Diffraction scans. This approach enables the construction of representative microstructures that capture the statistical and morphological features observed in real materials, providing a physically faithful numerical environment for studying wave-macrozone interactions. Grain statistical information extracted from two-dimensional micrographs is used to synthesise representative grains and macrozones, which are validated using finite element wave propagation simulations and two-point correlation measurements.

Finally, the framework is extended into the geometric regime to investigate wave-microstructure interactions at higher frequencies using finite element models, with reference to analytical descriptions. This regime is relevant to macrozone characterisation as operation at higher frequencies offers the potential for improved spatial resolution and sensitivity to finer microstructural features. Overall, this study establishes a comprehensive framework for advancing the fundamental understanding and ultrasonic characterisation of macrozones in Ti-64 through controlled investigation of wave-microstructure interactions.

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List of Acronyms

2D	Two-Dimensional
3D	Three-Dimensional
ANOVA	Analysis of Variance
BCC	Body-Centred Cubic
CDF	Cold Dwell Fatigue
CFL	Courant-Friedrichs-Lewy
DOE	Design of Experiments
DOF	Degrees of Freedom
EBSD	Electron Backscatter Diffraction
FE	Finite Element
FOM	Figure of Merit
FWHM	Full Width at Half Maximum
HCP	Hexagonal Close-Packed
ISM	Independent Scattering Model
MDF	Misorientation Distribution Function
MTR	Macro-Textured Region

NDE	Non-Destructive Evaluation
ODF	Orientation Distribution Function
RMS	Root Mean Square
RUS	Resonant Ultrasound Spectroscopy
SOA	Second-Order Approximation
Ti-64	Titanium-6Al-4V
TOF	Time-of-Flight
TPC	Two-Point Correlation

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Chapter 1

Introduction

1.1 Industrial Motivation

Titanium-6Al-4V (Ti-64) is a widely used alloy in the aerospace sector, particularly in aircraft engines for components such as inlet fan blades and compressors. This preference is attributed to Ti-64's exceptional strength-to-weight ratio and excellent corrosion resistance, making it ideal for demanding environments and critical applications [1, 2]. However, these favourable mechanical properties are largely a result of the complex and sophisticated manufacturing processes required to produce the alloy. Given its application in critical engine components, ensuring the reliable performance of the Ti-64 alloy is crucial to meeting stringent aerospace safety and certification standards.

Conventionally, Ti-64 alloys undergo sample-based destructive testing during manufacturing to ensure that their mechanical properties meet the required standards. Ti-64 components within the aircraft engines are inspected periodically based on the estimated fatigue life calculated using established mechanistic models. However, the material is susceptible to Cold Dwell Fatigue (CDF), a phenomenon that significantly reduces fatigue life when the material is subjected to stress for an extended period at moderate temperatures [3], potentially leading to unexpected engine failures. Compared to other fatigue conditions, CDF is less understood and cannot be easily detected using conventional methods, necessitating more frequent inspections

for potential crack initiation sites. Consequently, this approach increases operational costs and may still fail to guarantee early detection.

There is growing evidence that macrozones, also known as Macro-Textured Region (MTR), are a potential contributing factor to CDF [4–6]. Macrozones originate from larger, recrystallised grains that are not fully broken down during thermo-mechanical processing, resulting in clusters of grains with a preferred C-axis orientation (direction parallel to the height of the hexagonal prism - [0001] axis). These macrozones can vary considerably in size, shape, and crystallographic orientation.

To evaluate such polycrystalline features at the micron level, sophisticated techniques such as Electron Backscatter Diffraction (EBSD) [5, 7] are required. EBSD, a scanning electron microscopy technique, analyses crystallographic orientations by detecting electron diffraction patterns. However, the technique involves laborious surface preparation and provides only surface-level information, capturing Two-Dimensional (2D) sections of inherently Three-Dimensional (3D) macrozones. Full microstructural characterisation would require serial sectioning along the depth, which is both time-consuming and costly.

Additionally, because EBSD is destructive in nature, it cannot be applied directly to in-service components but only to sacrificial samples, which are implicitly assumed to be representative of in-service components. This assumption may not always hold in practice, as localised microstructural features that are spatially heterogeneous can critically influence component behaviour and may not be captured through limited sampling, as highlighted by recent catastrophic engine failure investigations [8].

Therefore, there is a clear need for a Non-Destructive Evaluation (NDE) method capable of characterising such complex polycrystalline features in engineering components. Ultrasonic testing is a promising NDE technique due to its superior penetration depth compared to surface-based microstructural characterisation methods, as well as its relatively low operating and capital costs, making it well-suited for industrial applications.

The benefits of incorporating such an NDE method into manufacturing and in-service inspection workflows are multi-fold. First, it enhances the reliability of in-service inspections by enabling direct evaluation of Ti-64 components rather than relying on sacrificial samples. Next, ultrasonic testing can be integrated into manufacturing lines to provide early-stage screening of fabricated components, allowing potentially harmful microstructural features to be identified before components enter service. Hence, this direct and integrated inspection framework has the potential to reduce unnecessary inspection frequency by enabling condition-based assessment of microstructural risk at the component level, while simultaneously lowering the likelihood of CDF-related engine failures.

1.2 Aim and Scope

The aim of this thesis is to address the challenges associated with characterising macrozones using ultrasound. The complex combination of grains and macrozones - each with varying size distributions and morphologies - poses significant difficulties for reliable characterisation.

To tackle these challenges, the first step is to develop a deeper understanding of how macrozones interact with ultrasound. This is achieved through the use of Finite Element (FE) models, which provide an ideal platform for evaluating complex phenomena. Although empirical studies could be undertaken by fabricating samples with different macrozone characteristics, this approach is constrained by two major barriers: the manufacturing process is difficult to control, and full microstructural characterisation using EBSD requires numerous destructive tests.

Therefore, to systematically investigate wave-microstructure interactions, this study adopts a simplified polycrystalline 2D FE wave propagation modelling approach. A parametric study is conducted to evaluate the range of physical interactions between ultrasound waves and idealised macrozones. The modelling results are corroborated with analytical predictions and validated through water-immersion experiments, enabling the assessment of how well experimental observations can support the characterisation of macrozones in Ti-64.

In addition, a methodology for generating realistic synthetic microstructures is proposed, using actual 2D EBSD datasets as statistical references. The goal is to demonstrate the reliability and representativeness of this approach by replicating Ti-64 samples containing macrozones and examining their influence on ultrasound responses. Unlike the earlier work with idealised models, these realistic models yield results that are directly comparable to experimental data, provided the testing conditions are consistent. This framework lays the foundation for developing future inversion techniques capable of characterising macrozones from ultrasonic measurements.

Finally, this thesis investigates ultrasonic wave propagation in the geometric scattering regime, where the wavelength becomes smaller than the characteristic microstructural length scales. In this regime, coherent-wave descriptions break down and attenuation is governed by energy redistribution due to multiple scattering rather than coherent decay. Through numerical simulations, Chapter 5 examines the transition between scattering regimes, identifies fundamental limits on ultrasonic characterisation, and clarifies the physical interpretation of attenuation in highly scattering media. While such conditions represent an extreme operating regime, the analysis provides important insights into the information content of ultrasonic signals and establishes conceptual bounds relevant to macrozone characterisation.

1.3 Thesis Outline

Chapter 2 presents the literature review underpinning this thesis. It encompasses theoretical models developed to estimate elastic wave scattering in polycrystalline materials and macrozones, FE model configurations, and signal processing methods relevant to ultrasonic analysis.

Chapter 3 introduces the 2D FE methodology for simulating wave propagation in Ti-64 polycrystalline materials with varying macrozone characteristics, presented as a parametric study. This chapter provides physical insights into the scattering behaviours associated with macrozone interactions and identifies key factors that influence ultrasonic responses. Experimental investigations conducted on actual Ti-64 cubic samples validate the FE results and demonstrate their applicability for potential macrozone characterisation.

Chapter 4 examines the feasibility of representing actual Ti-64 samples using a synthetic microstructural approach. The process begins with the extraction of grain and macrozone statistics from EBSD datasets, followed by their integration into commercially available software to generate realistic synthetic microstructure. These synthetic features are then validated using FE simulations and Two-Point Correlation (TPC) measurements to ensure that both wave interactions and morphological features are accurately reproduced.

Chapter 5 investigates the scattering effects within the geometric regime, given the potential for large macrozones to extend scattering behaviour beyond the stochastic range. As the geometric regime remains relatively underexplored, 2D FE models are used to examine how the scattering characteristics vary with grain-to-wavelength ratio, propagation distance, and anisotropy factor.

Chapter 6 summarises the key findings and contributions of this thesis, discusses its limitations and industrial implications, and outlines avenues for future work and further development.

Chapter 2

Literature Review

This chapter provides detailed background information on polycrystalline microstructure and elastic wave propagation, followed by an overview of FE simulation framework and signal processing methods used in this study.

2.1 Polycrystalline Microstructures of Titanium Alloys

In this section, the fundamental microstructural terms used throughout the thesis are first introduced. The primary features of polycrystalline materials such as Ti-64 include phases, grain geometry (size and shape), and crystallographic orientation. A phase denotes a distinct crystal structure or composition, while a grain refers to a region of uniform crystallographic orientation. Variations in these microstructural characteristics lead to spatial variations in elastic stiffness, which in turn give rise to ultrasonic scattering.

2.1.1 Phase Composition

In a microstructural context, a phase refers to a homogeneous region within a system that has uniform properties. Multiple phases with distinct properties can coexist within a metallic alloy due to variations in chemical compositions, forming what are known as heterogeneous

systems. In addition to composition, the volume fraction of each phase also depends on the thermo-mechanical history of the alloy [9]. In practice, phase composition is often tailored to modify and enhance certain mechanical properties.

For instance, titanium (alloys) can contain varying volume fractions of α and β phases, depending on type and concentration of alloying elements added [10]. Since the α and β phases have different crystal structures, densities, and elastic properties, changes in their relative proportions significantly affect the macroscopic behaviour of the alloy.

Examples of titanium alloys with different phase compositions are listed in Table 2.1 from reference [11]. α titanium alloys generally exhibit low strength but offer excellent creep and corrosion resistance at elevated temperatures. In contrast, β titanium alloys possess high strength but poorer creep and corrosion resistance at high temperatures. Consequently, a dual-phase alloy that combines both α and β phases generates a well-balanced microstructure, achieving good strength alongside adequate creep and corrosion resistance at high temperatures.

Table 2.1: Titanium alloys with varying phase compositions and their respective properties.

Types of Alloys	Example	General Properties
α	Commercially Pure Titanium (CP-Ti)	– Low to medium strength levels – Cannot be easily heat treated to obtain higher strength – Good creep and corrosion resistance up to 650°C
$\alpha + \beta$	Ti-6Al-4V	– Contains approximately 10% of β phase – Medium to high strength levels – Good creep resistance up to 400°C
β	Ti-6Al-2Sn-4Zr-6Mo	– Contains more than 20% of β phase – Can be hardened easily to achieve high strength levels – Good creep resistance up to 300°C

Particularly for Ti-64, the alloy is classified as an α - β titanium alloy [11]. At room temperature, the microstructure typically consists of a dominant Hexagonal Close-Packed (HCP) α phase with a smaller fraction of retained Body-Centred Cubic (BCC) β phase distributed along prior β grain boundaries. The coexistence of these two phases arises from the combined effects of

alloying additions—aluminium stabilising the α phase and vanadium stabilising the β phase—and the thermal history during processing, particularly cooling from the high-temperature β field.

2.1.2 Grain Morphology

Metals can exhibit grains of varying sizes, shapes, and distributions, depending on the manufacturing conditions. As shown in Figure 2.1, during the crystallisation process, small grain nuclei form and grow at random locations. As these grains are oriented in random crystallographic orientations, their growth eventually becomes obstructed by the adjacent grains. These constraints form grain boundaries that determine the size, shape, and distribution of grains [12].

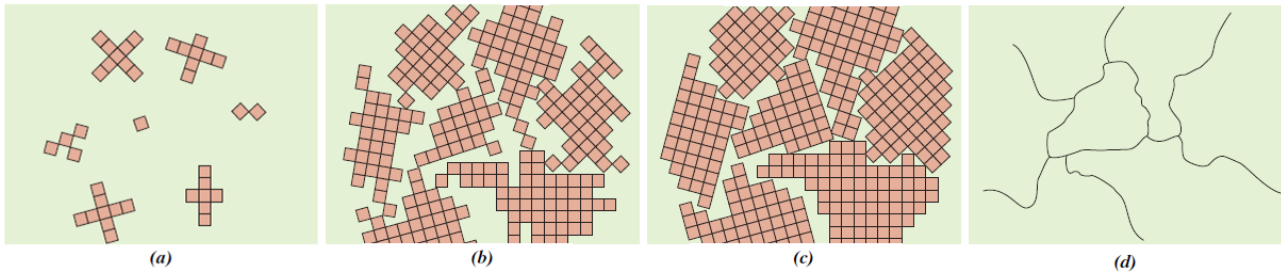


Figure 2.1: (a) Nucleation of grains, (b) grain growth, (c) irregular grains form as adjacent grains grow together, (d) grain boundaries formed upon complete solidification [12].

The two phases in Ti-64 alloy— α and β —each exhibits distinct grain morphologies [13]. Depending on the heat treatment and manufacturing conditions, the resulting grain morphology can differ drastically. As illustrated in Figure 2.2 (a) shows equiaxed α grains (white) with small fractions of β phases distributed along the α grain boundaries. (b) displays a Widmanstätten structure consisting of α platelets (white) in prior β grains. Lastly, (c) presents a bi-modal microstructure, where equiaxed α grains are surrounded by Widmanstätten platelets.

The Widmanstätten microstructure forms when the alloy is cooled from the high-temperature β phase field [13]. During this transformation, the α phase precipitates as thin platelets within the prior β grains following specific crystallographic orientation relationships. As a result, the crystallographic texture of the prior β grains is partially retained in the transformed α phase. When large prior β grains share similar orientations, this texture inheritance can give rise to

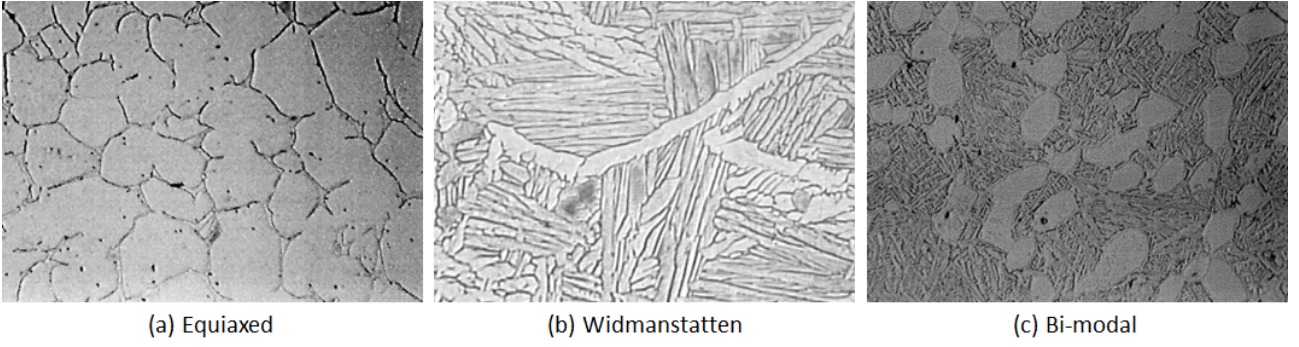


Figure 2.2: Possible grain morphologies in Ti-64 alloy: (a) equiaxed, (b) Widmanstätten, and (c) bi-modal structure, that are formed from varying heat treatment conditions [13].

extended regions of similarly oriented α platelets, commonly referred to as macrozones. These macrozones exhibit pronounced elastic anisotropy and are therefore of particular relevance to ultrasonic wave propagation and fatigue behaviour.

Typically, metals with smaller grain sizes exhibit higher tensile strength and fatigue resistance due to the increased number of grain boundaries that act as barriers to dislocations, and vice versa [14]. Therefore, obtaining an accurate measure of grain size is essential to provide reliable estimates of a metal's mechanical properties. For equiaxed (statistically spherical) grains, the mean grain size can be quantified using the TPC function [15]:

$$W(r) = e^{-r/L} \quad (2.1)$$

where r is the correlation distance, L is the spatially averaged correlation length, and $W(r)$ is the probability that two points separated by a distance r are located in the same grain.

In practice, the TPC function provides a statistical description of how material properties are spatially correlated within a polycrystalline medium. Specifically, it characterises the probability that two spatial points belong to the same grain as a function of their separation distance, thereby encoding information about average grain size, size distribution, and grain morphology. In analytical ultrasonic scattering models, the TPC function enters the formulation of attenuation and backscatter by governing the spatial correlation of elastic property fluctuations. As a result, the TPC serves as a compact statistical representation of the microstructure, enabling

complex grain morphologies to be incorporated into wave propagation models without explicitly resolving individual grains.

2.1.3 Crystal Elasticity

Each grain consists of a crystal structure that depends on the arrangement of atoms within it. Common crystal structures include cubic, tetragonal, orthorhombic, and hexagonal lattices [12]. In Ti-64, the α phase exhibits a HCP structure, whereas the β phase adopts a BCC structure, as shown in Figure 2.3.

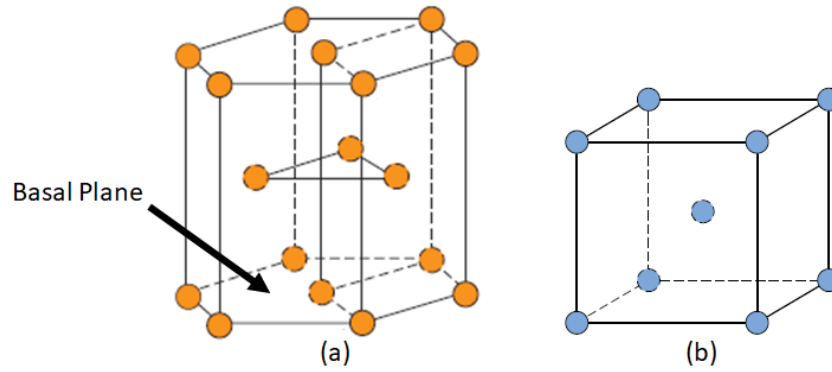


Figure 2.3: Crystal structures of the two phases in Ti-64, (a) HCP crystal structure for α phase, and (b) BCC crystal structure for β phase [12].

According to Hooke's law, the crystal structure deforms proportionally to the applied stress.

In 3D, Hooke's law is expressed as:

$$\sigma_{ij} = \sum_{k=1}^3 \sum_{l=1}^3 C_{ijkl} \epsilon_{kl} \quad (2.2)$$

where σ and ϵ represent stress and strain tensors, respectively, C is the elastic stiffness coefficients, and the subscripts i, j, k, l refer to the tensor directions [16]. Because of tensor symmetry—where off-diagonal components are equal (e.g., $C_{ijkl} = C_{ijlk} = C_{jikl} = C_{jilk}$)—equation (2.2) can be simplified using Voigt notation, yielding

$$\begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66} \end{pmatrix} \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \\ \epsilon_6 \end{pmatrix} \quad (2.3)$$

Due to tensor symmetry, the original 36 elastic constants can be reduced to 21 independent components. The number of independent elastic constants may further decrease depending on the crystal symmetry [12].

In Ti-64, the HCP α phase contains three mutually orthogonal planes of reflection symmetry and axial symmetry about the basal plane (as labelled in figure 2.3), meaning that the crystal is invariant under reflection across these planes. This symmetry constraints the elastic stiffness tensor, resulting in five independent elastic constants. Whereas the BCC β phase exhibits three mutually orthogonal planes with 90° rotational symmetry, reducing the number of independent constants to three.

Since both crystal types are anisotropic, their material properties vary with evaluation direction. The degree of anisotropy for each crystal structure can be quantified using the following equations:

$$A_{cubic} = \frac{2C_{44}}{C_{11} - C_{12}} \quad , \quad A_{hex} = \frac{C_{33}}{C_{11}} \quad (2.4)$$

where A is the anisotropy factor [16]. Values of the anisotropy factor close to unity indicate near-isotropic elastic behaviour, while increasing deviation from unity corresponds to stronger directional stiffness contrasts, which enhance orientation-dependent ultrasonic wave speeds and scattering at grain boundaries. In practice, common engineering metals typically exhibit elastic anisotropy factors of order unity, with values in the range of approximately 1–2 indicating moderate anisotropy, while substantially larger values are generally associated with highly anisotropic crystalline systems. To facilitate comparisons across different crystal systems, the universal elastic anisotropy index is proposed as an additional measure of anisotropy [17].

The elastic constants and corresponding anisotropic indices for both phases of Ti-64 are listed in Table 2.2. The anisotropy index for the α phase, which is predominant in Ti-64, is relatively low at 1.13, indicating weak single-crystal elastic anisotropy. At this level of anisotropy, simplified scattering models based on first-order or single-scattering assumptions can provide useful initial insight into ultrasonic attenuation and backscatter behaviour.

Table 2.2: Elastic constants and anisotropy indices for the α (HCP) and β (BCC) phases of Ti-64.

Phase	C_{11} (GPa)	C_{12} (GPa)	C_{33} (GPa)	C_{44} (GPa)	Anisotropy Index
α (HCP)	170	92	192	52	$A_{\text{hex}} = \frac{C_{33}}{C_{11}} \approx 1.13$
β (BCC)	134	110	—	36	$A_{\text{cubic}} = \frac{2C_{44}}{C_{11} - C_{12}} \approx 3$

2.1.4 Crystallographic Texture

Apart from grain morphology and phase variations, each individual crystallite also contains a specific orientation. As previously mentioned, HCP and BCC crystal structures are anisotropic and exhibit directional-dependent material properties. Therefore, the overall orientation distribution of crystals within a medium defines its crystallographic texture [18]. Figure 2.4 illustrates two examples: (a) an untextured (isotropic) medium with randomly oriented crystals, and (b) a highly textured medium, where the crystals are preferentially aligned along the normal direction.

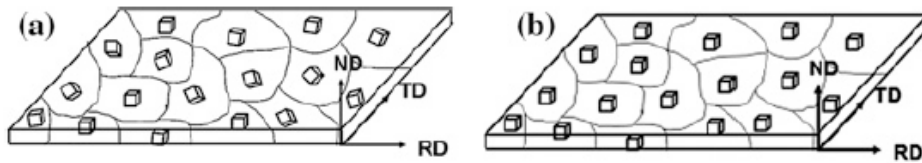


Figure 2.4: Illustration of crystallographic texture in a metal sheet with (a) randomly oriented cubic crystals (untextured) and (b) preferentially-oriented cubic crystals (textured) [18].

Texture is an important factor in anisotropic crystals, as it influences the macroscopic properties of the material. For example, nickel-based superalloys with a cubic crystal structure exhibit the highest creep resistance along the $\langle 001 \rangle$ direction. Hence, turbine blades in aircraft engines are manufactured from single-crystal nickel-based superalloy, where all crystals are oriented along the $\langle 001 \rangle$ direction and aligned with the blade axis to achieve optimal thermo-mechanical properties [19].

Texture can be represented mathematically using the Orientation Distribution Function (ODF)—a function that describes the frequency of crystal orientations in three-dimensional Euler space [20]. The ODF is expressed using generalised spherical harmonics in Bunge’s form as follows:

$$f(\varphi_1, \Phi, \varphi_2) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \sum_{n=-l}^{+l} C_l^{mn} T_l^{mn}(\varphi_1, \Phi, \varphi_2) \quad (2.5)$$

where $(\varphi_1, \Phi, \varphi_2)$ are the Euler angles, C_l^{mn} represents the orientation distribution coefficient, and $T_l^{mn}(\varphi_1, \Phi, \varphi_2)$ is the generalised Legendre functions. For an untextured polycrystal, the ODF $f(\varphi_1, \Phi, \varphi_2)$ takes a constant value of one for all orientations, reflecting an isotropic orientation distribution.

2.1.5 Macrozone Formation in Ti-64

During the production of aircraft engine fan blades and compressor discs, Ti-64 typically begins as a large ingot and undergoes multiple forging and heat treatment cycles to achieve the desired dimensions and microstructure, with the aim of minimising macrozone formation. However, during these processes, large Widmanstätten colonies originating from prior β grains may not be completely broken down. This leads to the formation of macrozones—clusters of grains with similar crystallographic orientations—whose size and shape are influenced by subsequent forging operations [21]. The final alloy microstructure therefore comprises a mixture of fine equiaxed grains and larger macrozone clusters. Although not all macrozones are detrimental, certain characteristics can adversely affect the structural integrity of the alloy.

CDF in Ti-64 is primarily driven by localised plastic deformation under sustained high-stress conditions, which promotes stress concentration and crack initiation [21]. The presence of macrozones further exacerbates this behaviour due to the anisotropic mechanical response associated with the HCP α phase [22–24]. In particular, heterogeneous crystallographic alignment within macrozones leads to uneven strain distribution across neighbouring grains, promoting localised plasticity and stress accumulation at macrozone boundaries, where micro-cracks are prone to initiate [6]. This effect is especially pronounced for highly elongated macrozones with its elongation axis aligned normal to the C-axis and the applied load. Under these conditions, the suppression of the basal slip plane and strong directional stiffness contrast cause the macrozones to resist deformation relative to the surrounding microstructure, resulting in enhanced strain incompatibility at their boundaries and increased susceptibility to CDF-related crack initiation [5].

This issue is of particular concern in aerospace applications, where safety-critical components such as rotating discs, fan blades, and structural forgings are subjected to prolonged high-stress and dwell loading during service. Under these conditions, the presence of macrozones is especially undesirable, as they can locally amplify fatigue damage through strain localisation while simultaneously introducing variability in ultrasonic inspection response. Such variability complicates reliable defect detection and life assessment, making the control, mitigation, and characterisation of macrozones essential for preventing CDF failures and ensuring robust inspection and maintenance strategies in aerospace components.

2.2 Fundamentals on Elastic Waves

Elastic wave theory integrates wave mechanics—which governs ultrasonic wave propagation—with the elastic properties of the material. Accordingly, this section discusses the fundamental theories of elastic wave propagation in isotropic, anisotropic, and scattering media.

2.2.1 Elastic Wave Equation for Isotropic Media

The elastic wave equation for isotropic media can be defined using Hooke's law in equation (2.2) and the momentum equation:

$$\nabla \cdot \sigma = \rho \frac{\partial^2 u}{\partial t^2} \quad (2.6)$$

where ρ is density, u is displacement, and t is time. Since an isotropic medium only has two elastic constants, λ and μ (known as Lamé's constant), the stiffness tensor can be expressed as:

$$C_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) = \begin{pmatrix} \lambda + 2\mu & \lambda & \lambda & 0 & 0 & 0 \\ \lambda & \lambda + 2\mu & \lambda & 0 & 0 & 0 \\ \lambda & \lambda & \lambda + 2\mu & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu & 0 & 0 \\ 0 & 0 & 0 & 0 & \mu & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu \end{pmatrix} \quad (2.7)$$

where δ is the Kronecker delta function ($\delta_{ij} = 1$ when $i = j$ and 0 otherwise). The strain tensor in equation (2.2) can be written in terms of the displacement gradient as:

$$\epsilon_{kl} = \frac{1}{2} \left(\frac{\delta u_k}{\delta x_l} + \frac{\delta u_l}{\delta x_k} \right) \quad (2.8)$$

where x is the spatial coordinate. By combining equations (2.2), (2.6), (2.7) and (2.8), the isotropic elastic wave equation can be expressed as:

$$(\lambda + 2\mu) \nabla (\nabla \cdot u) - \mu \nabla \times \nabla \times u = \rho \ddot{u} \quad (2.9)$$

This is also known as the Navier equation and is used to describe wave propagation in isotropic media [25]. The first term on the right-hand side corresponds to longitudinal wave propagation, while the second term represents shear wave propagation. To decouple these waves modes, a

scalar potential (ϕ) and a vector potential (ψ) are defined such that:

$$\mathbf{u} = \nabla\phi + \nabla \times \psi \quad (2.10)$$

Substituting equation (2.10) into (2.9) gives:

$$\nabla \left[(\lambda + 2\mu) \nabla^2 \phi - \rho \frac{\delta^2 \phi}{\delta t^2} \right] + \nabla \times \left[\mu \nabla^2 \psi - \rho \frac{\delta^2 \psi}{\delta t^2} \right] = 0 \quad (2.11)$$

Using the homogeneous Helmholtz decomposition method, this expression yields two independent wave equations (see [25] for full derivation):

$$\rho \frac{\delta^2 \phi}{\delta t^2} - (\lambda + 2\mu) \nabla^2 \phi = 0 \quad , \quad \rho \frac{\delta^2 \psi}{\delta t^2} - \mu \nabla^2 \psi = 0 \quad (2.12)$$

The first equation represents longitudinal (compressional) waves, and the second corresponds to shear (transverse) waves. Their respective wave velocities are determined by the material properties as follows:

$$c_L = \sqrt{\frac{\lambda + 2\mu}{\rho}} \quad , \quad c_T = \sqrt{\frac{\mu}{\rho}} \quad (2.13)$$

These relations illustrate how the elastodynamic principles can be employed to infer material properties (λ and μ) from variations in wave velocity and displacement fields within the medium.

2.2.2 Christoffel Equation for Anisotropic Media

In an anisotropic medium, the ultrasonic wave velocity changes with direction of propagation. This directional dependence can be determined by solving the Christoffel equation, which is derived from Hooke's law in equation (2.2) and the momentum equation in (2.6) to give:

$$\rho \ddot{u}_i = \frac{1}{2} C_{ijkl} \left(\frac{\delta^2 u_l}{\delta x_j \delta x_k} + \frac{\delta^2 u_k}{\delta x_j \delta x_l} \right) \quad (2.14)$$

Owing to the symmetry of the strain tensor, the indices k and l in equation (2.14) are interchangeable, simplifying the expression to:

$$\rho \ddot{u}_i = C_{ijkl} \frac{\delta^2 u_l}{\delta x_j \delta x_k} \quad (2.15)$$

Next, a plane harmonic wave solution is introduced which is defined as:

$$u_i = A_i e^{i(kn_j x_j - \omega t)} \quad (2.16)$$

where A_i is the amplitude, k is the wave number, and ω is the angular frequency, and n_j is the direction cosine. Substituting equation (2.16) into (2.15) gives:

$$(\rho \omega^2 - C_{ijkl} n_j n_k) A_i = 0 \quad (2.17)$$

This is the Christoffel equation for anisotropic media, which can be formulated as a classical eigenvalue problem. To obtain non-trivial solutions, the determinant of the coefficient matrix is set to zero:

$$|C_{ijkl} n_j n_k - \rho v^2 \delta_{il}| = 0 \quad (2.18)$$

Solving equation (2.18) provides the wave velocities (eigenvalues) and polarisation directions (eigenvectors) corresponding to three orthogonally polarised modes: one quasi-longitudinal and two quasi-shear waves.

To illustrate this, the Christoffel equation was solved in MATLAB for Ti-64 α and β phases across all angles of incidence. The results produced a 3D velocity surface, as shown in Figure 2.5. Since both phases are anisotropic, the longitudinal velocity varies with propagation direction. The β phase exhibits greater anisotropy, with larger velocity variations ranging from 5500 to 6500 m/s, compared to the α phase, which ranges from 6150 to 6550 m/s.

By characterising the directional velocity profile of the medium of interest, the crystallographic orientation or texture of single- and polycrystalline materials can be inferred from ultrasonic velocity measurements.

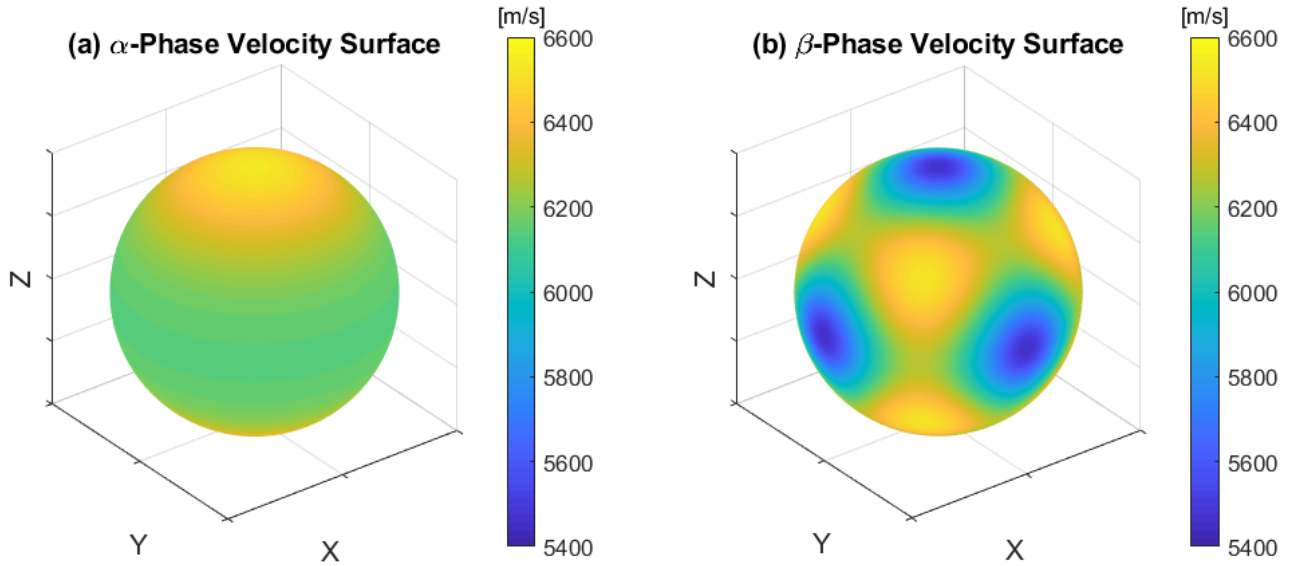


Figure 2.5: Single-crystal longitudinal velocity surfaces of titanium (a) α phase and (b) β phase, with velocity variation represented by colour contours.

2.2.3 Wave Propagation in Polycrystalline Materials

Wave scattering occurs when a propagating wave encounters a disturbance or variation in material property. In polycrystalline material, such disturbances arise from velocity mismatches across grain boundaries, causing part of the incident wave to be scattered in multiple directions. Scattering in an inhomogeneous medium can be represented by the inhomogeneous Helmholtz equation:

$$\Delta\phi(r, w) + k^2\phi(r, w) = -k^2O(r)\phi(r, w) \quad (2.19)$$

$$O(r) = c_0^2\rho(r)\kappa(r) - 1 \quad (2.20)$$

where $O(r)$ is the object function, comprising the background velocity (c_0), density (ρ), and compressibility (κ) of the object [26]. The total field, ϕ_t , is the sum of the incident and scattered fields:

$$\phi_t(r, w) = \phi_i(r, w) + \phi_s(r, w) \quad (2.21)$$

$$\phi_t(r, w) = \phi_i(r, w) - \int_V G(r, r')O(r', w)\phi_t(r', w)dr' \quad (2.22)$$

where $G(r, r')$ is the Green's function. Equation (2.22) is known as the Lippmann-Schwinger equation [27]. The scattering term is a product of the total field and the object function, which can be interpreted as a superposition of secondary sources, each represented by the Green's function. The Green's function describes the propagation of sound from a point source to a field point, and is defined as:

$$G(r, r') = -\frac{i}{4} H_0^{(1)}(k|r - r'|) \quad (2.23)$$

However, the scattered field in equation (2.22) cannot be solved directly due to its non-linearity, since ϕ_t lies within the integral. To address this, the Born approximation is applied, assuming that the total field is approximately equal to the incident field ($\phi_t \approx \phi_i$). This assumption is valid when the scattering strength is weak and the perturbation to the incident field is small. Substituting this approximation simplifies the equation into:

$$\phi_t(r, w) \approx \phi_i(r, w) - \int_V G(r, r') O(r', w) \phi_i(r', w) dr' \quad (2.24)$$

Assuming the incident field is known, the corresponding scattered field can be written as:

$$\phi_s(r, w) = - \int_V G(r, r') O(r', w) \phi_i(r', w) dr' \quad (2.25)$$

In practice, the phase of ϕ_t differs from that of ϕ_i due to velocity variations between the object and the homogeneous background. This phase error increases with object size and velocity contrast. For large objects or strong contrasts, the phase difference may approach π , causing $\phi_t \approx -\phi_i$, thereby invalidating the Born approximation. Therefore, for the Born approximation to hold, the maximum phase distortion induced by the inhomogeneity must remain below π [27].

In polycrystalline materials such as Ti-64, grain boundaries are formed due to crystallographic misorientation. As shown earlier in Figure 2.5, the wave velocity varies with crystal orientation. Thus, the velocity mismatch across grain boundaries leads to wave scattering, analogous to the scattering effect described in inhomogeneous media. This Born approximation is therefore commonly adopted in grain-scattering models to simplify the analytical formulations used

for microstructural characterisation. Its validity relies on the assumption of weak scattering, whereby the incident wave is only minimally perturbed by elastic property fluctuations. This assumption is generally reasonable for polycrystalline materials with small elastic contrast between neighbouring grains, where single-scattering effects dominate and multiple-scattering contributions remain limited.

The underlying elastodynamic principles cause ultrasound parameters, such as wave attenuation and velocity, to vary when interacting with different microstructural features. Numerous studies have established quantitative correlations between ultrasound responses and microstructural characteristics, including grain morphology and crystallographic texture [28]. These relationships are explored in more detail in the following sections.

2.2.3.1 Attenuation

Ultrasonic attenuation refers to the overall reduction in wave energy caused by grain scattering and absorption along the propagation path in a polycrystalline medium. Mason et al. [29] first identified the Rayleigh scattering regime, where scattering-induced attenuation increases with the fourth power of frequency. Shortly after, Mason [30] discovered the geometric scattering regime, where attenuation is independent of frequency and decreases with increasing grain size. Finally, Huntington [31] introduced the stochastic regime that bridges the gap between the Rayleigh and geometric regimes, with attenuation having a second-order frequency dependence. These three scattering regimes are represented by the following attenuation coefficients:

$$\text{Rayleigh Regime:} \quad \alpha_R \propto D^3 f^4 \quad \lambda \gg D \quad (2.26)$$

$$\text{Stochastic Regime:} \quad \alpha_S \propto D^1 f^2 \quad \lambda \approx D \quad (2.27)$$

$$\text{Geometric Regime:} \quad \alpha_G \propto D^{-1} f^0 \quad \lambda \ll D \quad (2.28)$$

where f represents the operating frequency, λ the wavelength, and D the grain diameter in the polycrystalline medium. Following the identification of these scattering mechanisms, Stanke and Kino [32] developed a unified theory using Keller's approximation [33] to connect all three

scattering regimes. An equivalent model was later proposed by Weaver [34] using the Dyson equation. Figure 2.6 illustrates the three distinct scattering regimes with their varying frequency dependencies [35].

The transition zone between the Rayleigh and stochastic scattering regimes marks a shift in scattering behaviour. In the Rayleigh regime, where grain sizes are much smaller than the wavelength, scattering is dominated by longitudinal-to-shear mode conversion because small elastic inhomogeneities preferentially generate shear distortions—each grain effectively acts as a point scatterer that diffuses ultrasound in all directions [29]. In the stochastic regime, where grain sizes are comparable to the wavelength, scattering is dominated by longitudinal-to-longitudinal interactions due to the phase scrambling of wavefront as a result of wave speed variations within each grain [31, 32]. In the geometric regime, where grain sizes are much larger than the wavelength, attenuation results from reflections and refractions as the wave crosses grain interfaces [30].

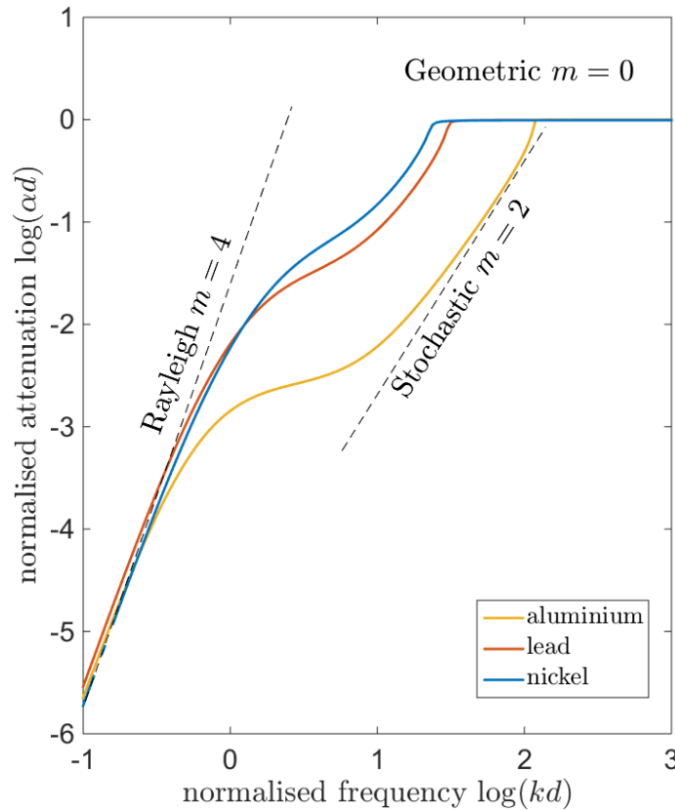


Figure 2.6: Unified theory for attenuation of three cubic materials (aluminium, lead, and nickel) with the three scattering regimes and frequency dependence (m) labelled [35].

The scattering effects can also be understood from a physical perspective. In the Rayleigh regime, where the wavelength is much larger than the grain size, each grain acts as a point scatterer that diffuses ultrasound in all directions [29]. In the stochastic regime, where the wavelength is comparable to the grain size, attenuation occurs due to phase scrambling along the wavefront caused by variations in wave speed within each grain [31]. In the geometric regime, where the wavelength is much smaller than the grain size, attenuation results from reflections and refractions as the wave crosses grain interfaces [30].

Analytically, Arguelles et al. [36] modified Weaver’s model to study the effects of varying grain size distribution by altering the two-point correlation function. They discovered that in the Rayleigh regime, a larger grain size distribution increases the attenuation level but decreases the slope of the attenuation curve. This finding underscores the importance of grain size distribution in accurately estimating grain sizes within the Rayleigh regime. Van Pamel et al. [37] modified the Weaver’s model further and developed the Second-Order Approximation (SOA) method. The SOA method, which does not require iterations, is applicable to a wider range of crystal structures and grain morphologies.

To validate the analytical solutions, Van Pamel et al. [38] developed a polycrystalline FE model using Pogo, which showed good agreement to the unified theory. Notably, the model successfully replicated the transition zone between the Rayleigh and stochastic regimes. Additionally, Van Pamel et al. [39] investigated the effects of dimensionality using FE models and confirmed the existence of dimensional dependence within the Rayleigh regime. In this regime, the scattering dependence on frequency scales with $D+1$ (D represents the dimensionality), as scattering is inherently a 3D phenomenon tied to the volume of the grains. This effect is reduced when the model is simplified to 2D [40]. In contrast, within the stochastic regime, scattering is driven by phase scrambling along the wavefront and remains independent of dimensionality.

Huang et al. [41] further advanced the development of FE models to maximise the accuracy of the wave propagation models while minimising computational resources. Using the optimised FE models, Huang et al. evaluated the wave scattering effects in polycrystals with high anisotropy factors [42] and morphological elongation [43]. Both factors were deemed to increase

scattering and estimated attenuation, leading to an earlier transition from the Rayleigh to stochastic scattering regimes.

Numerous experimental studies have been conducted on metallic samples to explore the correlation between ultrasonic attenuation and grain size, with a general consensus that attenuation increases with grain size [44–50]. Nowacki et al. [44] compared attenuation results with conventional microscopy and found good consistency between the two methods. Zeng et al. [45] correlated experimental data with theoretical models, demonstrating similar trends, particularly in the transition zone between the Rayleigh and stochastic regimes. Liu et al. [50] emphasised the importance of grain size distribution, noting that structures with different mean sizes and standard deviations could produce similar attenuation levels, highlighting the potential for non-uniqueness in grain size characterisation.

2.2.3.2 Backscatter

When an incident wave encounters a grain boundary, it is scattered in all directions. Ultrasonic backscatter refers to the portion of the scattered wave that propagates back to the transducer, as illustrated in Figure 2.7. Unlike attenuation and velocity measurements, backscatter can provide depth-dependent information.

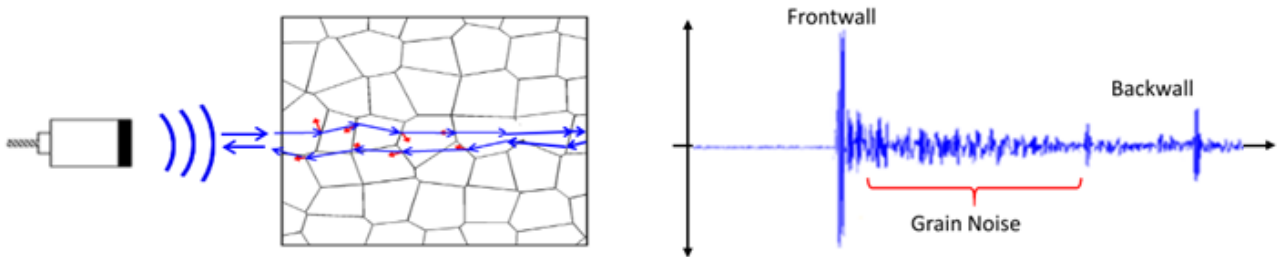


Figure 2.7: Ultrasonic backscatter from grain boundaries in a polycrystalline sample with the corresponding A-scan signal depicting the front-wall and back-wall reflections, as well as the backscattered grain noise arising from microstructural scattering [51].

The generation of backscatter with ultrasound is a complex phenomenon that has been extensively investigated to characterise microstructural features such as grain size. Numerous analytical models were developed to create reliable and accurate methods for grain size predictions. Margetan et al. [52] introduced the Figure of Merit (FOM) to quantify the time-domain

Root Mean Square (RMS) noise in an A-scan signal. For example, a material with an FOM of 2 produces a signal with noise levels double that of a material with an FOM of 1. The RMS approach is based on the assumption that the total noise signal is an incoherent superposition of signals from individual grains, where the phases of the individual signals are uncorrelated [52]. Therefore, the FOM is determined by the density of the grains and the average scattering capability of the individual grains, expressed as:

$$FOM = \sqrt{n}A_{rms} \quad (2.29)$$

where n is the number of grains or scatterers and A_{rms} is the average scattering amplitude. Up to this point, FOM can quantify experimental noise but cannot be used to predict or characterise microstructural properties. Rose [53] addressed this limitation by developing the backscattering coefficient, which includes the effects of grain orientations in polycrystalline materials using the Born approximation. Margetan et al. [54] subsequently validated Rose's model experimentally using titanium alloys and further developed it by introducing the Independent Scattering Model (ISM), which enables the analytical prediction of grain noise. Margetan et al. [55] also conducted multiple experimental validations and evaluated the effects of different toneburst durations, types of beam models, and varying frequencies.

Over the decades, ISM has been widely adopted by researchers and has demonstrated reliable results in relation to grain size characterisation. Li et al. [56] showed that the peak position of the RMS backscatter profile depends on the focal point of the transducer, with the most accurate FOM estimation occurring near the focal point. Adjustments can be made to the focal point to enable the extraction of depth-dependent information. Panetta et al. [57] applied the FOM model to actual Inconel specimens and obtained relatively good results, demonstrating the potential of using backscatter for spatial grain size measurement. However, the accuracy of these results is limited to a finite frequency range and grain sizes below $40 \mu m$. At higher frequencies and larger grain sizes, the scattering effect becomes more pronounced, causing the Born approximation to lose validity. Additionally, Inconel's high anisotropy factor of 2.82 amp-

lifies the scattering effect, further diminishing the accuracy of Born approximation methodology [57].

When investigating complex phenomena, analytical models always involve assumptions, and experimental methods come with inherent uncertainties, which can lead to inconclusive results. Therefore, FE models are essential for addressing intricate responses such as backscatter, as they provide a controlled environment for analysis. Ghoshal et al. [58] and Bai et al. [59] developed two-dimensional backscatter models and compared their numerical results with two-dimensional adapted ISM formulations. Ghoshal adjusted the correlation length in the analytical model to match the numerical results, concluding that the correlation length varies with the degree of scattering and the level of anisotropy. This indicates the presence of multiple scattering at high frequencies, which invalidates the Born approximation methodology that assumes single scattering events.

Bai conducted a more in-depth study, evaluating backscatter in grains with varying shapes and sizes [59]. Overall, there was good agreement in the backscatter coefficient across different grain morphologies, with slight variations attributed to deviations in the spatial correlation function. Additionally, Bai carried out a single-grain backscatter study, where individual grains exhibited varying levels of velocity mismatch relative to the homogeneous isotropic medium [59]. Interestingly, it was found that with the same velocity deviation, a grain slower than the reference background generated more backscatter than a grain faster than the reference background.

Liu et al. [60] advanced the field by developing a 3D FE model to predict grain noise levels. This model showed good agreement with a modified ISM for weakly-scattering polycrystals. However, when the anisotropy factor of the polycrystalline material increased, significant deviations from the ISM were observed, revealing the influence of multiple scattering. This underscores the FE model's superior capability to accurately capture complex phenomena compared to analytical models.

2.2.3.3 Velocity

Ultrasonic velocity is influenced by the crystal structure and the direction of wave propagation. Consequently, it has the potential to extract texture information from polycrystalline materials. Ultrasonic velocity is measured by calculating the ratio of distance to time. Lan et al. [61, 62] developed a spherical harmonics approach to extract texture information using ultrasonic velocity measurements. This approach is governed by the following simplified equation:

$$v = \sum_{i=1}^{N_\phi} f(\phi_i)g(\phi_i) \quad (2.30)$$

where v represents the velocity measured from the specimen in a particular direction, N_ϕ is the number of orientation samples, $f(\phi_i)$ describes the wave velocity through a single crystal with orientation ϕ_i in that direction, and $g(\phi_i)$ denotes the volume fraction of crystals with orientation of ϕ_i with respect to that direction. Lan applied the spherical deconvolution method to resolve this equation and successfully extracted bulk texture information experimentally by measuring velocity in multiple directions using a water immersion setup [63]. In addition to bulk texture, Lan was also able to extract indications of phase percentages within the Ti-64 sample using the water immersion method [63]. This advancement extended the texture measurement method, enabling the concurrent evaluation of both bulk texture and phase percentages.

Using the spherical deconvolution approach, Lan et al. [64] adopted the Resonant Ultrasound Spectroscopy (RUS) to extract bulk texture from titanium samples. RUS generates resonant frequencies of the sample, which are subsequently used to obtain the overall elastic coefficients. Combined with the Christoffel equation [25], the velocity v in equation (2.30) can be obtained. With f already known from the single-crystal elastic coefficients, the bulk texture g can be resolved. The results obtained from both experimental methods were compared with neutron diffraction, the conventional standard for bulk texture measurement, and showed good agreement.

Several studies explored the effectiveness of grain size characterisation using ultrasound velocity. A general inverse correlation between average grain size and bulk longitudinal wave velocity

was observed, primarily due to phase velocity dispersion with attenuation [65, 66]. However, further investigations using FE model revealed that this velocity variation is too subtle to be detected reliably in experiments due to inherent configuration and measurement errors.

High-frequency surface waves generated using laser ultrasound have proven effective in evaluating grain sizes and texture on sample surfaces [3, 67]. At high operating frequencies (hundreds of MHz), the ultrasound wavelength becomes comparable to grain sizes, allowing the generation of grain images similar to those produced by microscopy and EBSD. Experimental validations have shown good agreement in both orientation and grain size evaluation. However, like EBSD, surface waves are limited to near-surface assessments, and obtaining depth-related information would require serial sectioning, which is destructive in nature.

2.2.4 Wave Scattering in Macrozones

Characterising macrozones in Ti-64 alloy using ultrasonic testing presents several challenges. First, the mixture of small grains and the presence of large macrozones complicate the ultrasound responses. Additionally, the dual-phase nature of Ti-64, where the proportions of α and β phases can vary, further complicates the interpretation of the ultrasound signals. Lastly, scattering from grain boundaries is weaker than in conventional crack detection due to the low velocity mismatch between neighbouring grains, resulting in a low signal-to-noise ratio.

To circumvent these issues, several assumptions were made during the development of analytical methods to better predict variations in ultrasonic parameters due to the presence of macrozones [68–70]. Macrozones were approximated as regions of ellipsoids composed of multiple spherical crystallites to introduce macroscopic homogeneity, avoiding the need to account for the small grains and the large macrozones separately. Next, The β phases were ignored as they occupy only a small volume fraction and are much smaller in size, and therefore have negligible impact on the ultrasound response. Finally, directional backscatter ratios across the full signal time span were used to maximise the amplitude of the signals while reducing the number of microstructural and measurement system parameters required.

Using the developed analytical models and backscatter ratios, Rokhlin et al. successfully inverted bulk-averaged macrozone sizes, which showed good agreement with EBSD data [70, 71]. This approach was further refined by incorporating attenuation measurements to invert the elastic scattering factors of the bulk material [72]. Additionally, the methodology assumes that the sample is macroscopically untextured and homogeneous, with macrozones of uniform size evenly distributed throughout the sample and containing random crystal orientations.

Experimentally, Bhattacharjee [73] and Margetan [74] showed positive correlation between attenuation and the average macrozone sizes with normal incidence ultrasound scans. Bhattacharjee et al. [75] indicated that the main contributor to scattering-induced attenuation was the size of the macrozones, as opposed to the elastic modulus mismatch. Through EBSD data, he deemed that the overall elastic mismatch between the macrozones and the crystallites was negligible. Conversely, Humbert et al. [76] related the high level of backscatter to sharp velocity variations between the macrozones and the isotropic base material. This suggests that the scattering-induced attenuation and backscatter might be more sensitive to macrozone size and velocity mismatch respectively. Interestingly, it was shown that when the ultrasonic propagation direction was parallel to the macrozone elongated axis, low backscatter and high attenuation were obtained. Identical conclusions were made by Bhattacharjee [73] and Humbert [76].

Hubert discovered a periodic behaviour in macrozones by processing signals using a spatial correlation function [76]. This observation was later corroborated by Moreau et al. [7], who employed an autocorrelation function on velocity fluctuations to quantify the macrozones, identifying similar periodic bands. Moreau also attempted to measure the size of the macrozones using the autocorrelation function. However, he encountered difficulties in achieving quantitative agreement with EBSD data, as the ultrasonic testing results were approximately five times larger than those obtained through EBSD. This discrepancy is likely attributable to the differences in the operational modes of EBSD (surface measurement) and ultrasound (bulk measurement). Blackshire et al. identified the presence of coherent backscattered signals through a polycrystalline model with actual EBSD data which showed strong reflections in the

presence of a macrozone [77, 78]. This was also validated experimentally which highlights the potential for depth-dependent measurements.

In this study, the analytical models described by Rokhlin et al. are referenced [69, 71, 72, 79] to characterise macrozones. Both backscatter and attenuation approaches were used to estimate bulk macrozone sizes in Ti-64. The backscatter model was based on the longitudinal backscattering coefficient, given by:

$$\eta_L(p) = \frac{k_L^4 Q_{LL}(\sigma)}{4\pi^2} V_{MTR} \left\{ \frac{1}{[1 + k_L^2 l^2(p)]^2} + q(\sigma) \right\} \quad (2.31)$$

$$Q_{LL}(\sigma) = \frac{\langle \delta C_{3333}^{MTR}(\sigma) \delta C_{3333}^{MTR}(\sigma) \rangle}{4 \langle c_{11} \rangle^2} \quad (2.32)$$

$$q(\sigma) = \frac{V_{cryst}}{V_{MTR}} \left(\frac{\delta C_{3333}^{cryst} \delta C_{3333}^{cryst} |_{Iso}}{\langle \delta C_{3333}^{MTR} \delta C_{3333}^{MTR}(\sigma) \rangle} - 1 \right) \quad (2.33)$$

where k_L is the longitudinal wave number, Q_{LL} characterises the fluctuation strength (variance of elastic constant C_{3333}) at a given texture parameter, V_{MTR} is the volume of the macrozone, $l(p)$ is the effective correlation length, $q(\sigma)$ is a correction factor to account for single crystal effects in the macrozones, and V_{cryst} is the volume of single crystals. The attenuation analytical model is based on the Far-Field Born approximation model:

$$\alpha_L = \pi \omega^2 \sum_{N=L,T2,T3} \frac{k_N^2}{4\rho^2 V_L^3 V_N^3} \int_0^{2\pi} \int_0^\pi I_{P_L \rightarrow N}(\theta_S, \varphi_S) W(\mathbf{p}, s_N) \sin \theta_S d\theta_S d\varphi_S \quad (2.34)$$

$$I_{P_L \rightarrow N}(\theta_{PS}) = A_{LN} + B_{LN} \cos^2 \theta_{PS} + C_{LN} \cos^4 \theta_{PS} \quad (2.35)$$

where α_L is the longitudinal wave attenuation coefficient, ω is the angular frequency, the sum over $N = L, T2, T3$ covers the different scattering modes (longitudinal and two transverse modes), k_N is the wave number, ρ is the density, V_L and V_N are the phase velocities for the various modes, I_P is the scattering intensity function across various angles, W is the spectral power density, and θ is the scattering angle.

The analytical framework developed by Rokhlin et al. represents the main work to-date than enables quantitative characterisation of macrozones in bulk Ti-64 using ultrasonic attenuation

and backscatter measurements [69, 71, 72, 79]. However, the applicability of these models relies on several simplifying assumptions that may not hold in practical engineering materials. In particular, the assumption of macroscopic homogeneity and texture-free behaviour contrasts with experimental observations of strong crystallographic texture in Ti-64, as highlighted by bulk ultrasonic velocity measurements [63]. Furthermore, the treatment of macrozones as uniformly distributed and statistically homogeneous regions neglect spatial heterogeneity, which has been shown to play a critical role in the generation of coherent backscatter signals [77, 78]. These limitations suggest that while existing analytical models provide valuable bulk-averaged insights, they are insufficient to capture the spatially-resolved scattering behaviour observed in real macrozone samples. This motivates the need for numerical and experimental investigations that explicitly addresses these gaps, as pursued in the subsequent chapters.

2.3 Finite Element Models

The explicit time-domain FE method is commonly used to model wave propagation in solid media [80]. To simulate realistic polycrystalline structures, the model is discretised with a mesh size of at least ten elements per wavelength or per grain, whichever is smaller. This requirement leads to a large number of nodes and degrees of freedom, resulting in high computational costs and long processing times [40]. This challenge is addressed by Pogo, an FE solver developed at Imperial College, which leverages parallel processing on graphics processing units to efficiently handle large-scale models at high speed [80].

The following is a derivation for the explicit time-domain method, starting with the equation of dynamic equilibrium [27]:

$$[M]\ddot{u} + [C]\dot{u} + [K]u = [F] \quad (2.36)$$

where $[M]$ is the mass matrix, $[C]$ is the viscous damping matrix, $[K]$ is the stiffness matrix, and $[F]$ is a vector describing the force applied in the system. $\ddot{u}$, $\dot{u}$, and u are the acceleration, velocity, and displacement, respectively. The size of the matrices, defined by the number of rows and columns, is proportional to the number of Degrees of Freedom (DOF) in the model.

Using a finite difference scheme to advance the solution in time yields the following:

$$[M] \frac{u_{next} - 2u_{curr} + u_{prev}}{\delta t^2} + [C] \frac{u_{next} - u_{prev}}{2\delta t} + [K]u_{curr} = [F] \quad (2.37)$$

where u_{prev} , u_{curr} , and u_{next} are the displacement vectors in the previous, current, and next time steps, respectively. By rearranging this equation, the displacement in the next time step can be calculated as:

$$u_{next} = \left(M \frac{1}{\delta t^2} + C \frac{1}{2\delta t} \right)^{-1} \left[F + \left(C \frac{1}{2\delta t} - M \frac{1}{\delta t^2} \right) u_{prev} + \left(M \frac{2}{\delta t^2} - K \right) u_{curr} \right] \quad (2.38)$$

where δt is the time step. This equation is further simplified using modified matrices with lumped mass and damping matrices (full derivation in [80]). The resulting equation becomes:

$$u_{next} = F' + C' u_{prev} + K' u_{curr} \quad (2.39)$$

where F' , C' , and K' are the modified force, damping, and stiffness matrices, respectively, and are represented by:

$$F' = \left(M \frac{1}{\delta t^2} + C \frac{1}{2\delta t} \right)^{-1} F \quad (2.40)$$

$$C' = \left(M \frac{1}{\delta t^2} + C \frac{1}{2\delta t} \right)^{-1} \left(C \frac{1}{2\delta t} - M \frac{1}{\delta t^2} \right) \quad (2.41)$$

$$K' = \left(M \frac{1}{\delta t^2} + C \frac{1}{2\delta t} \right)^{-1} \left(M \frac{2}{\delta t^2} - K \right) \quad (2.42)$$

By solving this simplified finite difference equation, the displacement at each node for the next time step is extracted, and the process is repeated to solve the model over time to simulate the wave propagation behaviour. For the explicit finite-difference method to be stable and accurate, the time step must satisfy the Courant-Friedrichs-Lewy (CFL) condition [81], governed by the equation:

$$C = \frac{c\Delta t}{\Delta x} \leq 1 \quad (2.43)$$

where C is the CFL coefficient, c is the wave velocity, Δt is the time step and Δx is the size of the mesh. The time step also depends on the discretisation size of the mesh, which in turn is influenced by the ultrasonic wavelength [82].

2.4 Signal Processing

Time domain signals obtained from FE models and experiments are processed to extract ultrasound parameters such as wave attenuation, backscattered amplitude, and propagation velocity. A sample FE signal is shown in Figure 2.8, illustrating the input (numerically prescribed excitation), the backscattered, and the reflected backwall signal. These features are isolated by applying a tapered window for subsequent computations.

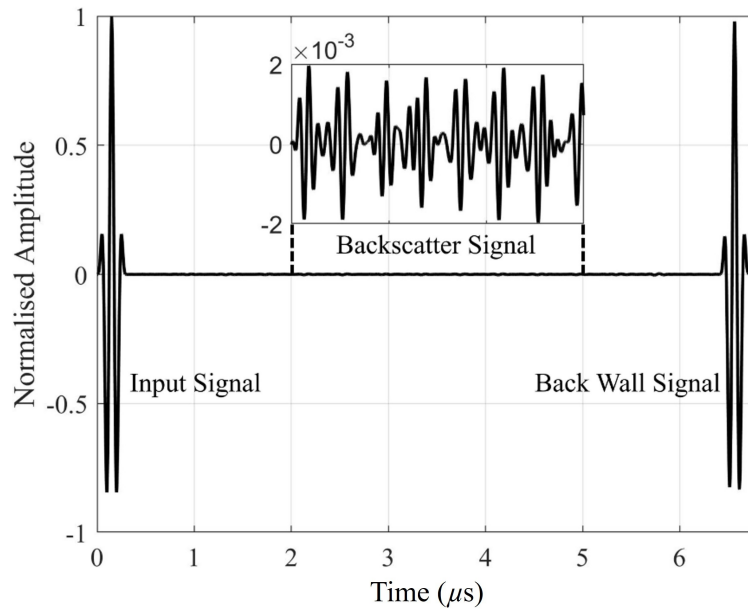


Figure 2.8: FE simulated time domain signal which comprises the input and back wall signal. The inserted figure represents the backscatter signal which is presented on a much smaller amplitude scale.

For general ultrasound attenuation measurements, the amplitude ratio between the front and back wall signals is used. Here, the front wall signal refers to the experimentally measured reflection from the sample front surface. This ratio is typically corrected by accounting for the interface transmission and reflection coefficients, as well as a beam-diffraction compensation factor to address beam spreading effects from a finite-sized transducer [83]. The corrected

attenuation is represented by the following formula [45]:

$$\alpha_s = \frac{1}{z} \ln \left(\frac{FD_1T_{01}R_{10}T_{10}}{BD_0R_{01}} \right) \quad (2.44)$$

where z is the propagation distance, F and B are the front and back wall signal amplitude in the frequency domain respectively, D is the beam diffraction coefficient, T and R are the transmission and reflection coefficients respectively, and the indices 0 and 1 refer to the water and Ti-64 media respectively.

Since the FE model consists of a single solid medium with plane wave propagation, effects such as beam spread, diffraction, and fluid-solid interface interactions—which are important in immersion-tank experimental setups—are not present. Therefore, the diffraction correction factor and the reflection/transmission coefficients are omitted and the resulting attenuation formulation is represented by:

$$\alpha = \frac{1}{z} \ln \left(\frac{F}{B} \right) \quad (2.45)$$

The isolated front and back wall signals are Fourier transformed to obtain their respective frequency contributions and subsequently used in equations (2.44) and (2.45) to compute the frequency-dependent attenuation profile.

Next, for backscatter signals, a common approach involves constructing a backscatter amplitude profile by computing the RMS amplitude across multiple spatial measurements in the time domain [54, 55]. Grain noise represents an incoherent scattering contribution arising from random microstructural variations and therefore exhibits strong spatial and phase variability between measurement positions. Consequently, individual A-scans are not representative of the underlying scattering strength. By performing an RMS operation over a defined scattering time window and across multiple spatial positions, position-specific interference effects are suppressed, yielding a statistically stable estimate of the average scattered energy which is directly related to the material microstructure.

In subsequent chapter, FE simulations generate a single time-domain backscatter signal for each model configuration, rather than multiple spatial realisations. To enable a consistent

and convenient comparison of the overall backscatter response between models, a scalar backscatter intensity metric is therefore computed. The region of interests corresponding to the backscattered signal is first isolated in the time domain and subsequently transformed into the frequency domain using Fourier transform. The magnitude spectrum is then integrated over the Full Width at Half Maximum (FWHM) bandwidth of the excited signal to yield a single backscatter intensity value.

Lastly, for ultrasound velocity measurements, the cross-correlation method is used. Cross-correlation measures the similarity between two signals as one is shifted in time [84]. This is represented mathematically by an inner product in the time domain:

$$R_{xy}(t) = \int_{-\infty}^{\infty} X(\tau)Y(\tau - t)d\tau \quad (2.46)$$

where R_{xy} is the cross-correlation function, X and Y are the two signals to be correlated, and t is the delay interval. Using cross-correlation, the relative delay interval is determined by sliding one signal with respect to the other and identifying the time lag at which the cross-correlation function attains its maximum value, corresponding to the strongest temporal alignment between the two signals. The wave velocity is extracted by dividing the Time-of-Flight (TOF) with the propagation distance.

2.5 Conclusion

Despite the extensive literature on ultrasonic scattering in polycrystalline materials, current industrial practice remains limited in its ability to characterise spatially extended microstructural features such as macrozones. In particular, many existing approaches assume statistically homogeneous microstructures and do not explicitly account for directional anisotropy at the macrozone scale. These limitations highlight a gap between established scattering theory and practical inspection needs, and motivate the investigations presented in the subsequent chapters aimed at developing methodologies for the characterisation of macrozones in realistic engineering materials.

Chapter 3

Parametric Study of Macrozone Effects on Wave Propagation

3.1 Introduction

The aim of this chapter was to investigate how macrozone morphology and orientation influence ultrasonic scattering behaviour. This goal was achieved by systematically isolating and varying macrozone descriptors within controlled FE models, enabling clear attribution of observed directional variability in ultrasonic responses to specific macrozone features. This chapter is based on work previously published by the author, with additional explanations and context provided here for completeness.

A parametric study was first conducted to identify potential relationships between macrozone characteristics and ultrasonic responses. The resulting trends were subsequently validated experimentally to confirm that the predicted behaviours are observable in physical samples and to demonstrate the reliability of the modelling approach. The experimental results were also benchmarked against EBSD data to assess the feasibility of the proposed methodology for macrozone characterisation.

In doing so, this chapter addresses a practical gap in current understanding: while existing scattering theories predict anisotropic behaviour in textured materials, they do not explicitly relate realistic macrozone morphologies to the direction-dependent variability observed in ultrasonic inspections of engineering components. The results therefore provide physically grounded insight that bridges theoretical scattering concepts and practical inspection interpretation.

3.2 Methodology

3.2.1 Finite Element Model Configuration

In this FE study of wave propagation in polycrystalline Ti-64, the objective is to understand the physical interactions between ultrasound wave propagation and macrozones of various characteristics. To enable a comprehensive parametric exploration of macrozone descriptors, 2D models are employed to achieve tractable computational cost while allowing systematic variation across a large parameter space. Although it is well documented that 2D and 3D models exhibit different quantitative behaviours in attenuation and backscatter—attenuation for instance was shown to have a dimensional dependence when operating in the Rayleigh regime [39, 85]—the qualitative physical insights remain transferable. Hence, the 2D framework is therefore sufficient for identifying dominant behaviours, which can subsequently guide more targeted 3D modelling where higher-fidelity quantitative prediction is required.

The polycrystalline microstructure is generated using open-source Neper software [86]. Neper is an off-the-shelf polycrystal generation tool that constructs representative grain structures using a Voronoi tessellation, whereby the domain is partitioned into cells based on proximity to a set of seed points, with each cell representing an individual grain. This approach enables controlled specification of grain size, morphology, and crystallographic orientation and is widely adopted for the FE modelling of polycrystalline materials.

The model configuration is shown in Figure 3.1 which features an average grain size of $20\ \mu\text{m}$ [5], within a $20\ \text{mm} \times 20\ \text{mm}$ computational domain, containing approximately 1.15 million grains.

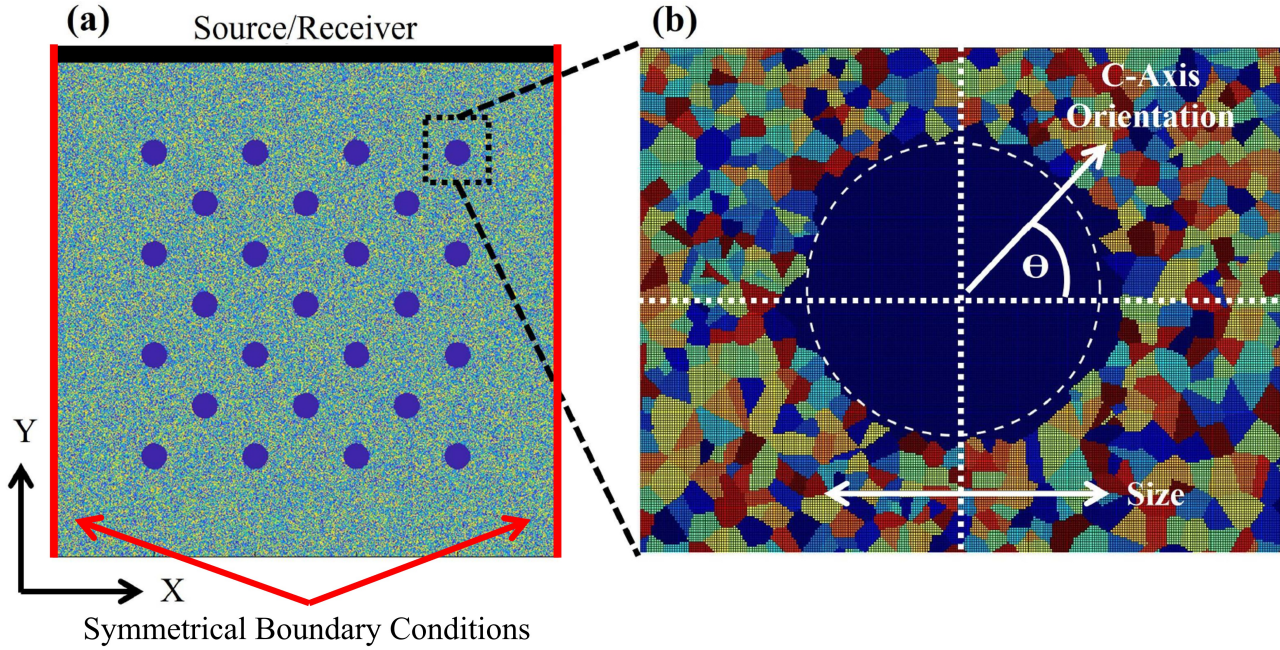


Figure 3.1: (a) 2D FE model setup with multiple macrozones (blue) located in the medium in a background filled with polycrystals. The top surface (in black) is the location for the excitation and monitoring nodes, and symmetrical boundary conditions on the sides (in red) to support plane-wave propagation (b) A zoomed-in image of a single macrozone surrounded with individual polycrystals of random orientations as depicted by the colour codes, with the size and C-axis orientation of the macrozones with respect to the wave propagation direction labelled.

The crystal orientations of the grains are defined using Roe's formulation and passive rotations [62], with the following stiffness matrix (unit: GPa) for the Ti-64 α phase [61]:

$$\mathbf{C} = \begin{pmatrix} 170 & 92 & 70 & 0 & 0 & 0 \\ 92 & 170 & 70 & 0 & 0 & 0 \\ 70 & 70 & 192 & 0 & 0 & 0 \\ 0 & 0 & 0 & 52 & 0 & 0 \\ 0 & 0 & 0 & 0 & 52 & 0 \\ 0 & 0 & 0 & 0 & 0 & 39 \end{pmatrix} \text{ GPa.} \quad (3.1)$$

The Ti-64 α phase has a HCP crystal structure, which is transversely isotropic with symmetry about the C-axis. The corresponding velocity profile in the 2D X-Y plane can be obtained by solving the Christoffel equation using the stiffness matrix. The resulting profile is illustrated in Figure 3.2, where velocity is highest along the C-axis and lowest normal to the C-axis.

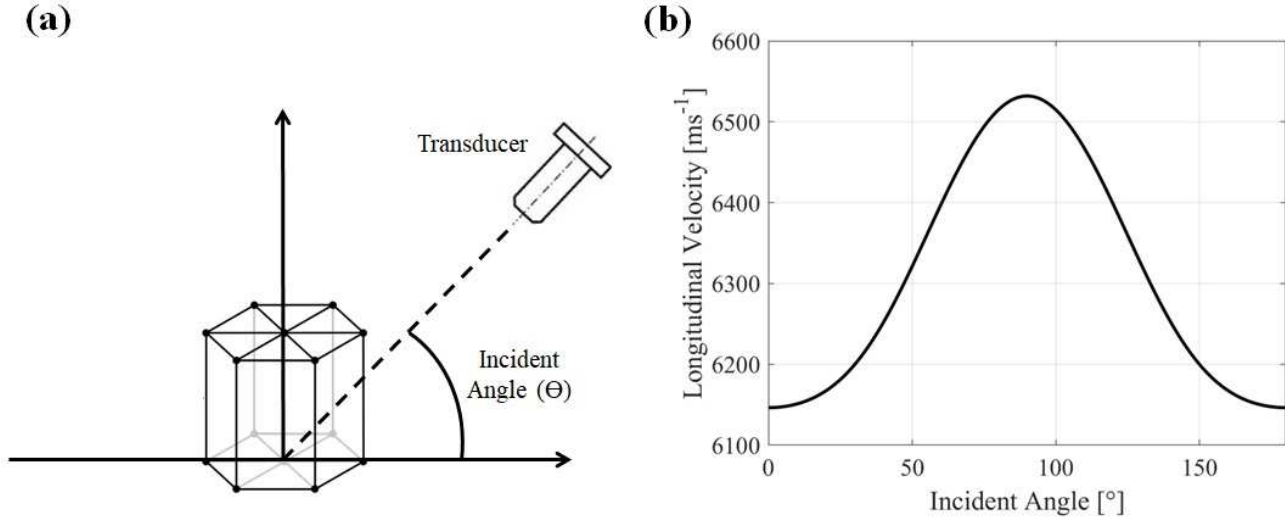


Figure 3.2: (a) A hexagonal crystal structure with the incident angle defined and (b) the corresponding longitudinal wave velocity with varying incident angle [61].

The grains are initially assigned randomised crystallographic orientations to generate an untextured medium with a Voigt-averaged velocity of 6244 m/s. Subsequently, regions of interest are defined, and the grains within these regions are assigned identical crystal orientations to form larger aggregates representative of macrozones. This idealisation is considered reasonable for the present study, as grain orientations within real macrozones typically exhibit a preferred orientation with limited statistical distribution [87].

For generalisation, macrozones are arranged in a periodic configuration with a prescribed density, defined here as the number of macrozones per unit area within the computational domain. In practice, macrozones in real components are often irregularly distributed; however, explicitly modelling such effects introduces additional stochastic variability that makes it difficult to attribute observed changes in ultrasonic response uniquely to a given macrozone descriptor. As a result, the controlled periodic arrangement enables systematic and repeatable comparison between models with varying macrozone size, shape, and orientation, while avoiding confounding effects arising from random spatial placement. While this idealisation may lead to

quantitative differences compared to real microstructures, the qualitative trends and governing mechanisms identified are expected to remain representative. In addition, single-macrozone models are employed throughout this study to further simplify the analysis and elucidate fundamental wave-macrozone interaction mechanisms, which manifest in a more complex and coupled manner in multi-macrozone configurations.

Based on the numerical studies reported in [88], the mesh size should be smaller than one-twentieth of the simulated wavelength and one-tenth of the average grain diameter to ensure numerical accuracy. An excitation frequency of 10 MHz is used and the Voigt-averaged longitudinal velocity is 6244 m/s. This corresponds to a wavelength of approximately 0.6 mm at the operating frequency, and a range of 0.5 to 1 mm over the excitation bandwidth. Using the aforementioned criteria, the model is spatially discretised using a structured mesh of $2\ \mu\text{m}$ square elements. Previous studies [38] demonstrated that both structured and unstructured meshes offer similar performance. Hence, a structured mesh is selected in this work for simplicity and consistency.

An explicit time-domain computation is implemented, coupled with a central difference time marching scheme which incrementally solves the system of equations with a time step of 0.1 ns to satisfy the CFL condition [89]. A 10 MHz 3-cycle Hann-windowed cosine toneburst is applied to the surface nodes of the model along the Y-direction to generate a longitudinal wave as shown in Figure 3.1 (a). This frequency and pulse was adopted as it provides macrozone-sensitive wavelengths, controlled bandwidth, and good time-frequency localisation consistent with practical ultrasonic inspection conditions. To support plane wave propagation, symmetrical boundary conditions are applied to the left and right boundaries of the model by constraining the X-direction displacements. This simulates an infinitely wide medium that is ideal for isotropic materials. For polycrystalline media, the use of symmetrical boundaries provides an approximate plane wave condition, which has been validated as a reasonable assumption and extensively tested to ensure numerical accuracy and stability [41].

Upon completion of each simulation, the time-domain signals recorded at the monitoring nodes are extracted for post-processing. The excited wave propagates downward, reflects from the

bottom boundary, and is subsequently received back at the top surface. The signals recorded across all the receiving nodes are summed to form a single time domain signal. As described in Section 2.4, the signals are subsequently processed to extract ultrasonic attenuation, backscatter, and velocity information.

3.2.2 Computational Analysis Approach

To better understand the physical phenomena arising from wave propagation through complex macrozone features, and to identify the relative influence of each contributing factor, an empirical approach is adopted. This is implemented using Design of Experiments (DOE) or experimental design, a systematic and efficient tool that evaluates the sensitivity of multiple parameters on various response metrics across a series of simulations or experiments [90].

The statistical software Minitab [91] uses the Analysis of Variance (ANOVA) method, followed by F-tests to determine the significance of the factors and their impact on the responses with a predefined confidence interval (95%) [90]. The resulting conclusions are valid within the defined ranges of the modelled parameters, as the DOE framework characterises parameter sensitivities locally within the sampled design space and does not assume extrapolation beyond these limits.

To evaluate the relative sensitivity of the various macrozone characteristics, multiple models with different macrozone shapes, sizes, and crystal orientations are generated, as summarised in Table 3.1. A total of 125 FE models are generated, with each parameter varied independently following the procedure described previously. The resulting time-domain signals are captured and processed to evaluate the ultrasonic attenuation, backscatter, and velocity responses.

The definitions of these macrozone characteristics are illustrated in Figure 3.1(b). The size refers to the cylindrical diameter, varying from 0.1–1 mm which covers a range of possible macrozone sizes [5]. The shape of the macrozones is denoted with X and Y representing the axis of elongation, and the number representing the elongation ratio (e.g., X4 denotes an elongation ratio of 4 along the X-direction, while XY1 represents an equiaxed configuration).

The total area occupied by the macrozones is held constant. The C-axis orientation of the macrozone is defined with respect to the normal of the wave propagation direction.

Table 3.1: Macrozone characteristics used in the parametric study.

Size (mm)	Shape	MTR Crystal Orientation (°)
0.1	X4	0
0.25	X2	30
0.5	XY1	45
0.75	Y2	60
1	Y4	90

The ultrasound responses obtained from the FE models were used as inputs in Minitab [91], which generates statistical output describing the correlations between macrozone characteristics (factors) and the ultrasonic responses. The following equations outlined the steps used to compute the sum of squares (SS), sum of squares error (SSE), mean squares (MS), mean squares error (MSE), and the F-ratio (F). SS measures the variation attributed to the varying macrozone characteristics, while SSE represents the variation attributed to error or the difference between the individual measurements and the predicted values. They are represented by:

$$SS = \sum (\hat{X} - \bar{X})^2 \quad (3.2)$$

$$SSE = \sum (X - \hat{X})^2 \quad (3.3)$$

where X is the measured value, $\bar{X}$ is the mean value, and $\hat{X}$ is the predicted value. MS is used to estimate the variance between the sample means and MSE represents the variation within the sample means. They are calculated by taking the following ratios:

$$MS = \frac{SS}{DOF} \quad (3.4)$$

$$MSE = \frac{SSE}{DOF_{Err}} \quad (3.5)$$

where the DOF is governed by the number of data points available (sample size) and the number of terms being estimated. DOF_{Err} corresponds to the remaining DOF used to estimate the model error. The F-ratio is calculated by taking the ratio of the MS and the Mean Squares

Error (MSE):

$$F = \frac{MS}{MSE} \quad (3.6)$$

The F-ratio evaluates the statistical significance of each factor within the experimental design. The results are presented in the form of a Pareto chart that shows the order of significance of the factors, and a main effects plot that shows the trend and relationship between the factor and its corresponding responses [90].

3.3 Finite Element Modelling Results

This section presents the results of the FE simulation and statistical analyses. The Pareto Chart and Main Effects Plot generated in Minitab are evaluated to determine the relative significance of each macrozone characteristic and its correlation with the respective ultrasonic response.

3.3.1 Attenuation

The variation of ultrasonic attenuation with different macrozone characteristics is first examined. From the Pareto Chart in Figure 3.3, the different macrozone characteristics are labelled on the Y-axis, with the standardised effect on the X-axis. The standardised effect was a normalised scale that represents the significance of the factors, with bars exceeding the red-dotted line being deemed as statistically significant—the line is drawn at the $(1-\alpha/2)$ quantile of a t-distribution, where α is the level of significance [90]. From the results, macrozone crystal orientation has the greatest impact, followed by macrozone size, and lastly the macrozone shape which is deemed to be statistically insignificant within the range of modelled parameters.

The Pareto chart is accompanied by the main effects plot which showed the trends of the various macrozone characteristics with respect to attenuation. The main effects plot is illustrated in Figure 3.4, where each data point represents the mean attenuation calculated across all model configurations containing the macrozone characteristic indicated on the X-axis. The associated error bars correspond to the standard deviation of attenuation within this subset of models,

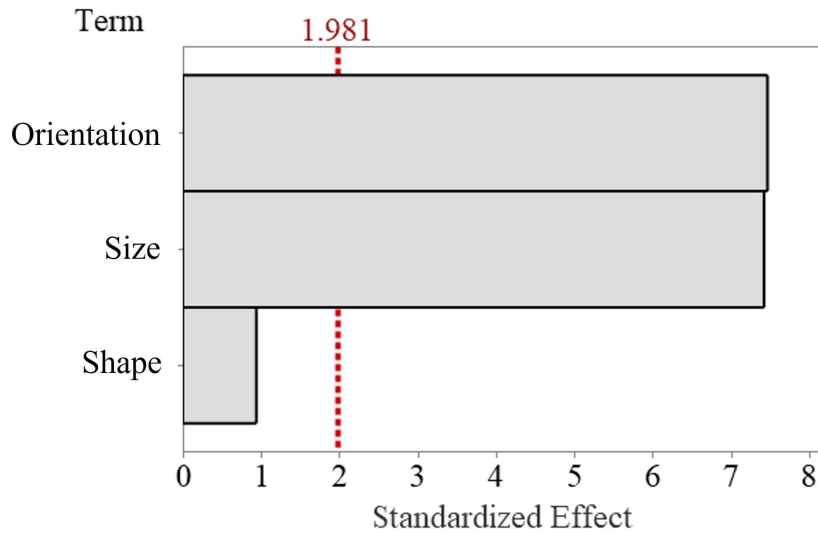


Figure 3.3: Pareto chart of the standardised effects for attenuation predicted at a 95% confidence interval. The red line (1.981) indicates that factors exceeding this are deemed to have a statistically significant impact.

reflecting variability that arise from the remaining macrozone parameters and their interactions, rather than numerical uncertainty. Several analyses can be made based on the mean values. An increase in macrozone dimension—which is dependent on the size and shape—along the wave propagation direction leads to an increase in attenuation. Crystal orientation affects the velocity mismatch between the macrozones and the surrounding materials and thus also results in varying attenuation values.

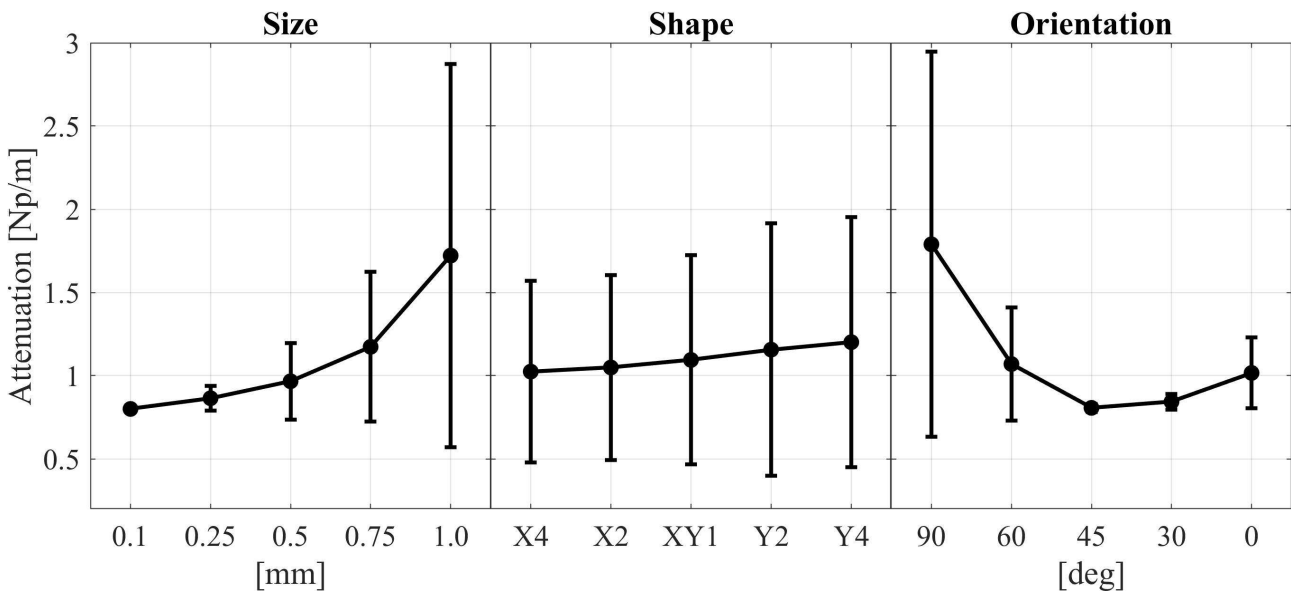


Figure 3.4: The main effects plot for attenuation highlights the correlation between ultrasound attenuation and the three macrozone characteristics: (a) size, (b) shape, and (c) orientation.

It is a well-known fact that any increment of grain sizes (or grain-size to wavelength ratio) leads to an increase in attenuation due to the larger grains and boundaries that scatters and distorts the propagating wave [32]. This is the case for macrozones as well, but with the additional preferred crystal orientation that exists within the macrozone as compared to the untextured polycrystalline background.

This can be represented by a beam profile shown in Figure 3.5. The beam profile was plotted by taking the maximum displacement at each spatial node within the model domain throughout the time period of the simulation. The colour code indicated the normalised displacement amplitude which varies after the wave interacts with the macrozone. On the left, the model contains a single macrozone embedded in a Voigt-averaged homogeneous medium. The macrozone C-axis is parallel to the wave propagation direction which travels from the top to the bottom. Wave velocity along the Ti-64 hexagonal crystal C-axis is higher at about 6550 m/s and thus the macrozone becomes a region of higher velocity. This leads to a local focusing effect which increases the wave amplitude across the wake of the macrozone, and vice versa. This results in a phase perturbation of the wavefront, causing destructive interference to occur when the whole beam is captured by a receiver and this is represented as attenuation. Attenuation is greater along the C-axis orientation (90°) because of the higher velocity mismatch with the Voigt-averaged background velocity of 6244 m/s, leading to a stronger distortion effect. With increased macrozone sizes, the larger grain boundary increases the scattering effects [45] while the larger grain area increases the beam distortion effect, both of which contribute to higher attenuation.

With changes in macrozone shapes from X4 to Y4, the macrozone-length along the wave propagation direction increases. Past study has shown that grain elongation within the stochastic regime (wavelength being comparable to grain size) results in increased attenuation due to greater phase perturbation [92]. Even though the models only have a limited number of macrozones embedded in an equiaxed polycrystalline medium, the phase perturbation effects due to macrozone elongation are also present. To quantify this perturbation effect, an RMS value representing the wave displacement fluctuations is calculated across the receiving nodes for each of the models. The displacements across the receiving nodes are normalised by the spatially

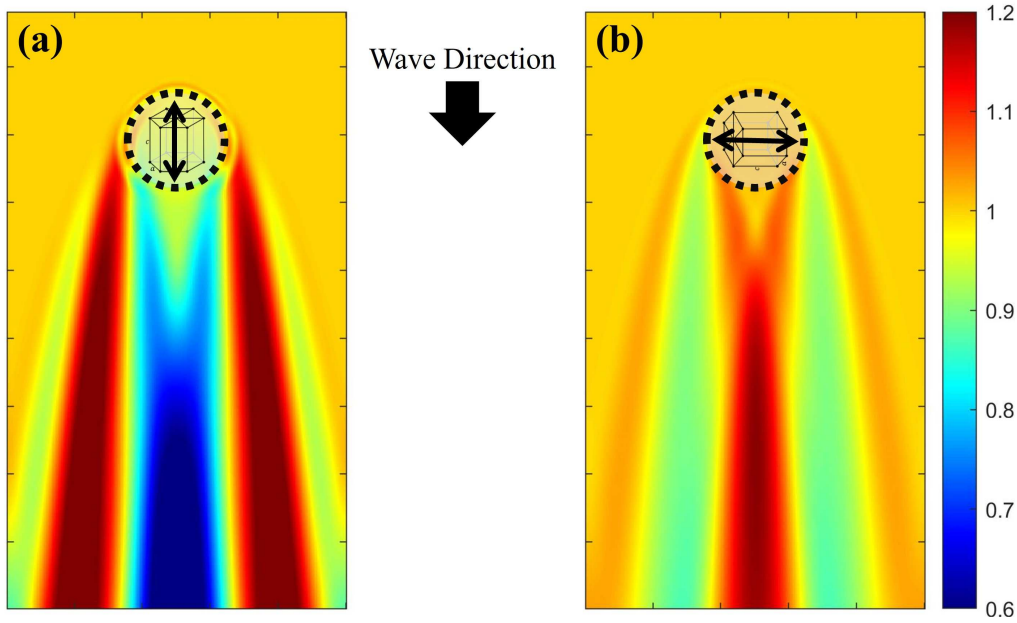


Figure 3.5: Beam profiles generated in 2D FE models by taking the maximum amplitude at each spatial node within the model, where the colour code represents the normalised arbitrary wave amplitude at 10 MHz centre frequency with a 3-cycle Hann-windowed cosine toneburst. The profiles show the distortion of the plane longitudinal wave after it interacts with a single circular macrozone of (a) parallel and (b) normal C-axis crystal orientation, generating a defocusing and focusing effect respectively.

averaged displacement to have a mean value of 0. Hence, the RMS values calculated from the normalised displacement correlates to the wave field fluctuations [92]. As seen in Figure 3.6, the RMS value increases from 1.835 to 1.971 when the grain-length increases by a factor of 16 (from X4 to Y4). This indicates that macrozones with longer grain-length along the wave propagation direction results in stronger local distortions and thus a higher measured attenuation.

Lastly, for the case of the macrozone crystal orientation, the attenuation profile has a minimum point at about 45° as shown in Figure 3.4. This is linked to the velocity mismatch between the macrozones and the untextured polycrystalline background in the model [93]. The velocity profile of a Ti-64 single crystal is illustrated in Figure 3.7 (a) by a solid line, with the Voigt-averaged velocity shown with a dashed line. In Figure 3.7 (b), the velocity difference between the single-crystal and the Voigt-averaged case is shown, with a minimum point at 39° and has a similar profile to the main effects plot illustrated in Figure 3.4. This velocity difference is positively correlated to ultrasound impedance which leads to the effects of wave scattering.

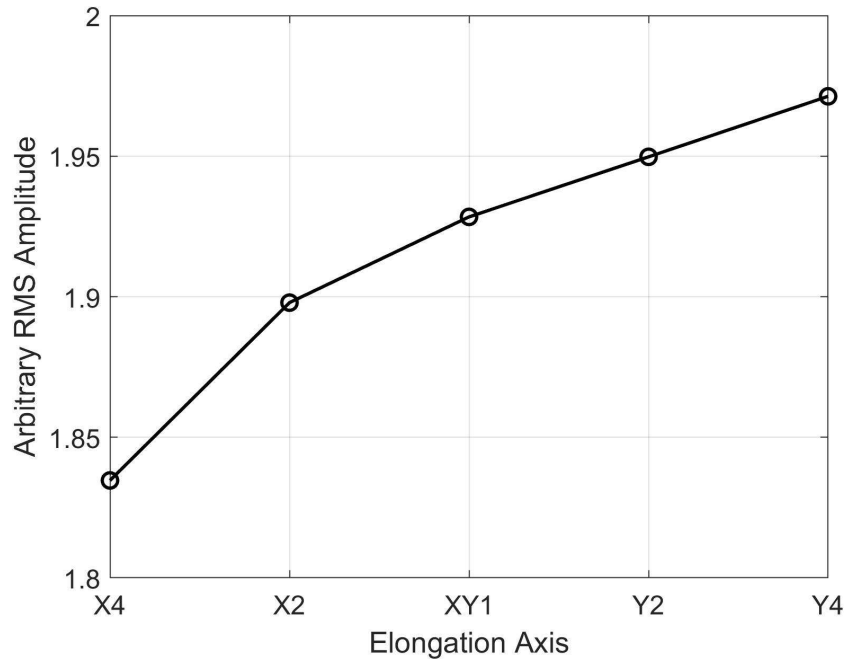


Figure 3.6: RMS values calculated from the individual nodal displacement values across the receiver located at the bottom of the model for macrozones of different shapes, indicating a positive correlation between macrozone-length along wave propagation direction and attenuation.

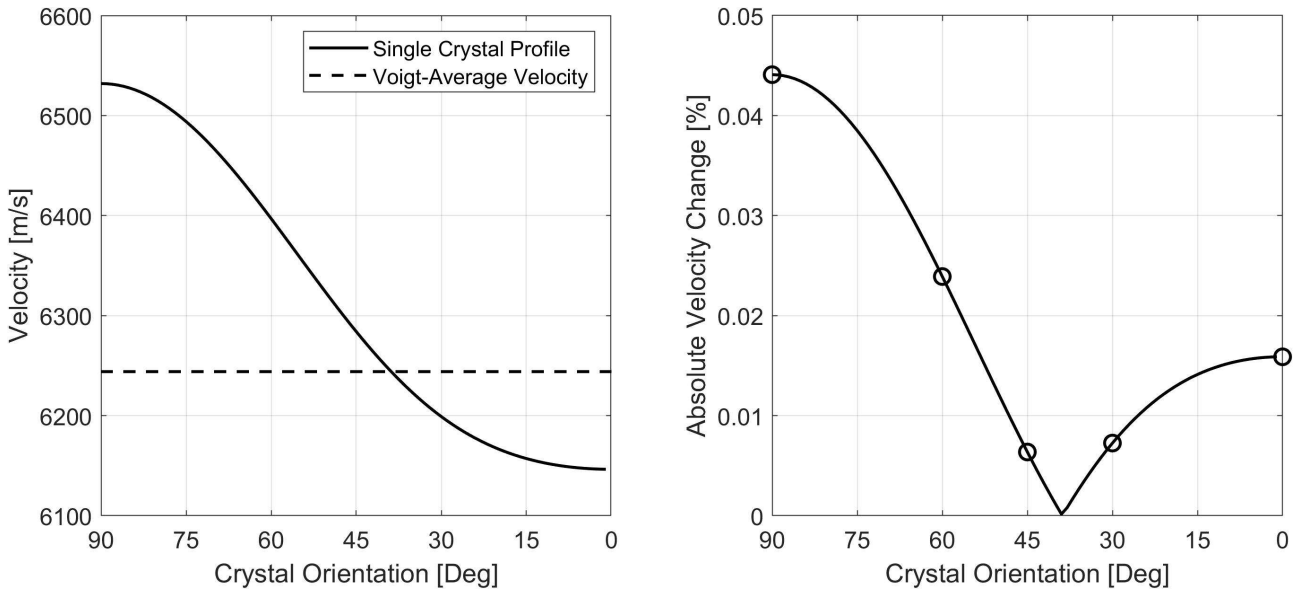


Figure 3.7: (a) Ti-64 single crystal velocity profile with different C-axis orientation and the Voigt-averaged velocity value, and (b) Velocity contrast with different C-axis orientation with respect to Voigt-averaged velocity.

The simulation model is populated with a finite number of macrozones with a predefined crystal orientation that introduces the presence of texture that affects the ODF. ODF is a measure of the overall orientation of the grains in a region of interest and is related to bulk texture. Liu et al. [94] demonstrated analytically that macroscopic texture in a polycrystalline mater-

ial generally results in a lower attenuation as compared to macroscopic isotropy due to the reduced crystal misorientations between neighbouring grains. In the model, apart from macroscopic texture, the location of the macrozones that are defined periodically also changes the Misorientation Distribution Function (MDF)—MDF measures the level of crystal misorientation between neighbouring grains and contains additional spatial information. Both ODF and MDF influences the attenuation of ultrasound through scattering and wave distortions and as such the simulated attenuation in the models are generally higher than the macroscopically isotropic case.

3.3.2 Backscatter

Next, the effects of different macrozones characteristics on backscatter amplitude are evaluated. From the Pareto chart in Figure 3.8, all three macrozone characteristics are deemed to be significant in generating backscatter signals, with orientation being the most significant, followed by macrozone shape and size.

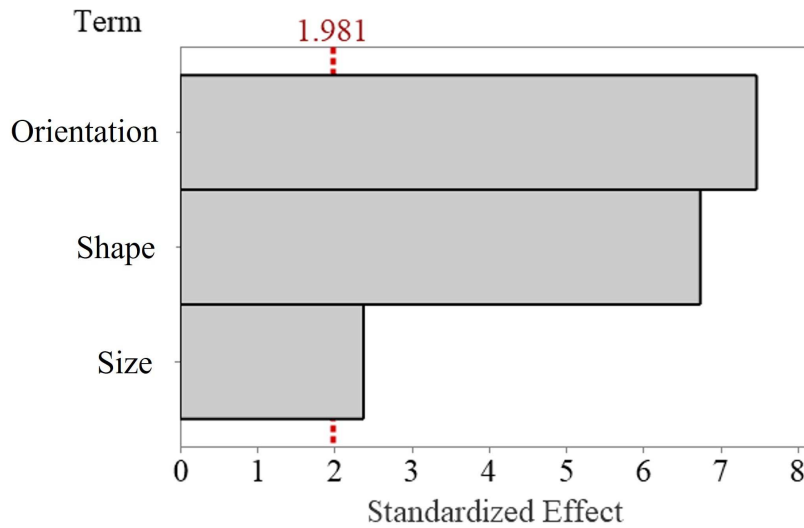


Figure 3.8: Pareto chart of the standardised effects for backscatter amplitude predicted at a 95% confidence interval. The red line (1.981) indicates that factors exceeding this are deemed to have a statistically significant impact.

Following up with the main effects plot in Figure 3.9, there is a general positive correlation between backscatter amplitude and macrozone size. Contrastingly, backscatter amplitude is inversely related to macrozone elongation, whereby macrozone length increases along the wave

propagation direction. Lastly, backscatter amplitude is highest when the macrozone C-axis orientation is parallel to the wave propagation direction as velocity and impedance mismatch is the greatest.

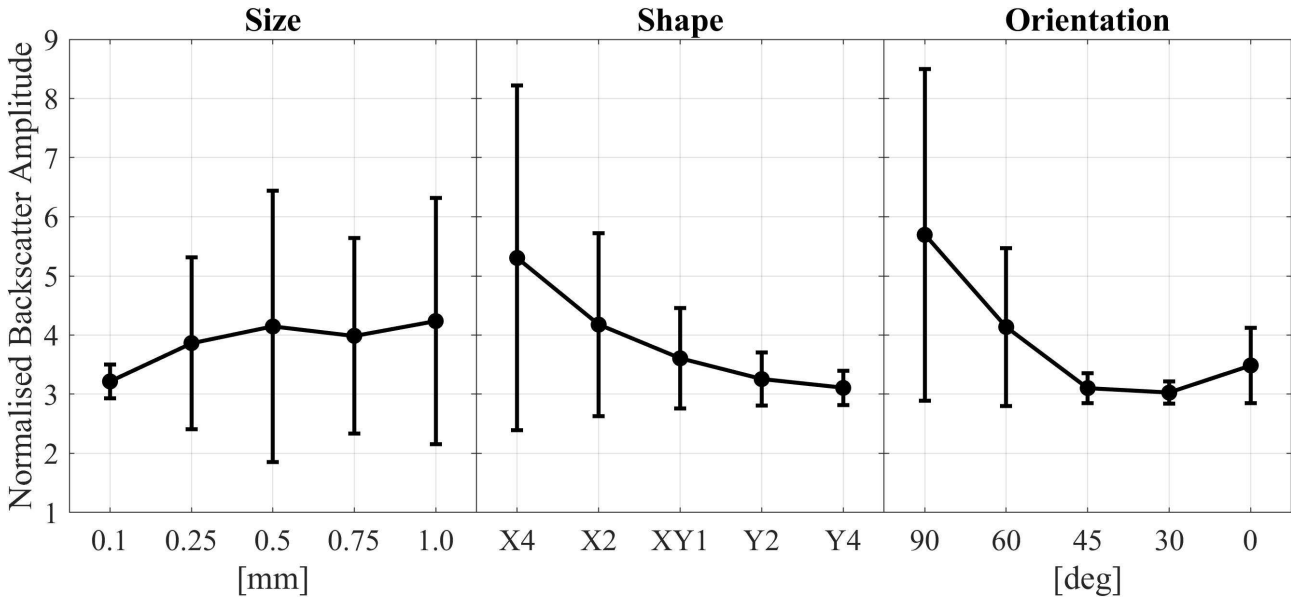


Figure 3.9: The main effects plot for backscatter highlights the correlation between ultrasound backscatter and the three macrozone characteristics: (a) size, (b) shape, and (c) orientation.

This backscatter variation due to macrozone size and shape can be further explained using a scattering profile. This was generated with FE simulation as illustrated in Figure 3.10. The setup is shown in (a) which consists of a circular ring of receivers represented by the white-dotted line with a longitudinal excitation source located at the top. In (b) at time = $1.25 \mu\text{s}$, the longitudinal wave is excited and propagates downwards. In (c) at time = $2.5 \mu\text{s}$, the wave interacts with the macrozone located at the centre which generates longitudinal and mode-converted shear scattered signals in all directions which are captured by the ring of receivers. The longitudinal scattered signals are Fourier transformed to obtain the scattering amplitude at the excitation frequency (10 MHz).

The scattering profiles generated for three different macrozones are illustrated in Figure 3.10 (d), with the incident wave from the 90° direction. The macrozones are shown in the legend and contain different sizes and shapes but with the same cross-sectional length. Their scattering profiles are represented by the respective coloured lines, with particular focus on the backscattered signals directed along the 90° angle. Even though the X-elongated macrozone (red)

is the smallest, it generated the largest backscattered amplitude compared to the other two macrozones because of its preferential pancake shape that presents a large effective scattering surface normal to the incident wave direction. Hence, this demonstrates why macrozone shape has a greater impact on backscatter amplitude than macrozone size.

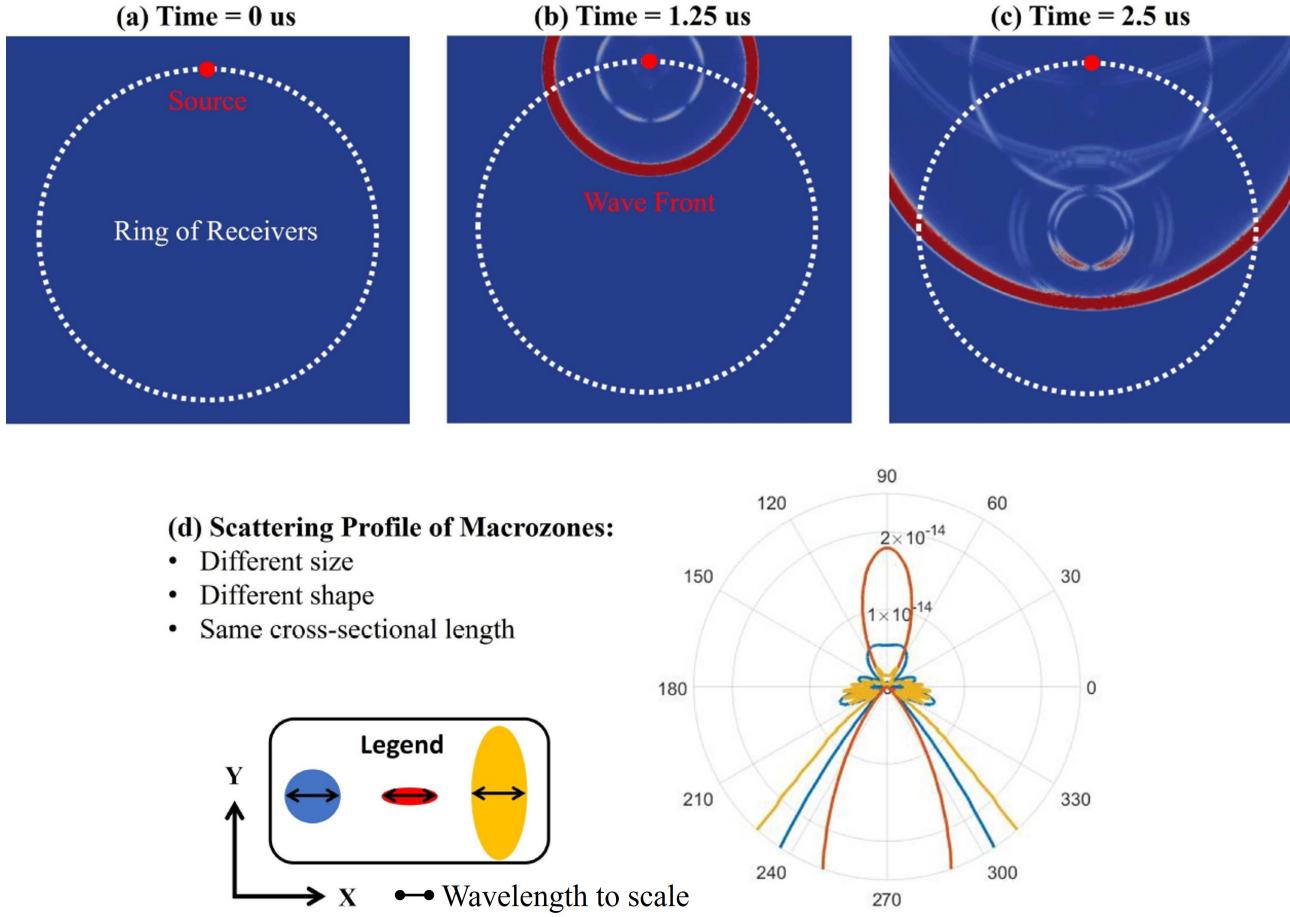


Figure 3.10: (a) The model setup contains a ring of receivers represented by the white-dotted line with a source located at the top. (b) A longitudinal wave is excited which propagates downwards. (c) The propagated wave interacts with the macrozone at the centre which generates scattered signals in all directions. (d) The scattered profile generated with the wave incident from the 90° direction. The coloured lines depict three macrozones with the same cross-sectional length but different sizes and shapes.

In Figure 3.9, a dip in the mean backscatter profile with respect to different macrozone sizes at 0.75 mm diameter was observed. The dip is a result of the macrozones having a dimension that is half the longitudinal wavelength along the wave propagation direction. This leads to a destructive interference between the backscattered signal generated from the top and bottom boundary of the macrozone. This effect is demonstrated using single-macrozone models as illustrated in Figure 3.11 which shows the backscatter (a) time-domain signal and (b) frequency

response of three pancake (X4) macrozones with varying sizes. From both figures, the amplitude response from the 0.75 mm pancake macrozone is the smallest as its dimension along the wave propagation direction is closest to half the longitudinal wavelength, resulting in a distorted time domain signal and reduced backscatter intensity in the frequency spectrum. A similar phenomenon was also observed by Liu et al. [60] whereby the backscatter amplitude from singular inclusions were modelled using FE and analytical solutions based on the Born approximations [53]. This also highlights the potential of being able to use backscattering amplitude and the Born approximation to quantify macrozone dimensions.

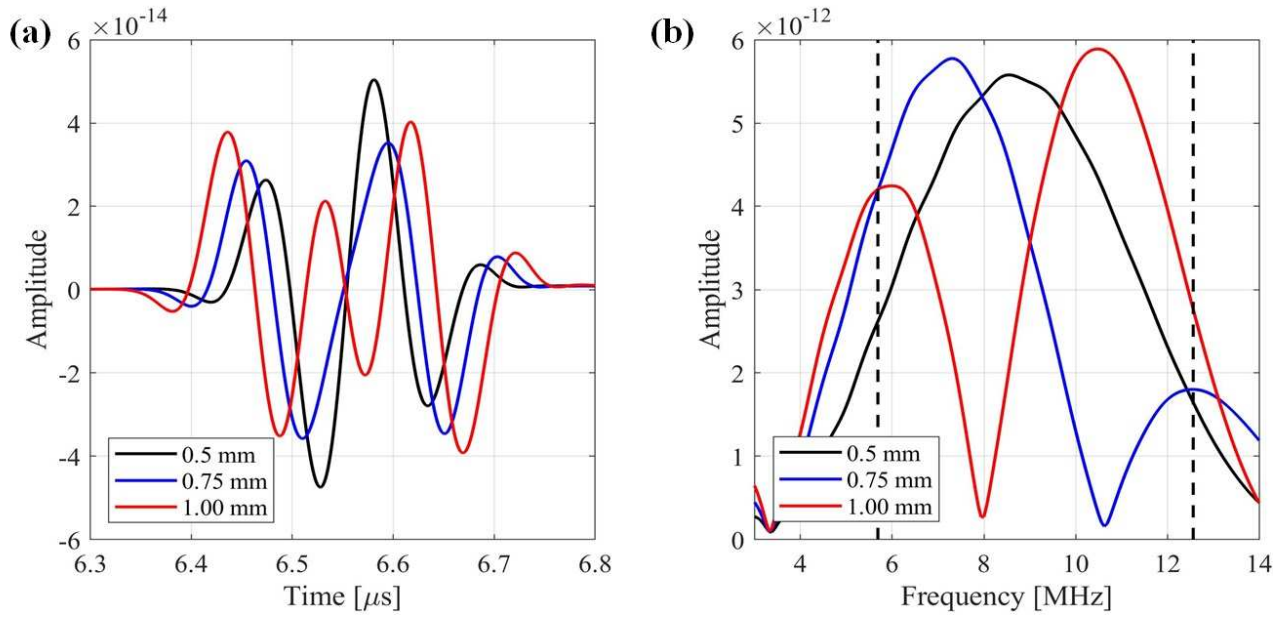


Figure 3.11: (a) Time domain backscatter signals and (b) the respective frequency spectrum of single-macrozone models with varying sizes only (same shape and crystal orientation).

3.3.3 Velocity

Lastly, effects of different macrozone characteristics on ultrasound velocity are discussed. From the Pareto chart in Figure 3.12, macrozone crystal orientation has the largest impact, followed by size, and lastly the shape of the macrozone that is deemed to be statistically insignificant.

Any variation in velocity is generally caused by the presence of texture (preferred crystal orientations) that is dependent on the area (2D) or volume (3D) of macrozones present [93]. As such, from the main effects plot in Figure 3.13, ultrasound velocity increases with macrozone

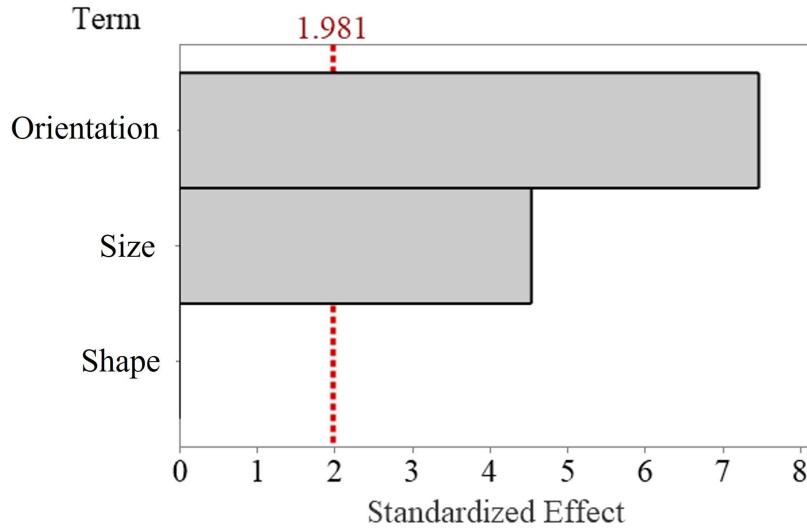


Figure 3.12: Pareto chart of the standardised effects for velocity predicted at a 95% confidence interval. The red line (1.981) indicates that factors exceeding this are deemed to have a statistically significant impact.

sizes, whereas any macrozone elongation does not affect the area of the macrozone and hence is insignificant towards ultrasound velocity. Lastly, velocity varies monotonically with crystal orientation, akin to the velocity profile in Figure 3.7 where velocity is highest along the macrozone C-axis (oriented at 90°).

The actual variation in the mean velocity within the range of modelled parameters is minute, with only an 8 m/s difference for an orthogonal shift in the crystal orientation of the macrozones. Even though bulk texture is not considered in this study, it does indicate that small changes in velocity might not be easily detectable in Ti-64 samples with small volumes (3D) of MTR.

3.3.4 Discussion

The parametric study demonstrates that crystal orientation exerts the largest influence on ultrasonic attenuation, backscatter, and velocity, followed by macrozone size, while macrozone shape plays a secondary role.

This hierarchy can be explained by the anisotropic nature of the Ti-64 polycrystalline structure. The directional dependence in the wave velocity of the HCP crystals indicates that any misalignment of the C-axis with or against the incident wavefront and surrounding polycrystals

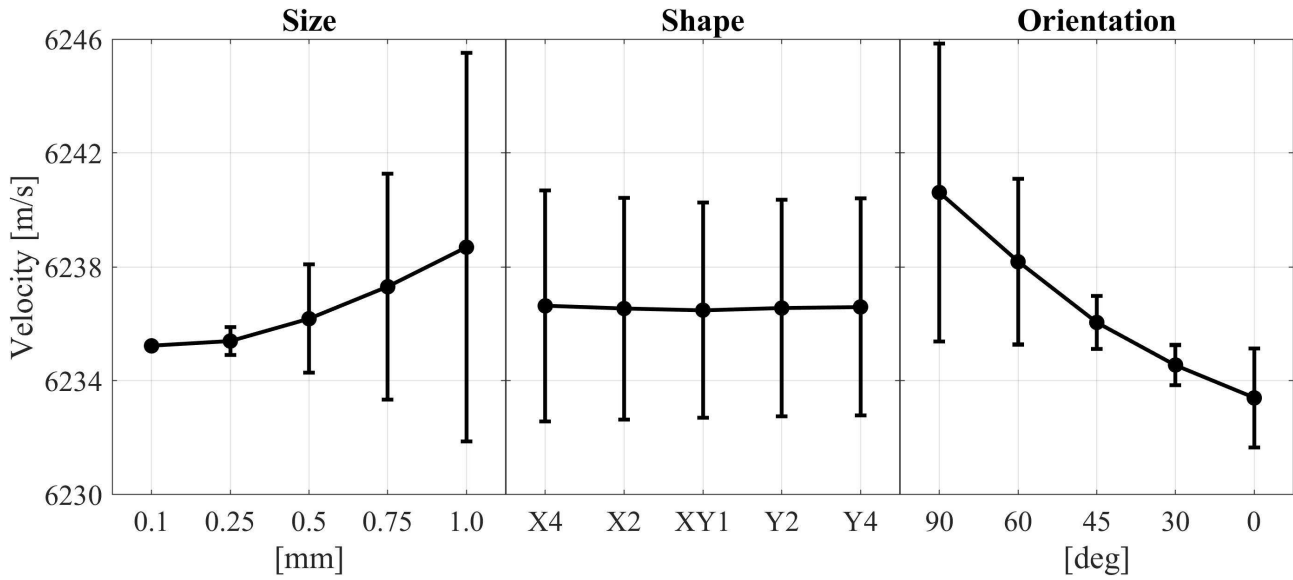


Figure 3.13: The main effects plot for velocity highlights the correlation between ultrasound velocity and the three macrozone characteristics: (a) size, (b) shape, and (c) orientation.

creates significant velocity and impedance mismatches. This velocity contrast results in scattering and mode-conversion along the grain boundaries, elevating attenuation levels, increasing backscatter amplitudes, and influencing the wave velocity.

In comparison, macrozone size affects the amplitude of scattering effects. Larger macrozones have stronger influence on ultrasound scattering due to the increased cross-sectional area and this amplifies the attenuation, backscatter, and velocity responses. However, the effect is weaker than crystal orientation because the size influences the magnitude of scattering, while orientation fundamentally changes the nature of scattering through crystal anisotropy and velocity mismatch between neighbouring grains.

Shape effects were found to be the least significant, particularly for velocity, since they do not affect the overall area of the macrozones. For attenuation effects, the low significance is attributed to the operating scattering regimes. The wave behaviour in Ti-64 is expected to follow the conventional Rayleigh and stochastic scattering mechanisms used to describe wave scattering from polycrystalline material [32, 34, 89]. Hence, macrozones with sizes much smaller than the wavelength operate within the Rayleigh regime ($kd \leq 1$), and macrozones with sizes comparable to the wavelength operate within the stochastic regime ($kd > 1$).

Within the Rayleigh regime, for the same size and crystal orientation, any shape variation in the macrozone has a limited effect on attenuation. However in the stochastic regime, any elongation of the macrozones increases attenuation due to additional phase perturbation along the length of the macrozones and vice versa [43].

A comparison of the simulated attenuation for different macrozone shapes (with respect to the circular macrozone) in the Rayleigh and stochastic regimes is shown in Figure 3.14. In each regime, the respective areas of the macrozones are held constant. In the Rayleigh regime, the percentage difference calculated using the equiaxed case (XY1) as a reference holds steady at about zero, whereas in the stochastic regime, attenuation increases monotonically with macrozone elongation along the wave direction.

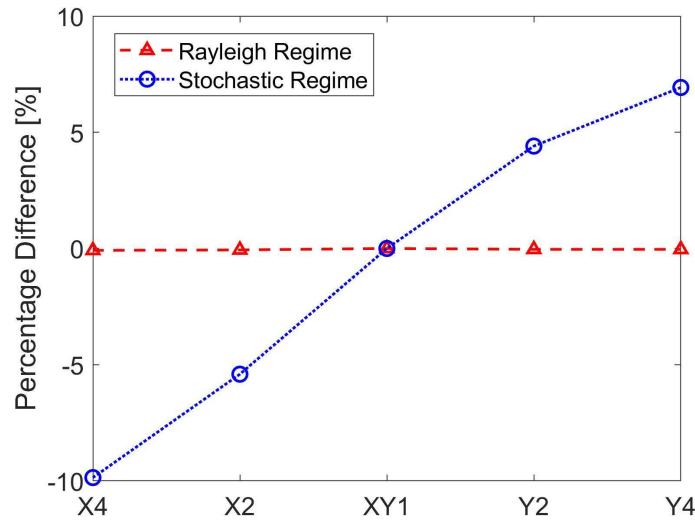


Figure 3.14: Percentage difference in the simulated attenuation of different macrozone elongation ratios with respect to the equiaxed macrozone in the Rayleigh ($kd \approx 1$) and stochastic regimes ($kd \approx 10$).

Hence, to use ultrasound measurements to characterise macrozones, it is advisable to operate within the stochastic regime, where the wavelengths are comparable to the morphologies of the macrozones, and have enhanced sensitivities to them compared to smaller grains in the background. Macrozone sizes typically range from microns up to the mm scale [5], so the operating frequency should be about 5 to 15 MHz to remain within the stochastic regime.

Looking back at the main effects plot for attenuation (Fig 3.4), backscatter (Fig. 3.9) and velocity (Fig 3.13), the large variation in standard deviation indicates certain compounded influence between the parameters. For example, in the attenuation plot with the largest macrozone size,

a combination of X4 elongation with 45° crystal orientation results in a small attenuation of 0.8 Np/m, whereas a Y4 elongation with 90° crystal orientation leads to a higher attenuation of 4.2 Np/m. Hence, having certain macrozone characteristic combinations leads to a non-linear variation in the measured attenuation. The lack of independence of the parameters imposes some limitations on the possibility of drawing rigorous conclusions from the Pareto charts. Nevertheless, this approach is effective in providing key insights to the behavioural trends.

The wave-macrozone interactions can be summarised into three general cases as highlighted in Figure 3.15:

1. In the first case, the C-axis of the macrozone is parallel to the grain elongation axis. High attenuation is expected along the Y-direction due to the preferred C-axis orientation leading to stronger wave distortion, and the elongated grain increases the phase perturbations further. Medium backscatter amplitude is obtained along the X-direction mainly due to the larger pancake shape and the preferable surface profile which leads to more coherent backscatter amplitude signals.
2. In the second case, the C-axis of the macrozone is normal to the grain elongation axis. High attenuation is expected along the X-axis due to the preferred C-axis orientation as a result of stronger wave distortion. Even though the grain is elongated along the Y-axis, the DOE study has concluded that crystal orientation plays a more significant role as opposed to grain shape when it comes to ultrasonic attenuation measurements. As such, attenuation along the Y-axis is of a medium level, since the elongated length increases phase perturbations. As for backscattering amplitude, it will be higher along the X-axis due to the preferable surface profile and C-axis orientation.
3. In the third case, the macrozone is spherical in shape. Since the macrozone is symmetrical in shape, the direction of higher attenuation and backscatter follows the C-axis orientation of the macrozone—which in this case is along the Y-axis—since there is a larger velocity mismatch between the macrozone and the background in this propagation direction.

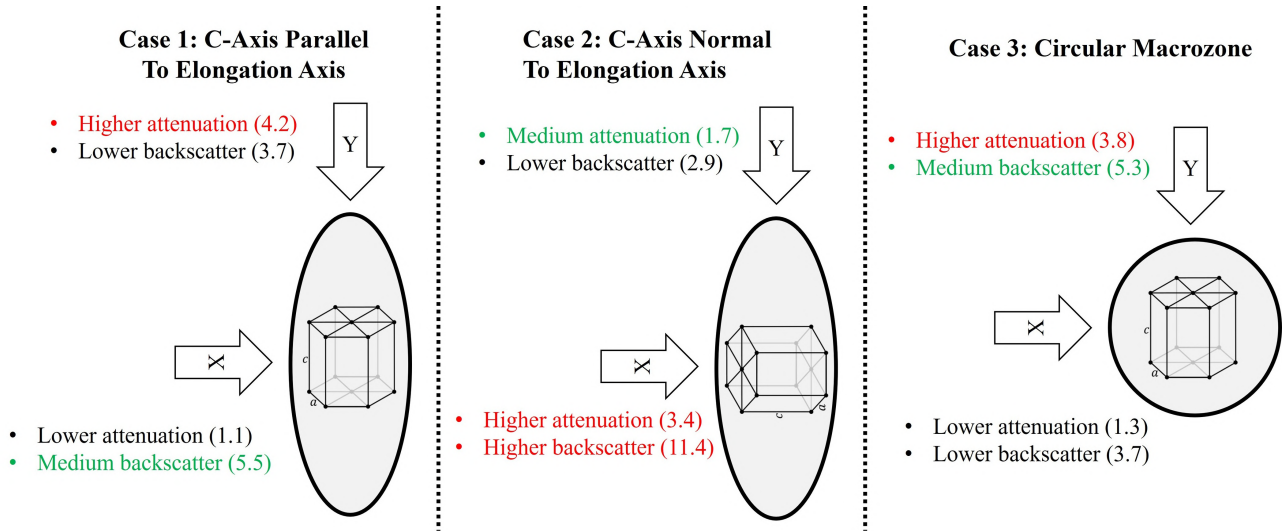


Figure 3.15: The ultrasound attenuation (Np/m) and backscatter (arbitrary normalised amplitude) response with respect to three general cases of macrozones of 1 mm size in equivalent diameter are summarised in this figure. For case 1, the macrozone C-axis orientation is parallel to the elongation axis. In case 2, the macrozone C-axis orientation is normal to the elongation axis. In case 3, the circular macrozone has its C-axis orientation along the Y-direction.

These cases demonstrate how different macrozone-parameter combinations give rise to varying ultrasound responses in orthogonal directions. Cases 1 and 2 both have the same elongated macrozones but due to them having a different C-axis orientation, the attenuation and backscatter responses vary significantly. It is crucial to note that the macrozones are normally generated through deformation processes such as rolling, and the preferred C-axis orientations usually follow the deformation and grain elongation direction [95]. As such, cases 1 and 3 are more common than case 2. Nevertheless, these various 2D cases serve as a reference for experimental measurements and can provide some qualitative insights toward the general 3D macrozone configuration.

The spatial density of the macrozones is defined arbitrarily as the goal was to include multiple macrozones to emulate realistic samples. Even though the density of the macrozones are not the goal of this study, it will influence the result. Having less-dense macrozones will generally result in lower attenuation and backscatter, whereas velocity will depend on the overall bulk texture. Hypothetically, there exists an upper limit to the effect of increasing macrozone size and density. In the limiting case where macrozones increasingly overlap, the material approaches effectively single-crystal behaviour. This reduces the number of grain boundaries, leading to diminished

microstructural scattering and therefore lower attenuation and backscatter responses. This represents a conceptual upper limit rather than a quantified maximum point in the present study.

3.4 Experimental Validations

Building on the parametric investigation of macrozones using FE models, this section validates the qualitative findings through experimental measurements. The aim is to confirm that the predicted behaviours can be reproduced on physical samples, thereby establishing the reliability of the modelling approach.

In the experimental study, ultrasonic attenuation, backscatter, and velocity measurements are all employed for qualitative macrozone characterisation, consistent with the modelling framework. Particular emphasis is placed on ultrasonic backscatter, as it uniquely provides depth-dependent information that cannot be obtained from bulk-averaged attenuation or velocity measurements. This capability is especially relevant for experimental validation, where spatial localisation of macrozones is important. The experimental results are subsequently benchmarked against EBSD data to assess the viability of this method for macrozone quantification.

3.4.1 Methodology & Configurations

Experiments were carried out on two cubic Ti-64 samples, each with dimensions of 45 mm. The specimens—referred to as the Big-MTR and Small-MTR samples—were provided by IHI and underwent different heat treatment and deformation processes to produce distinct macrozone populations. EBSD images of the three orthogonal surfaces shown in Figure 3.16 were also performed by IHI.

Ultrasonic measurements were performed using a water-immersion pulse-echo setup with a 10 MHz planar transducer (diameter: 6.35 mm, stand-off: 25 mm, step size: 0.2 mm). The transducer spot size on the sample surface, estimated via a Huygens' model, was approximately

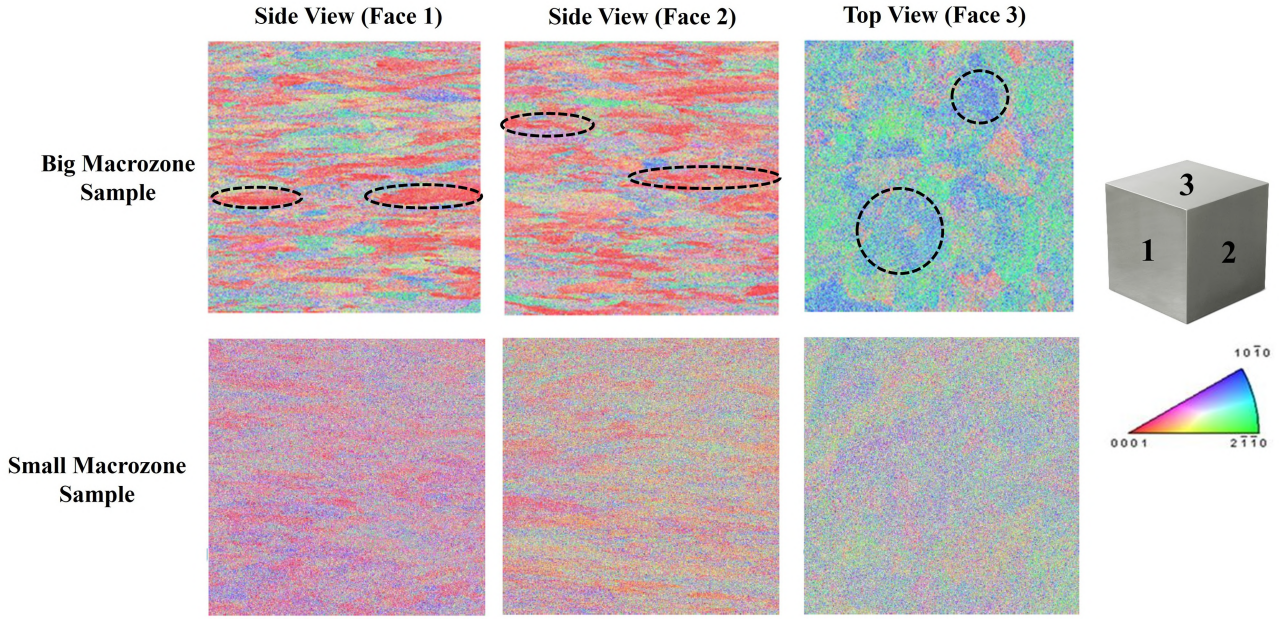


Figure 3.16: EBSD images of the three orthogonal surfaces of the Big-MTR and Small-MTR Ti-64 samples (10×10 mm area). The colour code represents the grain orientations as depicted by the Inverse Pole Figure. The macrozones with pancake-like geometries are outlined for illustration.

4 mm. The Peak NDT LT2 ultrasonic inspection system is used for signal acquisition at a sampling rate of 200 MHz to provide sufficient oversampling of the 10 MHz excitation to ensure accurate time- and frequency-domain analysis while avoiding aliasing effects. A total of 128 averages were applied to reduce uncorrelated electronic noise while improving the signal-to-noise ratio.

A representative time-domain signal from the Big-MTR sample is presented in Figure 3.17. The front and back wall reflections are used to calculate attenuation and velocity, while the low-amplitude backscatter response is highlighted through signal magnification.

Attenuation and velocity were determined using equation (4.1) [45] and the cross-correlation method [84]. The results are acquired and averaged over a 120×120 grid of spatial positions to further suppress incoherent noise. Backscatter signals were quantified via the RMS method in the frequency domain to generate a backscatter spectral response [55], with characteristic peaks around 9 MHz shown in Figure 3.18. Notably, the backscatter responses along face 3 were stronger than those along faces 1 and 2, indicating increased sensitivity to the presence of macrozones.

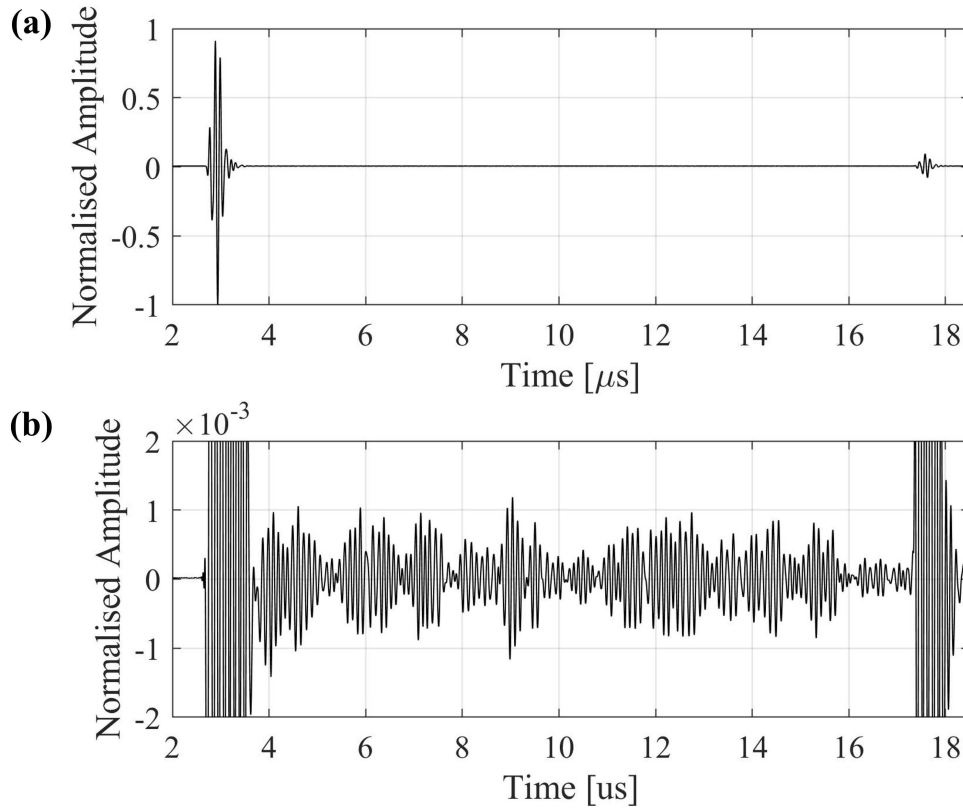


Figure 3.17: Experimental time-domain signal obtained from the Big-MTR sample. (a) Front and back wall reflections used for attenuation and velocity calculations. (b) Magnified view capturing the low-amplitude backscatter signals.

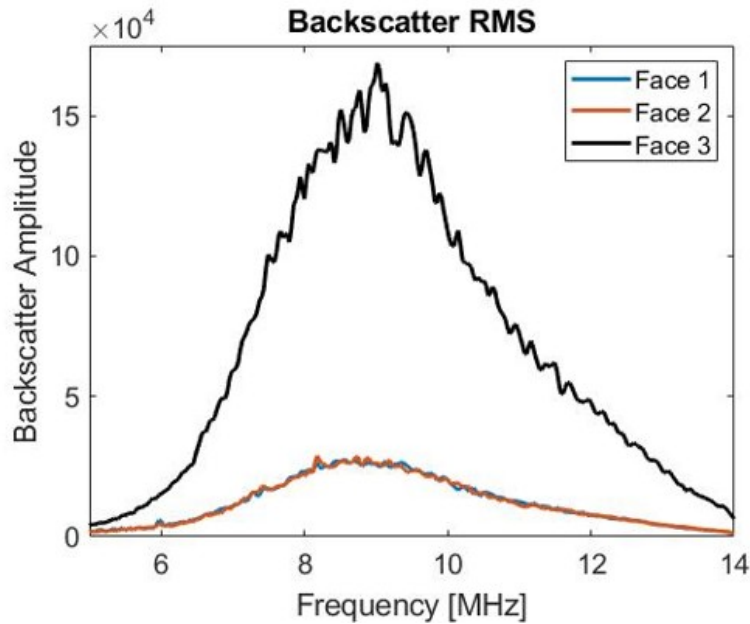


Figure 3.18: Experimental backscatter spectral response obtained for all three orthogonal faces on the Big-MTR sample, extracted through an RMS operation in the time-domain, followed by Fourier transform.

Since the higher backscatter response along faces 3 and 6 indicate higher sensitivity to the presence of macrozones, the signals along these faces are selected for further evaluation. Figure 3.19 (a) shows the backscatter RMS profile across depth for the two faces. The signal amplitude drops off rapidly with depth due to energy loss from beam spread and material scattering, both of which need to be compensated for.

Notably, the two RMS profiles in the time domain exhibit different gradients as observed in Figure 3.19 (a). If macrozones were uniformly and randomly distributed through thickness, the profiles would start at comparable values and decay at similar rates. Instead, the larger near-surface amplitude and faster decay on face 6 indicate a higher concentration of macrozones near that surface, implying a non-uniform depth distribution as illustrated in Figure 3.19 (b). Under such anisotropic conditions, conventional attenuation compensation is insufficient, motivating the cross-compensation approach introduced here.

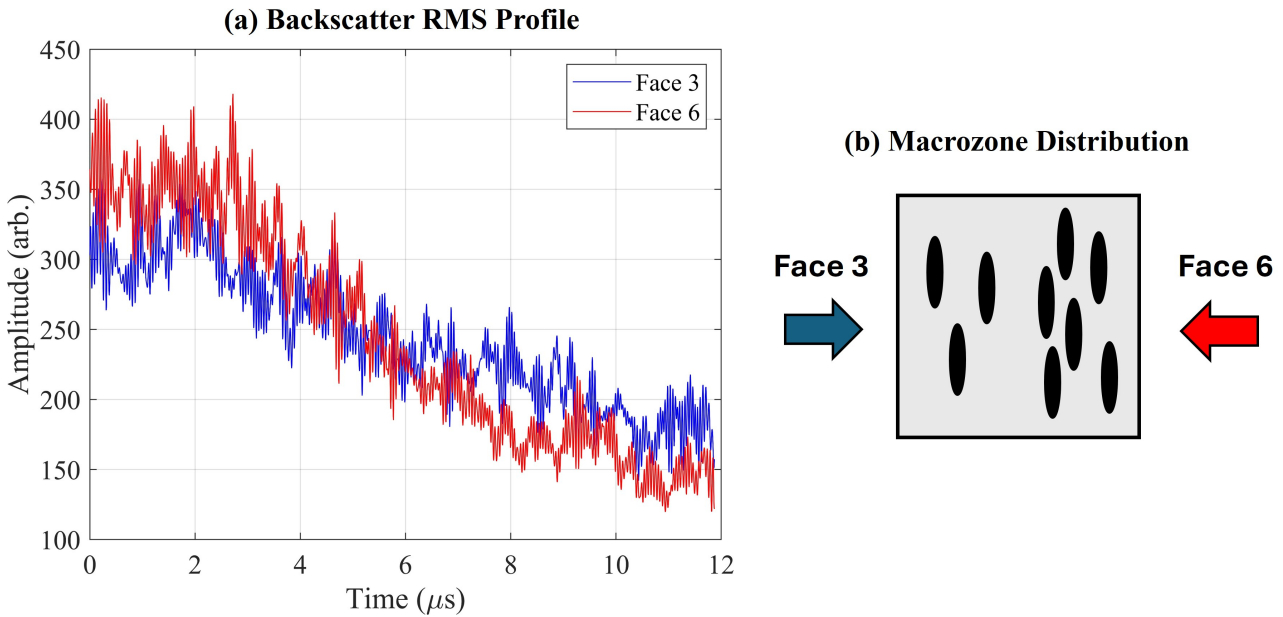


Figure 3.19: (a) Spatially averaged backscatter signal profile in the time domain through RMS operation across the two opposing scanning faces 3 and 6 from the big-MTR sample. (b) The difference in the starting amplitude and decay rate of the profiles indicates the presence of non-uniform macrozone distribution within the sample.

The cross-compensation method assumes that near-surface backscatter amplitudes represent the intrinsic microstructural scattering strength before significant propagation-related energy losses occur. Based on this assumption, near-surface time windows from faces 3 and 6 are selected as two reference levels, representing opposite sides of the sample, as illustrated in Figure

3.20. These reference values serve as anchor points for compensating the depth-dependent backscatter response.

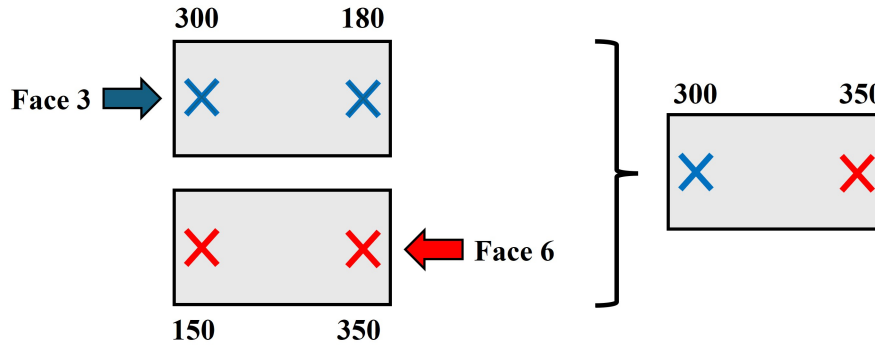


Figure 3.20: Near-surface backscatter amplitude (illustrated with arbitrary values) which serve as references to help compensate and reconstruct the original backscatter signals.

To account for gradual energy losses arising from beam divergence, attenuation, and distributed scattering, a smooth baseline profile is reconstructed between the two anchor points using a low-order polynomial interpolation. This polynomial does not represent a physical scattering model; rather, it provides an estimate of the slowly varying system- and propagation-induced amplitude decay. The raw backscatter profiles are subsequently normalised with respect to this baseline, yielding compensated backscatter signals that are less sensitive to non-microstructural effects, as shown in Figure 3.21.

Following the compensation strategy, a Hilbert transform is applied to obtain the envelope of the backscatter signals. Regions of elevated backscatter intensity are then identified using a threshold of 50% of the maximum envelope amplitude, which serves as a pragmatic detection criterion for identifying large macrozones.

3.4.2 Experimental Results

3.4.2.1 Bulk Characterisation

The experimental attenuation and backscatter measurements are summarised in Figure 3.22 and Table 3.2. For the Big-MTR sample, backscatter amplitudes are significantly higher along face 3, while attenuation is highest along faces 1 and 2. The elevated attenuation in these directions

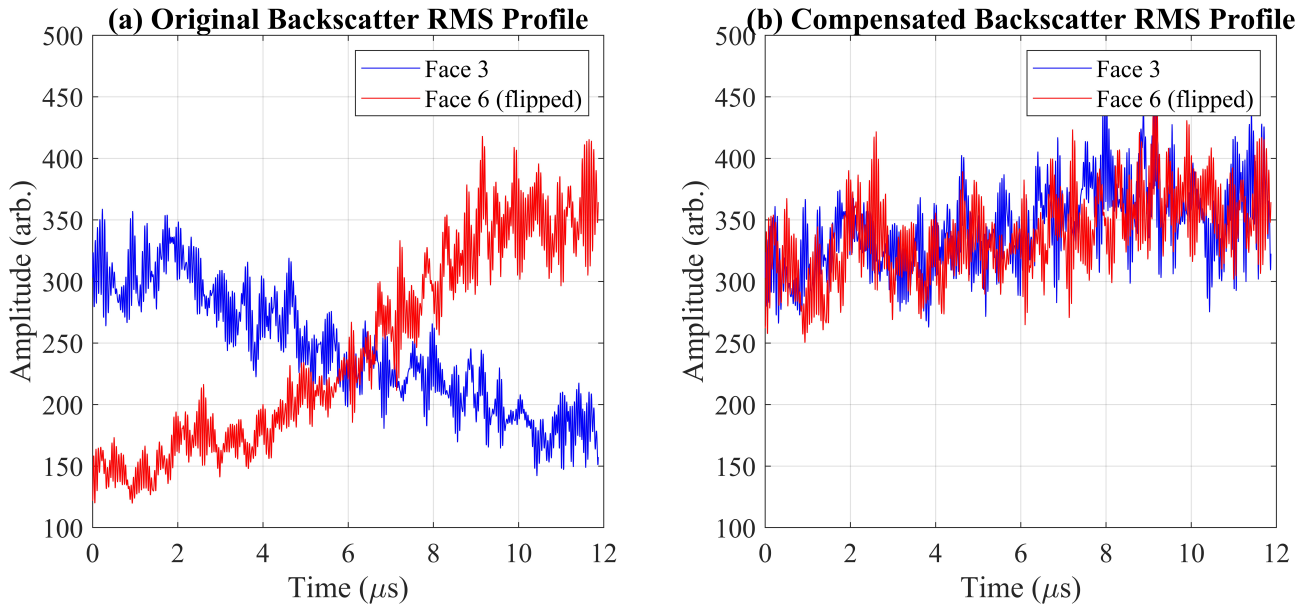


Figure 3.21: (a) Original backscatter RMS profiles from face 3 and face 6, exhibiting pronounced depth-dependent decay and directional mismatch. (b) Backscatter RMS profiles after cross-directional compensation, showing reduced depth bias and improved alignment of depth trends between opposing scans.

arises from preferred C-axis orientations, which enhance beam distortion and extend the mean grain length, thereby increasing phase perturbation. In contrast, the stronger backscatter along face 3 is attributed to a larger macrozone surface area normal to the propagation direction. Such opposing behaviours across orthogonal faces are consistent with previous studies [96, 97].

The variability observed in the attenuation profiles in Figure 3.22 (a), expressed by standard deviations, reflects the random spatial distribution of macrozones. The propagating wave encounters macrozones of varying sizes and densities at different positions. This variation affects the scattering of waves and therefore leads to varying attenuation measurements.

The measured velocities are listed in Table 3.2. For both samples, velocities are higher along faces 1 and 2, consistent with the macrozone C-axis alignment. The velocity variation in the Big-MTR sample is approximately 112 m/s, compared with 56 m/s in the Small-MTR sample. The reduced variation in the Small-MTR sample indicates smaller or less dense macrozones, consistent with weaker texture. These findings are supported by EBSD images in Figure 3.16, which show finer grain clusters in the Small-MTR sample, and align with both FE model predictions (Figures 3.4 and 3.9) and earlier experimental results [73].

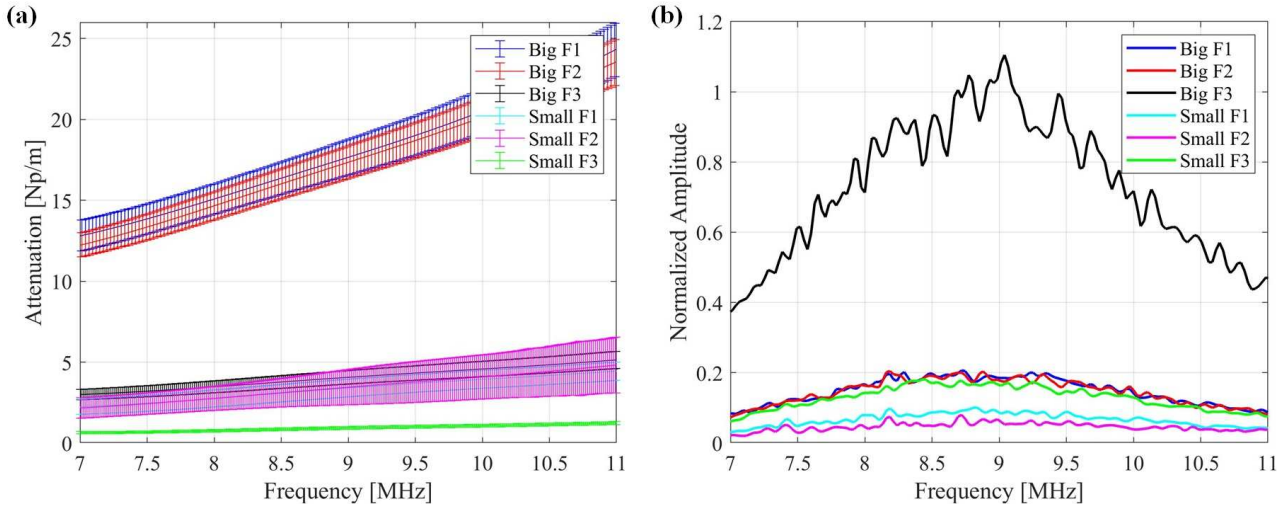


Figure 3.22: Experimentally measured (a) average attenuation and (b) backscatter RMS for both the big and small MTR samples along all 3 orthogonal faces.

To relate experimental results to the 2D FE predictions in the earlier section, ultrasound responses at 10 MHz are compared in Table 3.2. Backscatter ratios were obtained by dividing the corresponding RMS profiles illustrated in Figure 3.22 (b). This enables a direct comparison between the FE models and experiments as the effects of the receiver size are reduced. The results confirm the trends identified in the models: attenuation and velocity are elevated along elongation and C-axis directions (faces 1 and 2), while backscatter is highest perpendicular to elongation axis (face 3). These observations suggest a pancake-like macrozone morphology, which is corroborated by EBSD analysis (Figure 3.23) and consistent with prior literature [74, 98].

Table 3.2: Attenuation, backscatter ratio, and velocity measured from the 2D FE model and experiments with the Small- and Big-MTR samples at 10 MHz operating frequency.

		Attenuation (Np/m)	Backscatter Ratio (S/E)	Velocity (m/s)
2D FE Model	Elongated (E)	4.2	1.5	6250
	Shortened (S)	1.1		6230
Small MTR Sample	Face 1 (E)	3.5	2	6229
	Face 2 (E)	3.5		6216
	Face 3 (S)	0.9		6166
Big MTR Sample	Face 1 (E)	20.5	5	6254
	Face 2 (E)	20.1		6256
	Face 3 (S)	4.6		6143

Interestingly, in the Big-MTR sample, wave propagation along faces 1 and 2 yields high attenuation but low backscatter. This apparent loss of energy arises because needle-like macrozone profiles generate little backscatter but strongly distort the forward-propagating wavefront

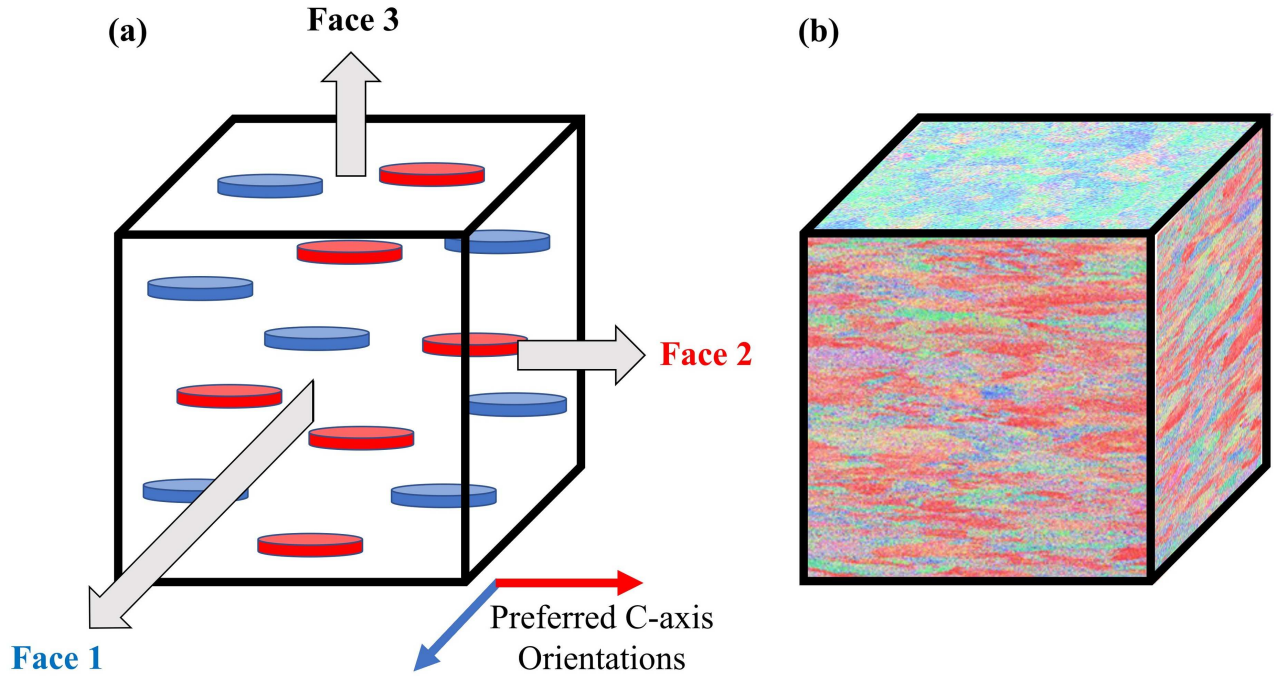


Figure 3.23: (a) Visualisation of pancake-shaped macrozones in the Big-MTR sample, with preferred C-axis orientations along Faces 1 and 2. (b) EBSD maps of the three orthogonal faces, where the colour red corresponds to grains with C-axes oriented normal to the surface.

through C-axis alignment, producing destructive interference at the receiver. This beam distortion phenomenon has been reported previously [74]. Energy conservation is nevertheless preserved, as confirmed by FE simulations at the experimental frequency.

Bulk characterisation using backscatter ratio inversion method [72, 97] was further applied to estimate the macrozone dimensions. By comparing the orthogonal backscatter data and fitting of analytical functions, dimensions on the order of 0.3×0.1 mm were obtained as listed in Table 3.3. These are consistent with the EBSD results that measures the average macrozone dimension within the 10 by 10 mm scanned region in Figure 3.16, with reference to face 1 of the big macrozone sample.

Table 3.3: Macrozone dimensions estimated via EBSD and backscatter ratio inversion method

	Diameter (mm)	Thickness (mm)
EBSD	0.35	0.11
Backscatter Ratio	0.27	0.08

However, it should be noted that the analytical backscatter ratio inversion method relies on several simplifying assumptions, most notably that the material can be treated as effectively

homogeneous and that crystallographic texture plays a negligible role in wave propagation. These assumptions are not fully satisfied for the Ti-64 sample considered in this study.

Evidence of significant crystallographic texture is apparent from the measured ultrasonic velocity variations between orthogonal inspection directions. In particular, longitudinal wave velocities of approximately 6254 m/s, 6256 m/s, and 6143 m/s were measured along the three orthogonal faces 1, 2, and 3, respectively, indicating direction-dependent elastic behaviour. Such velocity anisotropy is consistent with the presence of strong preferred crystallographic orientations and has also been reported in independent bulk texture measurements using established ultrasonic methods [63]. The observed velocity variations therefore suggest that texture effects cannot be neglected for this material, violating a key assumption of the analytical inversion framework.

In addition to the presence of texture, the EBSD measurements reveal a highly heterogeneous spatial distribution of macrozones. While the bulk-averaged EBSD statistics indicate average macrozone dimensions on the order of a few hundred micrometres, the EBSD map clearly shows clusters of elongated macrozones extending up to several mm in length. These large, spatially connected macrozones are particularly relevant from a fatigue and damage-tolerance perspective, yet they are inherently smoothed out by bulk-averaged inversion approaches that assume a statistically homogeneous distribution of scattering features.

As a result, the discrepancy between the macrozone dimensions estimated from backscatter ratio inversion and the visually observed macrozone morphology arises primarily from the breakdown of the underlying model assumptions. The combined presence of strong crystallographic texture and spatially heterogeneous, mm-scale macrozone clusters means that the material cannot be adequately represented by a homogeneous, weakly anisotropic medium with uniformly distributed scattering domains. Consequently, while the analytical inversion provides reasonable bulk-averaged estimates, it is not sensitive to the larger-scale spatially distributed macrozones that dominate the microstructural variability in this sample.

3.4.2.2 Spatial Characterisation

The cross-compensation method, applied to time-domain signals in Figure 3.21, was used to reconstruct three-dimensional volumetric datasets. The X–Y plane corresponds to the sectorial scanning grid, while the Z-dimension represents sample depth. Although the raw dataset contains convoluted scattering contributions, post-processing enables extraction of regions with coherent macrozone-related backscatter. This was carried out by applying an amplitude threshold at 50% of the maximum envelope amplitude.

The subsequent volumetric image revealed hotspots of high backscatter intensity when scanning from opposing faces (faces 3 and 6). As shown in Figure 3.24 (a), these regions demonstrate consistent localisation across faces, providing confidence that they originate from large macrozones. Though given the irregular geometry of microstructures in general, perfect symmetry is not expected and backscatter response will differ from opposing directions as illustrated in Figure 3.24 (b).

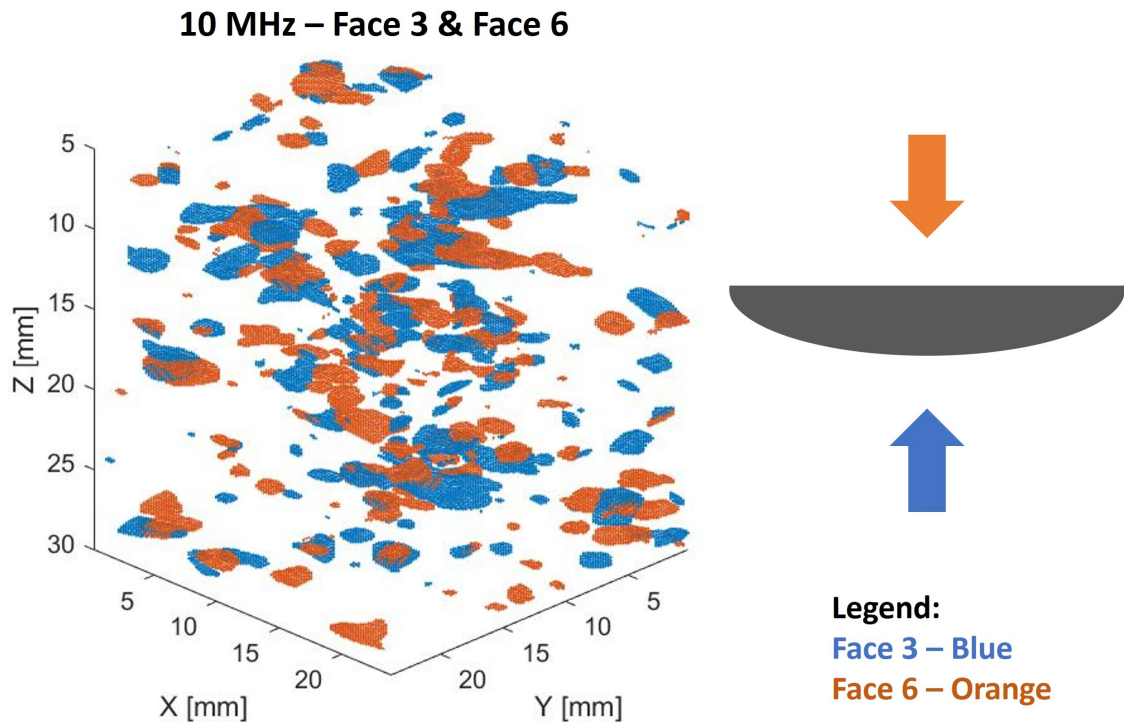


Figure 3.24: (a) Volumetric image of high backscatter intensities indicating the presence of macrozones. The colour code represents the scanning direction, with (b) showing the asymmetry of macrozones which affects backscatter amplitude in opposing directions.

Further isolation of the larger hotspots using a sizing threshold confirmed good agreement between opposing scans, as illustrated in Figure 3.25. The use of a threshold-based sizing approach is motivated by the need to identify spatially coherent regions of elevated backscatter that are less sensitive to local amplitude fluctuations and residual compensation uncertainties. By converting the backscatter response into connected regions above a consistent threshold, the method provides a robust first-order estimate of macrozone extent rather than relying on absolute amplitude values. The resulting hotspot sizes are estimated to be on the mm-scale which are consistent with EBSD observations. While refinements in compensation and threshold selection are still required to achieve precise sizing and localisation, these results demonstrate that the backscatter response coupled with the cross-compensation method can identify non-uniform macrozone distributions and provide spatially resolved characterisation.

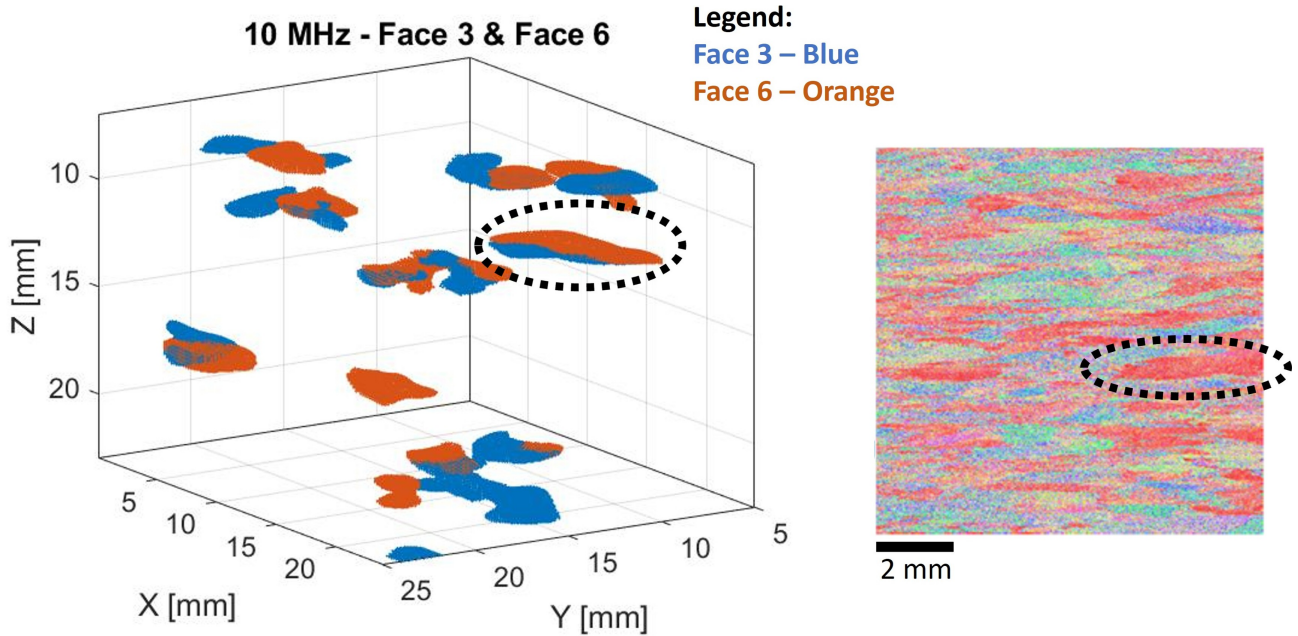


Figure 3.25: Enhanced volumetric image with sizing threshold applied highlights similar large hotspots indicative of large macrozones which are consistent with the large macrozones identified in the EBSD image.

3.5 Conclusion

This chapter set out to investigate the interaction between ultrasonic waves and macrozones through idealised 2D FE models that qualitatively represent complex grain-scale microstruc-

tures. The numerical findings were subsequently validated against experimental measurements, demonstrating not only qualitative agreement in observed trends but also quantitative consistency in relative attenuation, backscatter responses, and characteristic macrozone length scales. While absolute scattering magnitudes remain influenced by modelling assumptions and experimental conditions, the results establish the robustness of the approach for both qualitative interpretation and semi-quantitative macrozone characterisation.

Key physical insights into the wave-macrozone interactions were identified, along with the trends associated with different macrozone types. It is important to note that the general relationships observed here are also valid for general inclusions of varying sizes and shapes. The systematic study using DOE could also be expanded—if beneficial in other contexts—to include additional features, such as diagonally aligned macrozones or multiple preferred C-axis orientations. Finally, the experimental results demonstrated the potential for qualitative characterisation of bulk macrozones within the sample. Based on orthogonal experimental scans, the overall shape and texture directions of the macrozones can be inferred. More detailed information on the macrozone morphology may also be extracted from the backscattered signals.

From an industrial perspective, the methods presented in this chapter demonstrate how directional ultrasonic measurements can be used to identify microstructural anisotropy associated with macrozones. By comparing directional velocity and backscatter responses, macrozone crystal orientation and morphology can be inferred qualitatively, while their spatial extent can be estimated heuristically through subsequent EBSD verification and comparison with an idealised reference sample.

In practice, serviced aerospace components often impose angular constraints on inspection and may not be accessible for scanning in three orthogonal directions. In addition, the proposed methodology is inherently insensitive to macrozones oriented diagonally with respect to the inspected surfaces. To address these limitations, a beam-steering strategy using a tilted probe or phased-array transducer could be employed to enable multi-angle interrogation from a single surface. Such an approach would, however, require additional amplitude correction to account for beam-steering effects and energy losses at the coupling interface.

In summary, this chapter has established that the C-axis orientations of macrozones exert the greatest influence on wave scattering, followed by their size and, to a lesser extent, their shape. These findings were experimentally validated and serve to identify the key parameters governing subsequent synthetic model generation.

Chapter 4

Generation of Representative Synthetic Macrozones for Wave Propagation

4.1 Introduction

Building on the study in Chapter 3, which isolated how macrozone size, shape and C-axis orientations influence ultrasonic responses in idealised aggregates, this chapter extends the study to EBSD-derived microstructures that are representative of real titanium alloys. This chapter is based on work previously published by the author, with additional explanations and context provided here for completeness.

In this chapter, the same modelling philosophy is applied to the much more complex material microstructures of titanium alloys, by establishing a methodology to generate realistic synthetic hierarchical microstructures based on a 2D EBSD reference dataset. The reliability of this method is evaluated through replicating actual Ti-64 samples containing macrozones, followed by investigating their effect on the ultrasound wave response. This is no easy task: as will be demonstrated, solving the issues for the 2D cases is challenging enough and will therefore be the main focus of this chapter; nevertheless, the methods developed here lay down a solid foundation for the approach to be adapted into 3D and to include more diverse macrozone characteristics. With a well-defined material microstructure and definite wave response, this

approach will eventually serve as an ideal environment to systematically study the full wave-macrozone interactions and physical phenomena.

4.2 Methodology

The proposed methodology for generating realistic synthetic microstructure, based on a 2D EBSD reference dataset, is outlined in Figure 4.1. This 2D EBSD dataset is extracted from a Ti-64 billet that has undergone the full manufacturing procedure with specific tweaks to generate large macrozones. Starting from the 2D EBSD dataset, a C-axis misorientation and sizing threshold procedure is applied to extract the relevant crystal orientations and grain morphology data. Next, this data is fed into polycrystalline generation software to create a synthetic microstructure that emulates the statistical characteristics of the EBSD dataset. Finally, the synthetic microstructure is validated by comparing its morphological descriptors and simulated ultrasonic wave responses against those obtained from models derived directly from the original EBSD dataset, thereby assessing the fidelity of the synthetic representation.

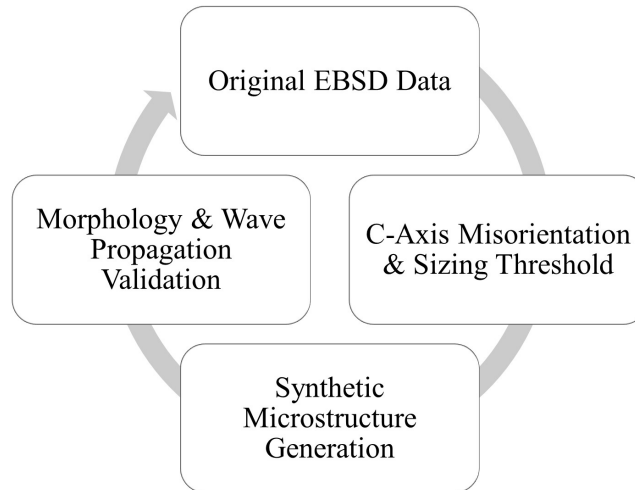


Figure 4.1: An overview of the methodology used to generate a realistic synthetic microstructure using EBSD data.

4.2.1 Finite Element Model Configuration

The basic configuration of the FE model, including meshing, boundary conditions, and loading, is similar to the one described in Chapter 3. A 10 MHz 3-cycle longitudinal plane wave is excited from a line source which is supported by symmetrical boundary conditions, coupled with the use of a structured mesh of $3\ \mu\text{m}$ to match the scanning resolution of the EBSD dataset.

The primary difference is that the 2D EBSD reference dataset is directly imported into the wave propagation model, as illustrated in Figure 4.2. The EBSD dataset has a dimension of 10 by 10 mm with a step size of $3\ \mu\text{m}$, with each pixel containing three Euler angles that describe its C-axis orientations. Since the features in the EBSD micrograph are asymmetrical, the ultrasound waves are generated in both X and Y directions to evaluate the wave response in both principal axes.

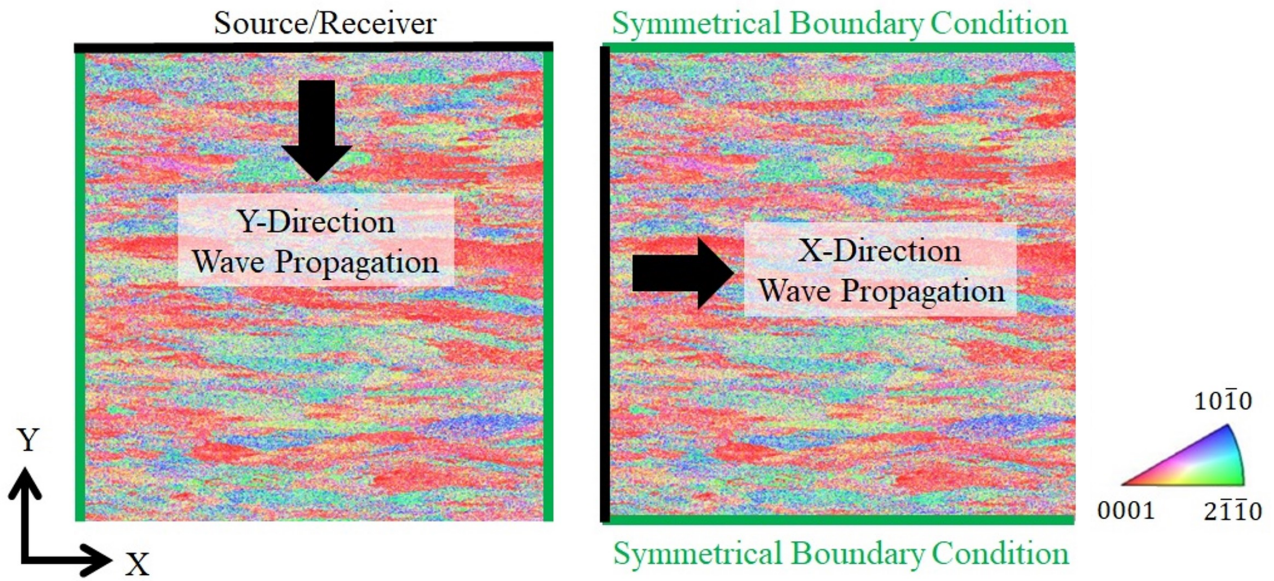


Figure 4.2: EBSD image of Ti-64 sample with the colour code indicating the orientations of the grains as depicted by the Inverse Pole Figure. The clusters of red indicate the presence of elongated macrozones. The EBSD data is configured in the FE model with a line source/receiver and symmetrical boundary conditions added on both sides to support plane wave propagation.

Once the FE wave propagation models are generated, the time-domain signals captured at the monitoring nodes are extracted for post-processing. Following the methodology described in Chapter 3, the input signal is generated by the line source on the excitation surface, represented by the black solid line in Figure 4.2. The signal propagates along the medium, reflects off the

back surface, and returns to the source, which also functions as a receiver. The received signal is obtained by summing the displacement values along the receiver line. The input and received signals are subsequently isolated for attenuation and velocity measurements.

For ultrasound attenuation measurements, the amplitude ratio between the input and back surface signals is used. Since the simulation model comprises a single medium with plane-wave propagation, the reflection/transmission coefficients and diffraction correction factor are neglected, which are both important considerations in experiments. This is represented with the simplified formula:

$$\alpha_s = \frac{1}{z} \ln \left(\frac{F}{B} \right) \quad (4.1)$$

where z is the propagation distance, and F and B are the input and back wall signal amplitudes in the frequency domain, respectively. As for ultrasound velocity measurements, the cross-correlation method is used [84]; the similarity between the input and back wall signals is measured as the latter is shifted in time. The time shift at which the best match occurs is the TOF, which, divided by the propagation distance, gives the wave velocity. Lastly, for backscatter amplitude, the backscatter signals are isolated in the time-domain, followed by a Fourier transform operation to convert the signal into the frequency domain. This is subsequently compensated by the input signal frequency response to generate a backscatter amplitude profile across the operating frequency range [72].

4.2.2 C-Axis Misorientation Threshold

Generally, the C-axis orientations of grains in actual macrozones contain certain degrees of preference statistically [87]. However, this poses a challenge in quantifying the macrozone sizes since it is difficult to identify their boundaries. To date, there is no standardised technique used to properly distinguish between the grains and macrozones and to quantify the respective feature dimensions. Consequently, an intermediate processing step is required to identify grains and macrozone regions, extract their representative dimensions and orientation statistics, and translate this information into statistically equivalent synthetic microstructures suitable for

controlled wave propagation modelling. Direct use of pixel-level EBSD orientations would not permit this level of abstraction or parametric control.

A common technique is to apply a C-axis misorientation threshold such that neighbouring crystals with misorientations below this threshold are regarded as part of the same macrozone [87]. Each grain in the synthetic microstructure is then assigned a representative crystallographic orientation, taken as the mean orientation of the corresponding macrozone region to preserve the dominant texture. However, it is also important to determine the appropriate angular threshold since it affects the measure of the overall sizes of the grains and macrozones, and as a result also impacts the wave interactions. As such, the angular threshold is varied from 5° to 25° to evaluate the suitable value for this application.

The micrographs with different angular thresholds are listed in Figure 4.3, whereby an increment in the angular threshold led to the identification of larger grains and macrozones. As evident from (a) to (c) with small angular thresholds, the macrozone boundaries are different compared to visual inspections of the original grain map, and subsequent sizing of the features proved challenging. However, an overly large threshold, such as in (f), can lead to overestimation of the grains and macrozone sizes. As such, certain criteria are needed to determine the optimal angular threshold value.

The first criterion is the preservation of macrozone morphology and crystallographic alignment consistent with the original EBSD observations, ensuring that the spatial extent and orientation continuity of macrozones are not artificially fragmented or merged. From the micrographs in Figure 4.3, only the 20° and 25° threshold cases reproduce mm-scale macrozone clusters comparable to those seen in Figure 4.2. Lower thresholds fragment these regions, while any higher thresholds lead to excessive merging of features.

The second criterion is the minimisation of artificial increases in simulated wave attenuation, which can arise if excessively large angular thresholds lead to unrealistically strong texture aggregation. The micrographs in Figure 4.3 are imported directly into the wave propagation model to simulate the wave behaviour. The resulting attenuation profiles is illustrated in Figure 4.4, where attenuation remains broadly consistent with the original profile for thresholds up to

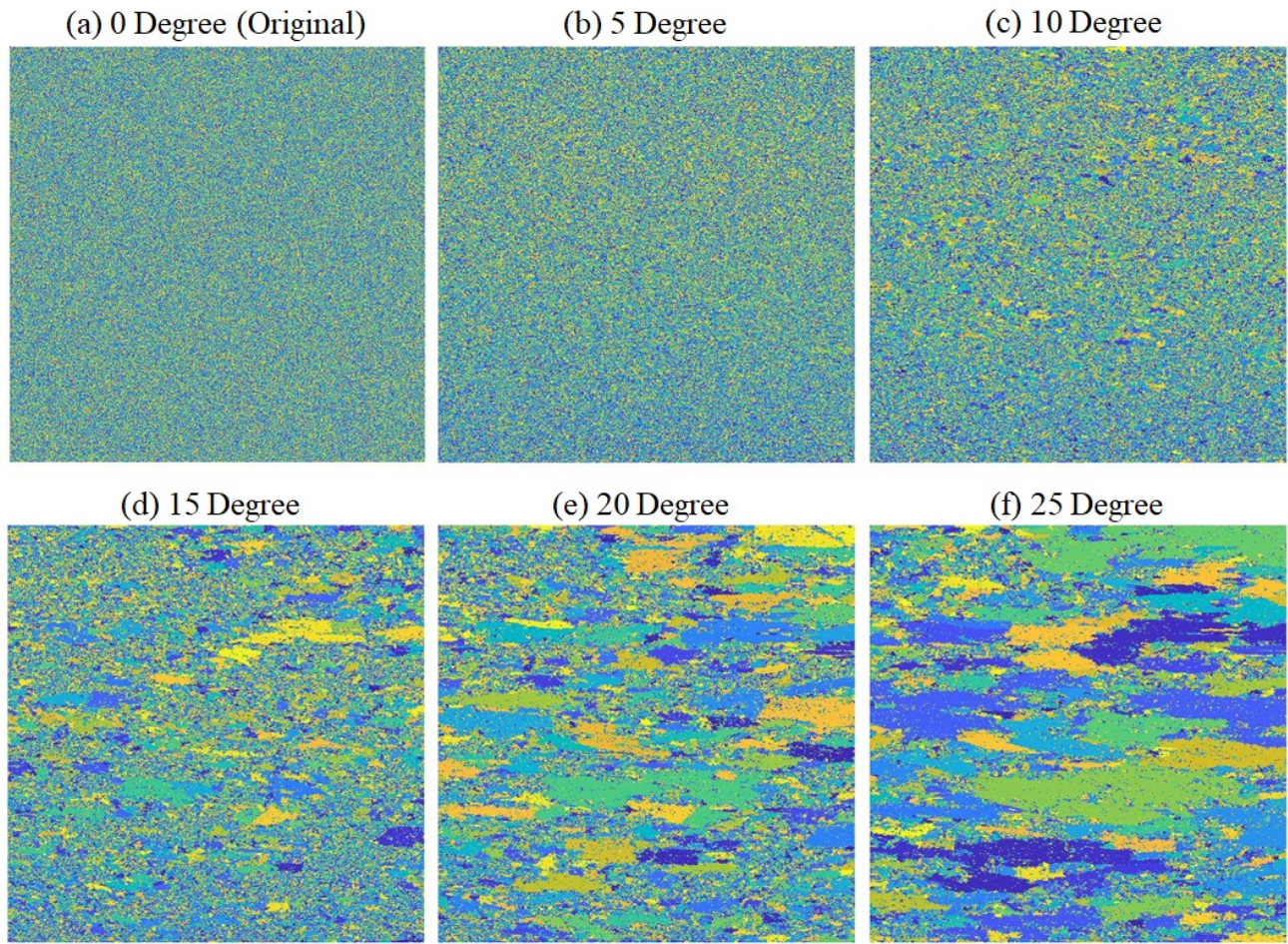


Figure 4.3: Micrographs of the EBSD data with varying angular thresholds applied from 5–25°. The colour code represents the indices of each individual feature.

20°, and a marked increase is observed at 25°, particularly in the X direction. This indicates that thresholds beyond 20° introduce artificially strong scattering due to overestimation of grain and macrozone dimensions.

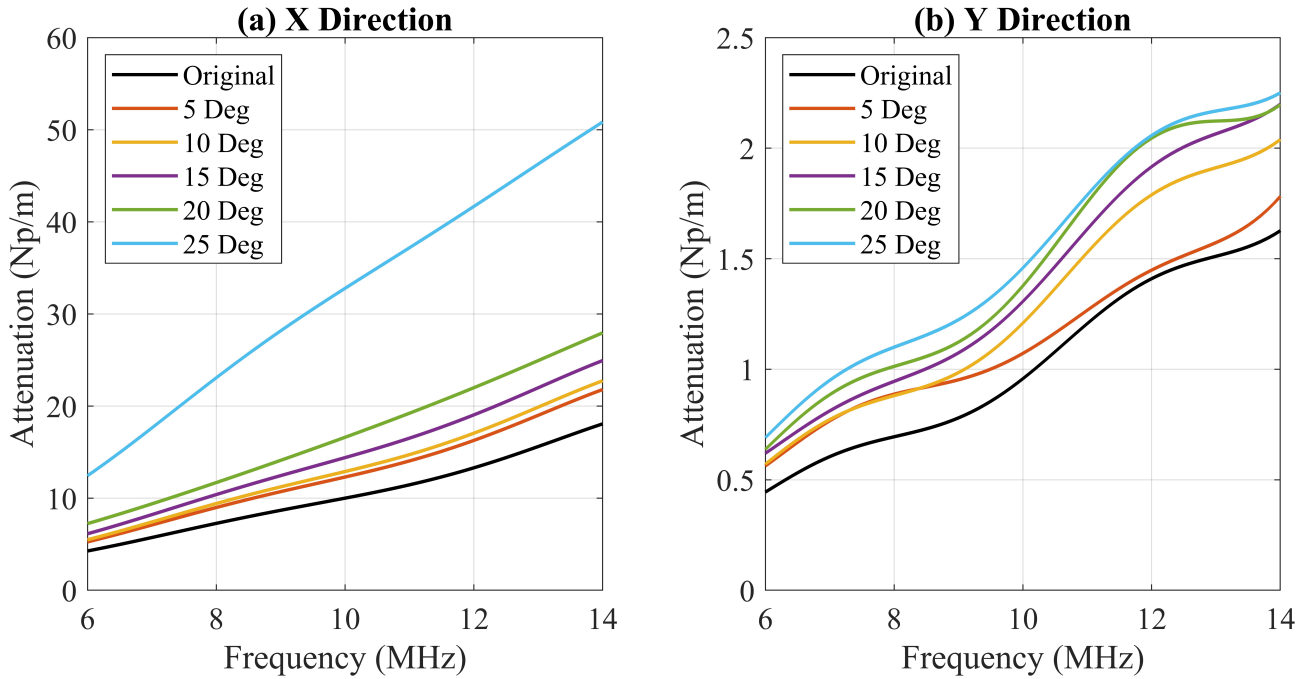


Figure 4.4: Simulated attenuation profile in (a) X-direction and (b) Y-direction for the original EBSD and the threshold cases (5–25°).

Based on these two criteria, a 20° angular threshold is selected as the most appropriate compromise. As illustrated in Figure 4.5, the 20° threshold reproduces macrozone regions that are consistent with the original EBSD data in terms of spatial extent, connectivity, and dominant C-axis orientation trends, while avoiding the excessive coalescence observed at higher thresholds. At the same time, it preserves quantitative consistency in the simulated attenuation response by limiting artificial increases associated with overestimated grain and macrozone dimensions. Hence, this 20° angular threshold provides a physically reasonable estimate of grain and macrozone morphology that is compatible with both the EBSD observations and the ultrasonic wave propagation behaviour.

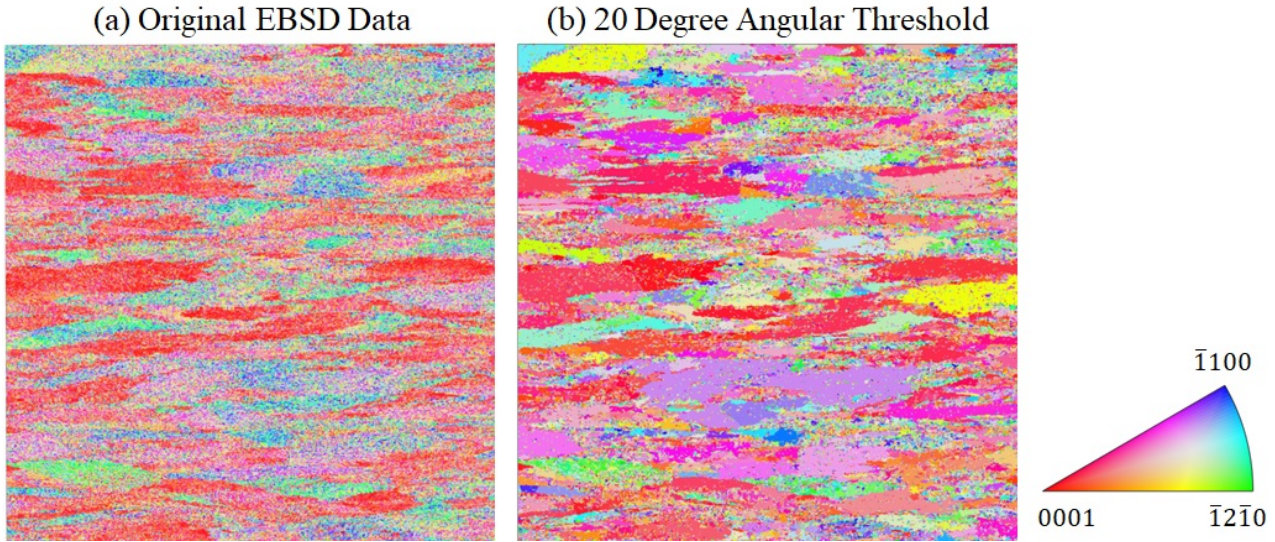


Figure 4.5: (a) Original EBSD image and (b) with 20° angular threshold applied, with consistent macrozone regions observed. The colour code indicates the orientations of the features as depicted by the Inverse Pole Figure.

4.2.3 Sizing Threshold

With the application of a 20° C-axis misorientation threshold, the grain and macrozone feature dimensions and C-axis orientations are extracted. Based on [87], a sizing threshold of 10,000 μm^2 is applied to separate the micrograph into two distinct features: the smaller-sized grains and the larger-sized macrozones.

However, this dual-segmentation approach is unable to accurately represent the macrozone population. Analysis of the EBSD-derived feature statistics reveals that macrozones do not form a single homogeneous population, but instead exhibit a continuous range of sizes accompanied by systematic variations in elongation ratio. This behaviour is illustrated in the 3D histogram shown in Figure 4.6, where macrozones with smaller equivalent diameters exhibit an average elongation ratio of approximately 3, while larger macrozones exhibit higher average elongation ratios of approximately 4. This size-dependent evolution in morphology demonstrates a fundamental limitation of dual segmentation—enforcing a single size distribution and elongation ratio leads to misrepresentation of both smaller and larger macrozones.

In addition to this statistical limitation, the polycrystalline generation software Neper [86] permits only a single elongation ratio to be specified for each generated microstructure. Con-

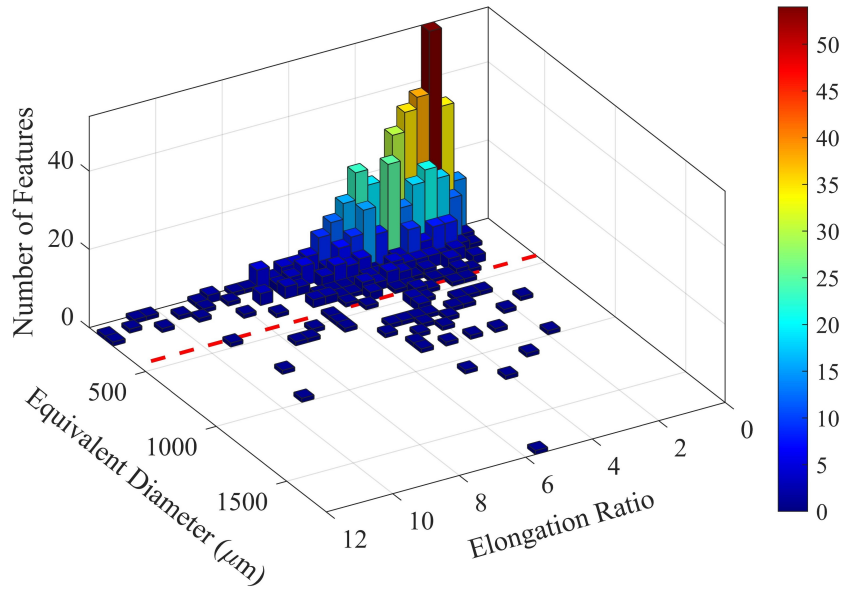


Figure 4.6: 3D histogram with elongation ratio on the Y-axis and the equivalent diameter on the X-axis. The Z-axis and colour code represents the number of features with the various grain characteristics. The red-dotted line represents the additional sizing threshold applied.

sequently, a dual-segmentation strategy would require all macrozones to share identical morphological descriptors, which is inconsistent with the observed EBSD statistics. As this limitation is inherent to the segmentation strategy itself rather than to specific parameter choices, the detailed visual outcomes of the dual-segmentation procedure are not presented here.

To address this limitation, a higher-order segmentation strategy is adopted. The original EBSD micrograph is instead separated into three distinct feature classes—small grains, medium macrozones, and large macrozones—as shown in Figure 4.7. Each class is treated independently during synthetic microstructure generation, allowing distinct size distributions and elongation ratios to be assigned and subsequently merged into a hierarchical structure.

Three partitions were selected as a practical compromise between descriptive resolution and statistical robustness. Using two partitions was found to be insufficient to separate the macrozone size populations cleanly, as each partition encompassed a broad range of sizes that could not be represented reliably by a single exponential size distribution and elongation ratio. In contrast, three partitions enabled the dominant size-dependent trends to be isolated while maintaining adequate population counts within each partition to ensure statistical stability. Increasing the number of partitions beyond three did not yield proportionally greater insight and

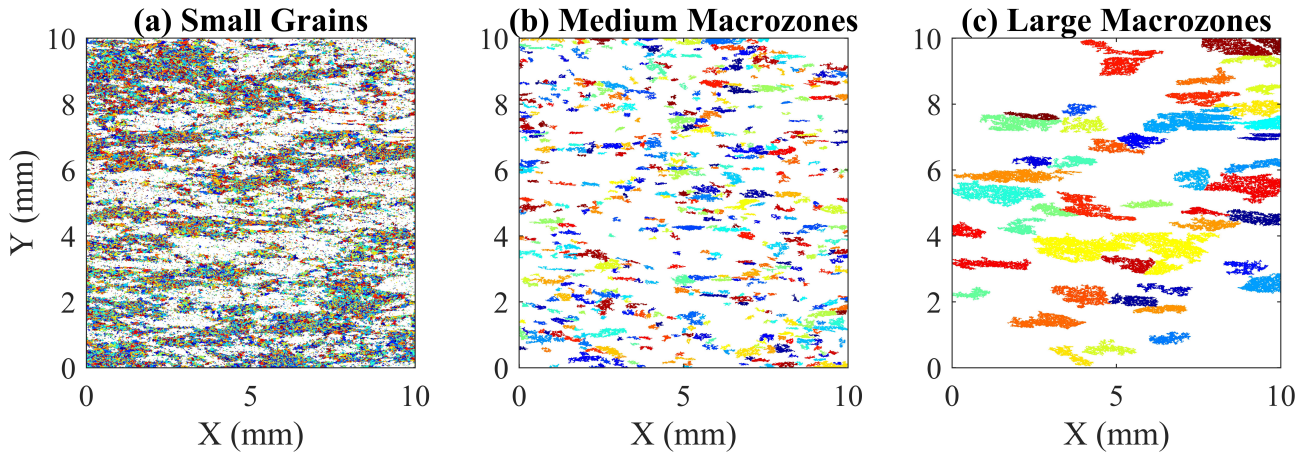


Figure 4.7: Micrograph for the individual features after the triple-segmentation procedure, with the (a) small grains, (b) medium, and (c) large macrozones. The colour code represents the index of each individual feature.

instead diluted the available macrozone population within each partition, leading to unstable sizing profiles for synthetic microstructure generation.

4.2.4 Formation of Synthetic Macrozone

Next, with the features segmented, their respective size distributions are represented in the form of a histogram in Figure 4.8. The histograms are fitted accordingly using exponential functions to obtain the respective size distribution profiles which are then imported into the Neper software [86] to generate the corresponding synthetic microstructures shown in Figure 4.9.

Apart from the morphology, crystal orientation is also equally important since it has a direct impact on the ultrasound wave response. Euler angles are extracted for each of the segments and used to generate the respective ODF plots in Figure 4.10. It is apparent that the macrozones contain a stronger texture than the smaller grains, since the presence of preferred orientations is a characteristic of macrozones during the manufacturing process. The ODF plots are randomly sampled in the orientation space to obtain a large set of Euler angles (in total a hundred thousand) which are assigned to the respective features such that the appropriate textures are replicated.

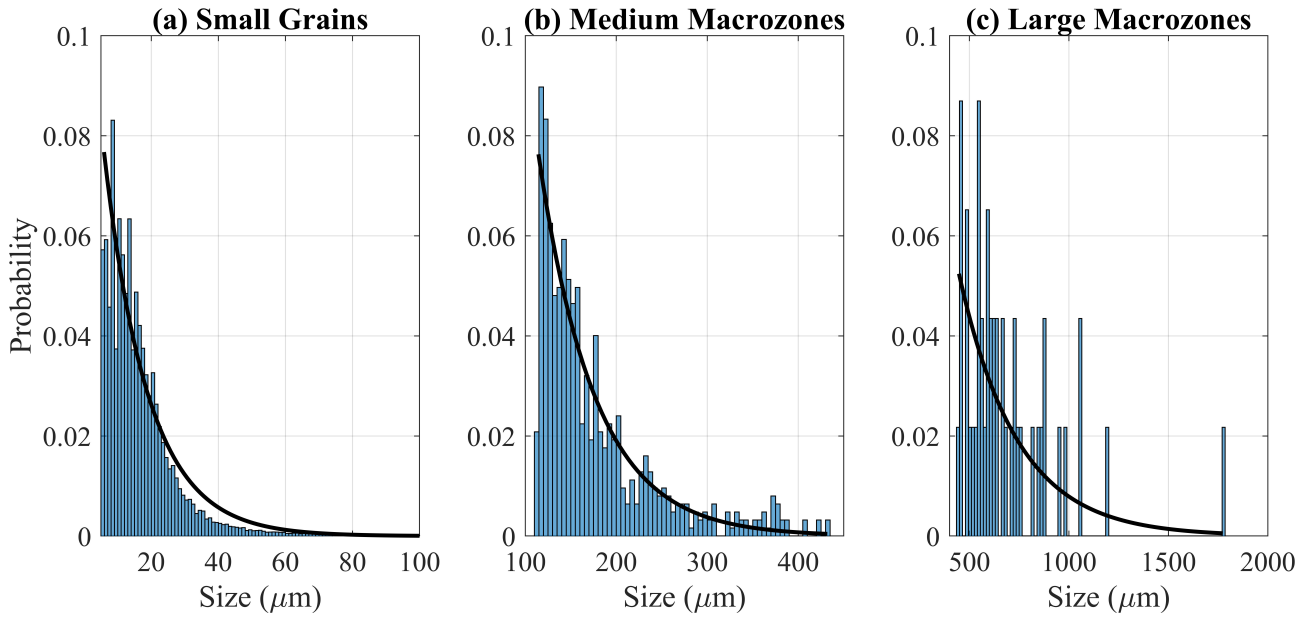


Figure 4.8: Sizing histogram for (a) small grains, (b) medium and (c) large macrozones with the respective fitted profiles using an exponential function.

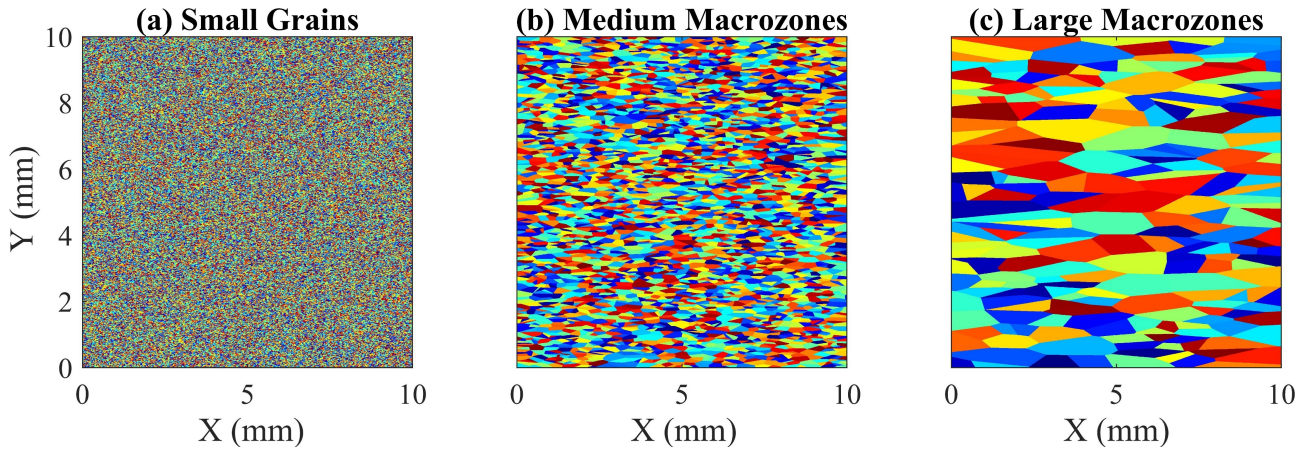


Figure 4.9: Synthetic microstructure for (a) small grains, (b) medium and (c) large macrozones generated with the extracted exponential profile using Neper.

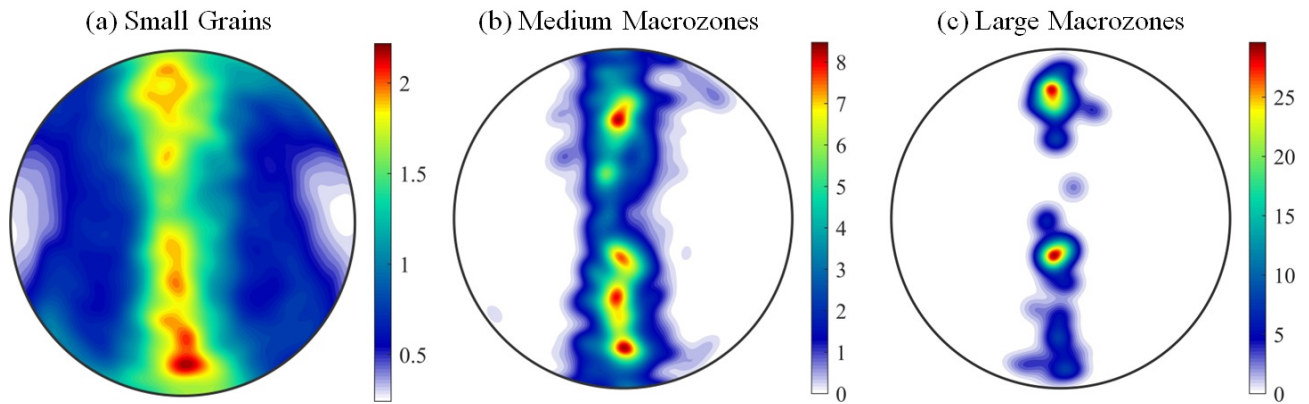


Figure 4.10: ODF plots for the respective features (a) small grains, (b) medium macrozones, and (c) large macrozones in the [0001] direction. The colour code represents the intensity of the orientations.

To create a realistic microstructure containing a mixture of grains and macrozones, the segments depicted in Figure 4.9 were merged. This involves randomly selecting a finite number of medium- and large-sized macrozones to replace the existing features in the small grain micrograph. The selection of medium and large macrozones is based on the area ratio they occupy in the reference 2D EBSD data. This process results in the formation of a synthetic microstructure, as shown in Figure 4.11 (a), closely resembles the reference EBSD dataset.

To validate the morphological accuracy of this synthetic microstructure, TPC calculations were employed. This calculation provides the probability of any two points, at certain distances apart, being situated within the same grain. The TPC profiles shown in Figure 4.11 (b) indicate a good agreement between the EBSD data and the synthetic Neper model, which are averaged across 20 realisations. This agreement suggests that the overall morphological statistics of the synthetic model in both the X and Y directions closely resemble those of the actual EBSD reference data.

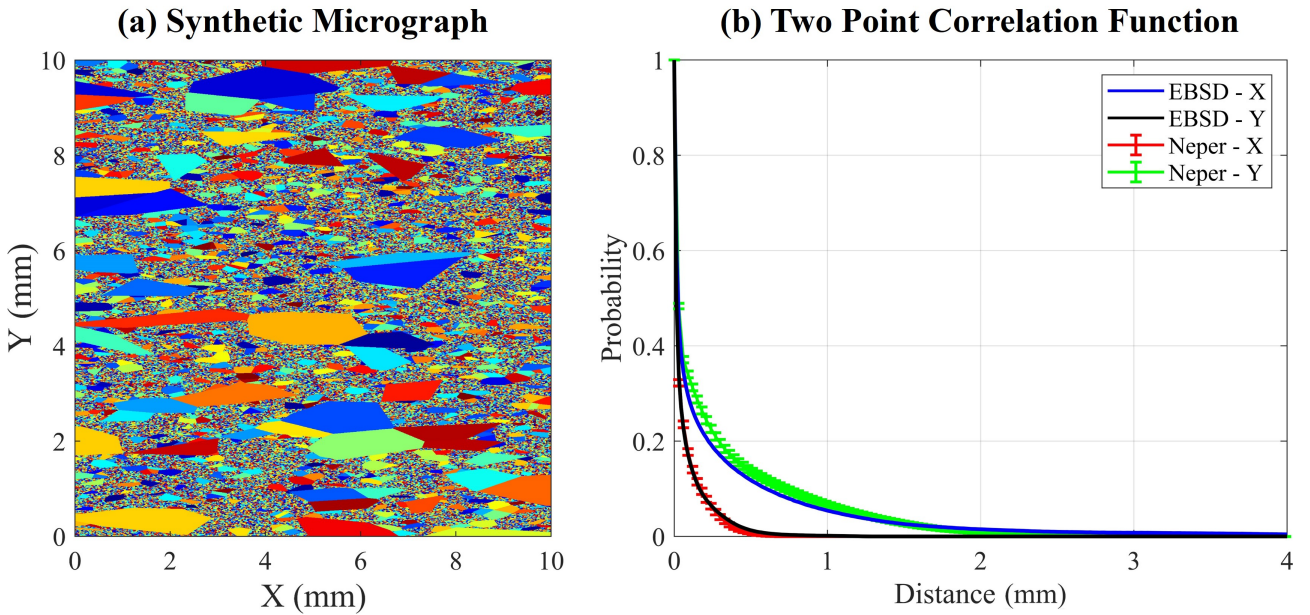


Figure 4.11: (a) The synthetic microstructure containing small grains, medium macrozones, and large macrozones. (b) The TPC profile comparing between the synthetic model and the actual EBSD data across the X and Y directions.

With the morphology defined and validated, the next step is to assign crystal orientations to each feature in the micrograph. Using the ODF plots generated in Figure 4.10, Euler angles are sampled with the corresponding weights to preserve the overall texture and are assigned to the

grains and macrozones in the synthetic micrograph. The ultrasound response of the synthetic microstructure is evaluated through the FE wave propagation model using the setup described in Section 2.1.

4.3 Results and Analysis

4.3.1 Ultrasound Responses

The attenuation results are illustrated in Figure 4.12, whereby the synthetic (Neper) profile is averaged across 20 realisations with each realisation configured by randomly selecting the macrozones and crystal orientations from the respective dataset. The attenuation values in the X direction are much greater than those in the Y direction, which is partly attributed to the macrozones being elongated in the X-axis. This phenomenon was demonstrated in [43, 99], where elongated grains lead to additional wave scattering and perturbations when operating within the stochastic regime. Within this regime, where the feature size is similar to the wavelength, ultrasound attenuation and backscatter become sensitive to morphological variations of the macrozones in orthogonal directions, which is an important characteristic to be determined.

The other contributing factor is the C-axis orientation of the macrozones. Based on the EBSD Euler angles, the C-axes of the macrozones are evenly distributed along the X-axis and in the out-of-plane direction. When the wave is excited in the X direction, it encounters macrozones with maximum and minimum velocities, resulting in higher velocity mismatches and stronger wave distortions. Whereas along the Y-direction, the C-axes of the macrozones are normal to the propagating wave, resulting in a lower velocity mismatch and weaker scattering effects.

This is corroborated by the simulated ultrasound velocities listed in Table 4.1, where the velocities for the EBSD data are simulated to be 6265 and 6184 m/s in the X and Y directions, respectively. Such observations were also reported in Chapter 3, where both macrozone shapes and C-axis orientations were deemed to have a significant impact on ultrasound attenuation.

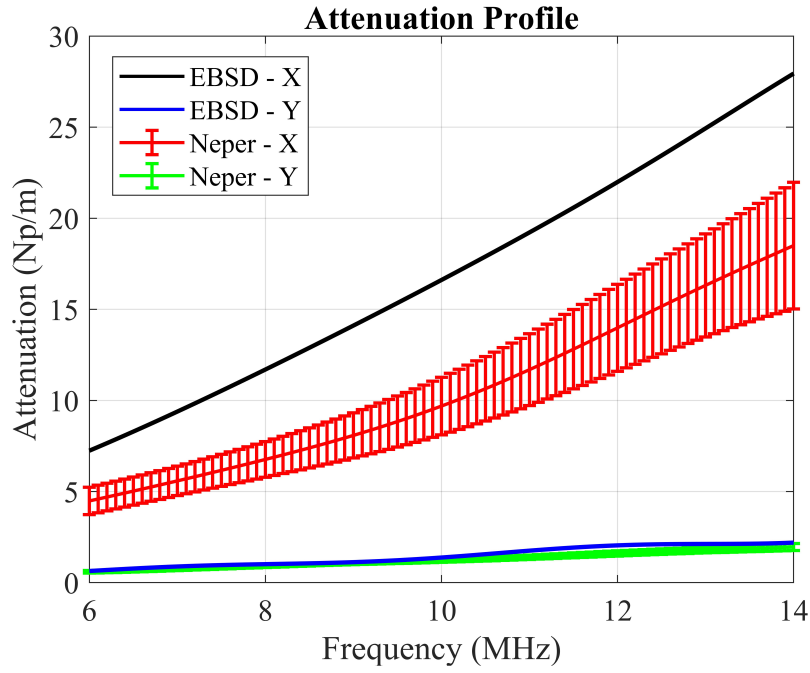


Figure 4.12: Attenuation profile comparing the synthetic (Neper) model to the EBSD reference model in both X and Y directions, with the synthetic results representing the mean and standard deviation across 20 realisations.

Ultrasound velocities simulated from the synthetic models across 20 realisations averages at 6275 and 6173 m/s in the X and Y directions, respectively which is similar to the EBSD simulated values. Compared to the velocity variation of ~ 100 m/s as a result of texture in the orthogonal directions, the difference of ~ 10 m/s between the two models is less significant. This agreement also indicates that the overall texture of the synthetic models is retained.

Table 4.1: Simulated ultrasound velocity for both the EBSD and Synthetic configurations in both X and Y propagation directions.

	Direction	Velocity (m/s)
EBSD	X	6265
	Y	6184
Synthetic	X	6275
	Y	6173

Overall, the ultrasound attenuation and velocity measurements between the two models are comparable, indicating that the synthetic model can capture the overall microstructural characteristics and wave responses that are reflected in the EBSD data. However, it was observed that the synthetic model tends to underestimate the simulated attenuation in both propagation directions. At the centre frequency of 10 MHz, the attenuation relative to the EBSD profiles

decreased by 4.7 Np/m (approximately 28%) and 0.2 Np/m (approximately 15%) in the X and Y directions, respectively. Since the wave perturbation effect in the Y direction is generally weaker, it is also less sensitive to variations between the models, which explains the smaller mismatch in attenuation.

Complete agreement is not expected, as there are bound to be some variations between the models. A prime example is the shape of the reference and synthetic microstructural features illustrated in Figures 4.7 and 4.9, respectively. The macrozones in the EBSD map have complex grain boundaries, whereas those in the synthetic micrograph are simplified with an elongated trapezoidal shape. Furthermore, the methodology also includes statistical sampling, whereby the feature sizes and crystal orientations are extracted from the reference EBSD data to generate multiple realisations of the synthetic microstructure. These potential sources of discrepancies are discussed further in the next section.

The simulated backscatter results are illustrated in Figure 4.13 which compares the responses for both the synthetic and EBSD models in the X and Y directions. Generally, the backscatter response is strongly dependent on grain morphology, as discussed in Chapter 3. Consequently, the responses are stronger in the Y direction, perpendicular to the macrozone elongation axis, as depicted by the red and green profiles. However, the distinction between the orthogonal directions for both model configurations is smaller than expected.

The absence of clear directional variation in the backscatter response is primarily attributed to artefacts introduced by the boundary conditions employed in the model configuration. The plane-wave model assumes an infinitely-wide domain, with the boundaries acting as reflectors. When a longitudinal wave propagates through a macrozone, it generates forward-propagating mode-converted shear waves. This behaviour is illustrated in Figure 3.10 (c) in Chapter 3, where two forward-propagating shear waves are observed at approximately 45° following the interaction with the macrozone.

In the plane-wave configuration, these shear waves undergo internal reflections at the model boundaries and propagate back towards the surface receiving nodes, where they contribute to the measured backscatter signal. This contribution is not associated with true microstructural

backscattering but is instead a consequence of the model geometry and boundary assumptions. The effect is particularly pronounced when the wave propagates in the X-direction, parallel to the macrozone elongation, where mode conversion is strongest.

As a result, the shear-wave artefacts mask the expected directional dependence of the backscatter response. In particular, higher backscatter levels were anticipated for propagation in the Y-direction due to the larger effective macrozone surface area normal to the incident wave. The inability to observe this trend indicates that the plane-wave model configuration is not well suited for evaluating directional backscatter behaviour in the presence of macrozones.

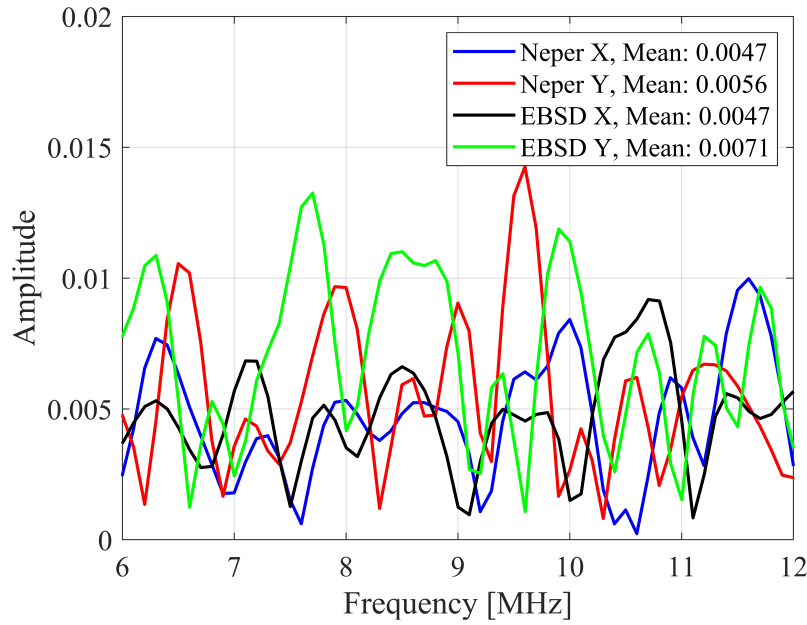


Figure 4.13: Backscatter amplitude for the synthetic (Neper) and the EBSD reference model in both X and Y directions in the frequency domain, with the mean amplitude values computed for comparison.

4.3.2 Sources of Discrepancy Between EBSD Data and Synthetic Models

Even though a close ideal match between the reference EBSD data and the synthetic model is not expected, it is still important to identify and determine the potential sources of errors, as they may affect how the methodology is used for characterisation purposes, and this section aims to investigate these.

4.3.2.1 Macrozone Shapes

First, the shape of the microstructural features was evaluated, specifically the large macrozones. In general, ultrasound attenuation is positively correlated to grain and macrozone sizes. Hence, the larger macrozones will have a considerably stronger impact on the wave response. To determine whether the complex shape influences ultrasound attenuation, a direct comparison is made to the large macrozones with a simplified elliptical profile.

These two setups are illustrated in Figure 4.14, and the elliptical shapes are generated using the morphological information extracted from the EBSD data, namely the size, elongation ratio, and central coordinates. The background consists of synthetic small-grains and medium-macrozones to complete the model configuration. Since the overall area of the large macrozones and their respective C-axis orientations are retained, the main variation between the two models is the large macrozone shape.

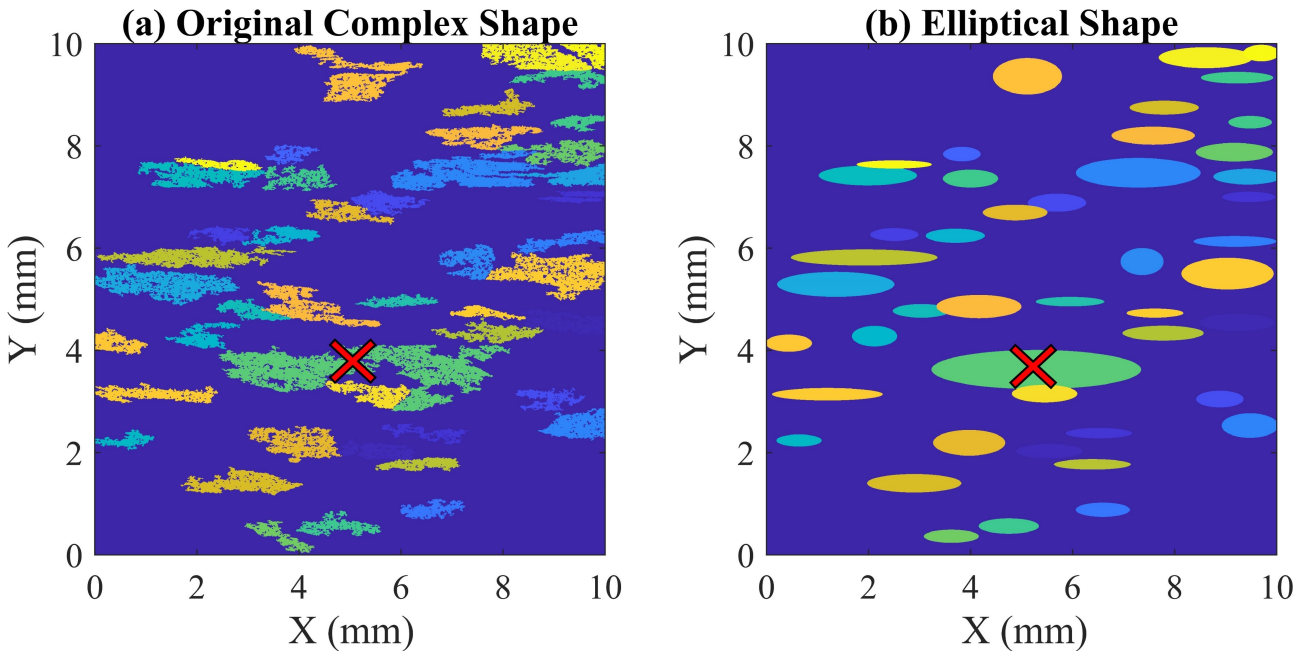


Figure 4.14: (a) Original complex-shaped macrozones and (b) the elliptical-equivalent. The colour code represents the feature indices, with the background grains removed for ease of comparison. The large macrozone in the centre is marked by a red cross to enable visual comparison of the original complex shape and its elliptical counterpart.

The overall morphology between the two is compared using the TPC function in Figure 4.15 (a), with the corresponding simulated wave attenuation in Figure 4.15 (b). Due to the complex

macrozone shape, the TPC profile is weighted towards longer distances. Statistically, even though the synthetic macrozones are generated based on the reference EBSD data, there are currently no means to duplicate the complex shape and boundary. These variations leads to infidelity in the replication procedure, and the original TPC profile contains slightly lower count of smaller grains and higher count of larger grains.

To further elaborate, in Figure 4.14 (a), the complex macrozone marked by the red cross has various concave and protruding features as opposed to the elliptical counterpart in (b). Hence, two random points at large distances can still fall within the same macrozone due to the protruding surfaces. Conversely, two random points at short distances may not lie within the same macrozone due to the concave surfaces and embedded grains.

Consequently, this difference in morphology also led to a variation in attenuation. Specifically, a reduction in attenuation is observed in the X-direction due to the simplification of the macrozone shape by $\sim 5\%$. The elliptical macrozones are akin to the Neper-generated synthetic macrozones and could potentially account for the underestimated attenuation values generated from the synthetic microstructural models.

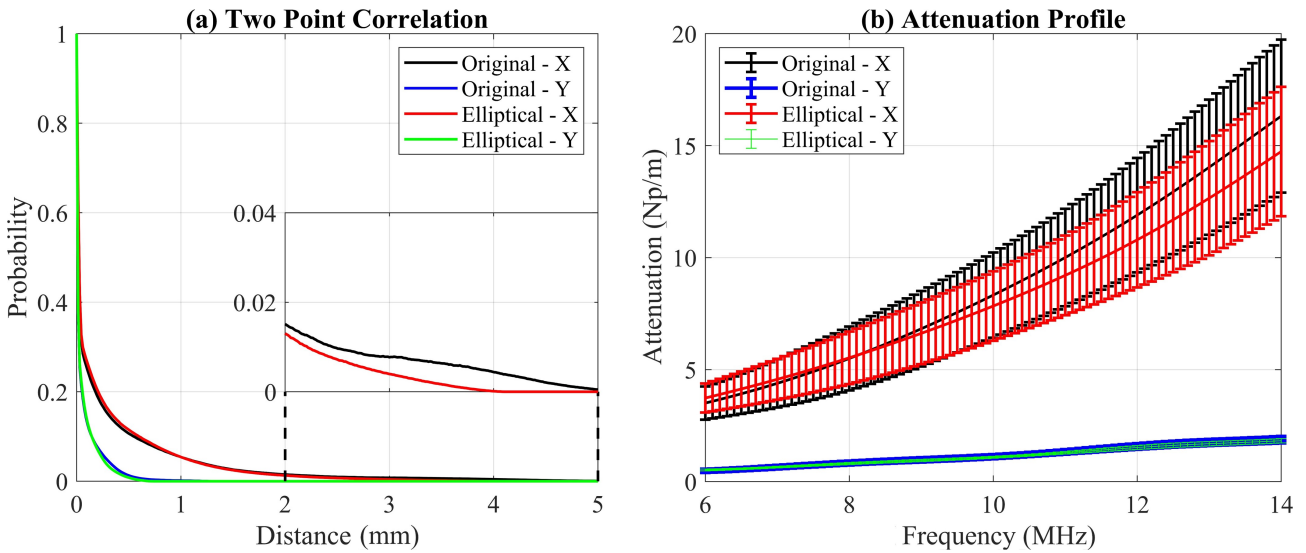


Figure 4.15: (a) The TPC profiles comparing between the original complex macrozone shape and the simplified elliptical macrozone shape in both X and Y directions. (b) Attenuation profile comparing between the original complex macrozone shapes and the simplified elliptical profile in X and Y directions.

From an analytical perspective, TPC can be used to account for the change in attenuation; TPC is widely used in analytical models to estimate the elastic wave attenuation in polycrystalline media [41]. The TPC profiles are fitted with an exponential function to generate a correlation length that, in theory, should positively correlate to the attenuation profiles. The corresponding correlation lengths are listed in Table 4.2, with the original complex macrozone shape in the X-direction having the highest value, and hence, the largest attenuation.

From a physical perspective, a longer correlation length relates to larger grain sizes along the wave propagation direction. Therefore, this leads to stronger wave perturbations and higher simulated attenuation. Likewise, this is also supported by the RMS values calculated based on the displacement variations across 50 model realisations; a higher RMS indicates stronger wavefield fluctuations and therefore is correlated to stronger simulated attenuation. From Table 4.2, the RMS values for the original macrozone configuration is higher than that of the simplified elliptical macrozone profile in both propagation directions.

Table 4.2: The correlation length derived from the TPC profiles and the RMS values computed based on the displacement variations across 50 model realisations for both macrozone shape configurations in the X and Y directions.

	Direction	Correlation Length (μm)	RMS Value
Original	X	195	1.1
	Y	54	0.5
Elliptical	X	192	1.0
	Y	51	0.4

4.3.2.2 Orientation Distribution Function

Apart from the morphologies, the C-axis orientations of the macrozones also play a significant role on the overall attenuation values. In the synthetic model, Euler angles that are sampled from the EBSD-generated ODF plots were used, which inherently causes distortions (in most cases reductions) to the levels of orientation preference compared to the original ODF plot. As illustrated in Figure 4.16, the stronger the texture, the more significantly the maximum intensity of the ODF drops; in the case of the large macrozones, the intensity has reduced by about 20%.

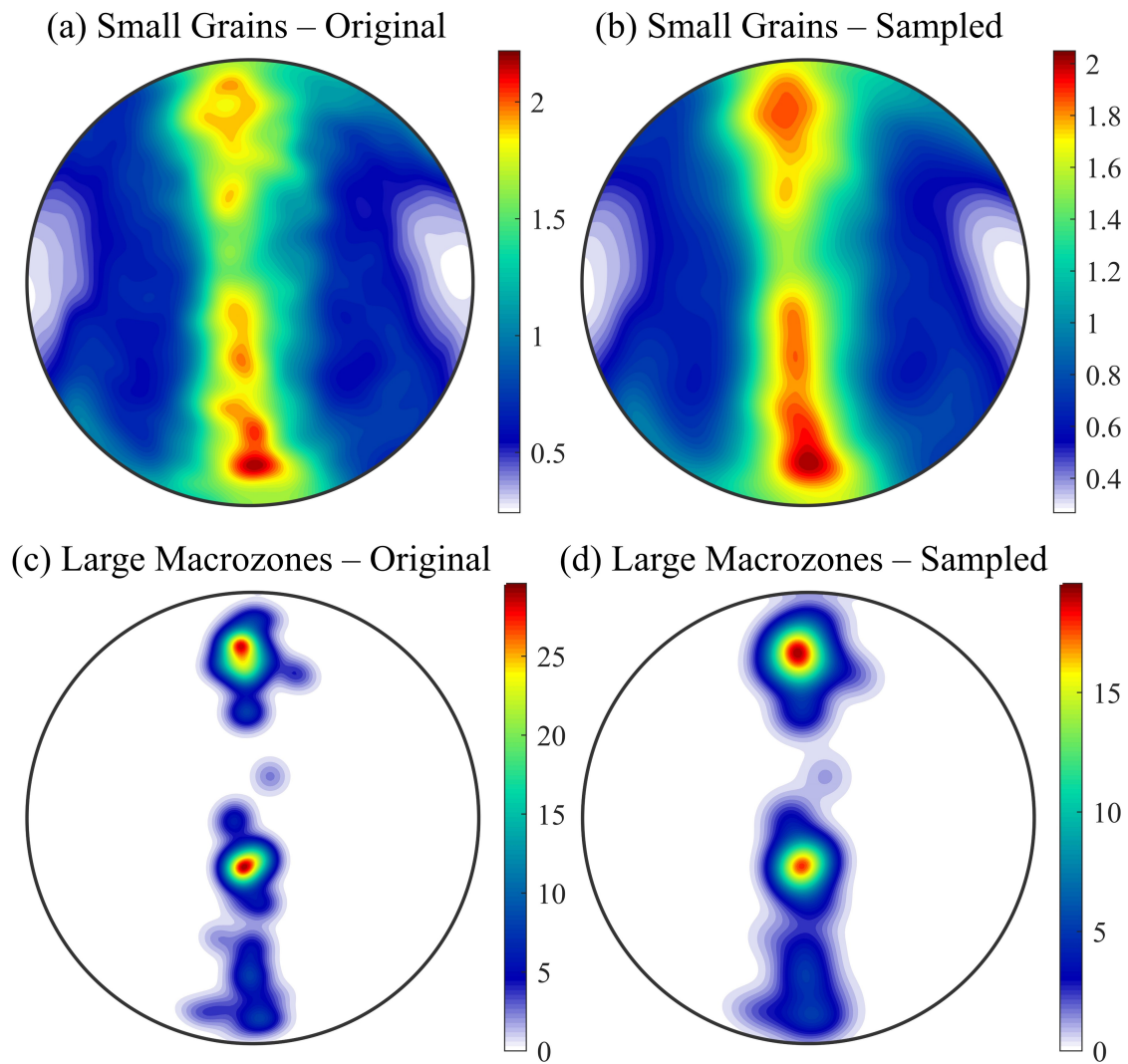


Figure 4.16: Pole Figures of (a,c) original EBSD data and the (b,d) sampled orientation data showing a dilution in texture due to the sampling process for the small grain and large macrozone features, respectively.

This can be understood by comparing to the sampling of a continuous 1D function $f(x)$: since the ODF are fundamentally probability density functions, the ODF of the strongly textured sample is similar to a series of strong and narrow peaks; and because the number of large macrozones are relatively few, the sampling gaps are rather coarse. Both of these factors combined result in a reduction of the original ODF intensity.

To evaluate the texture effect in the synthetic EBSD model, the grain and macrozone morphology from the original EBSD micrograph was retained, while only the crystallographic orientations were modified. Specifically, the orientations (from EBSD-scanned to sampled) of one category—the small grains, medium macrozones, and large macrozones—were altered at a time with everything else kept the same for the models. For instance, to evaluate the small grains, only the crystal orientations of the selected grains were modified using the sampled Euler angles. This process is then repeated for the medium and large macrozones, and each investigation comprises 20 model realisations, where the sampled Euler angles are randomly selected.

The respective attenuation profiles are plotted in Figure 4.17. It can be seen from (c), even though the texture dilution effect is the strongest for the large macrozones, the attenuation changes when compared to the original EBSD result are minimal, at about 5%. The slight decrease in attenuation does reflect the dilution in texture, since a weaker texture generally relates to smaller velocity variations between the features and hence less wave scattering and perturbations.

However, surprisingly, it is for the small grains in (a) where a large deviation in attenuation of $\sim 30\%$ is observed, and the level of decrease in attenuation is similar to the difference between the original and synthetic models shown in Figure 4.12. This indicates a lead to the fundamental reason for the discrepancy. Given that the texture dilution effect for the smaller grains is minimal and the grain size distribution is well represented, there must be another underlying factor that is fundamentally contributing to this reduction, which brings us to the next part of the investigation: the misorientation distribution function.

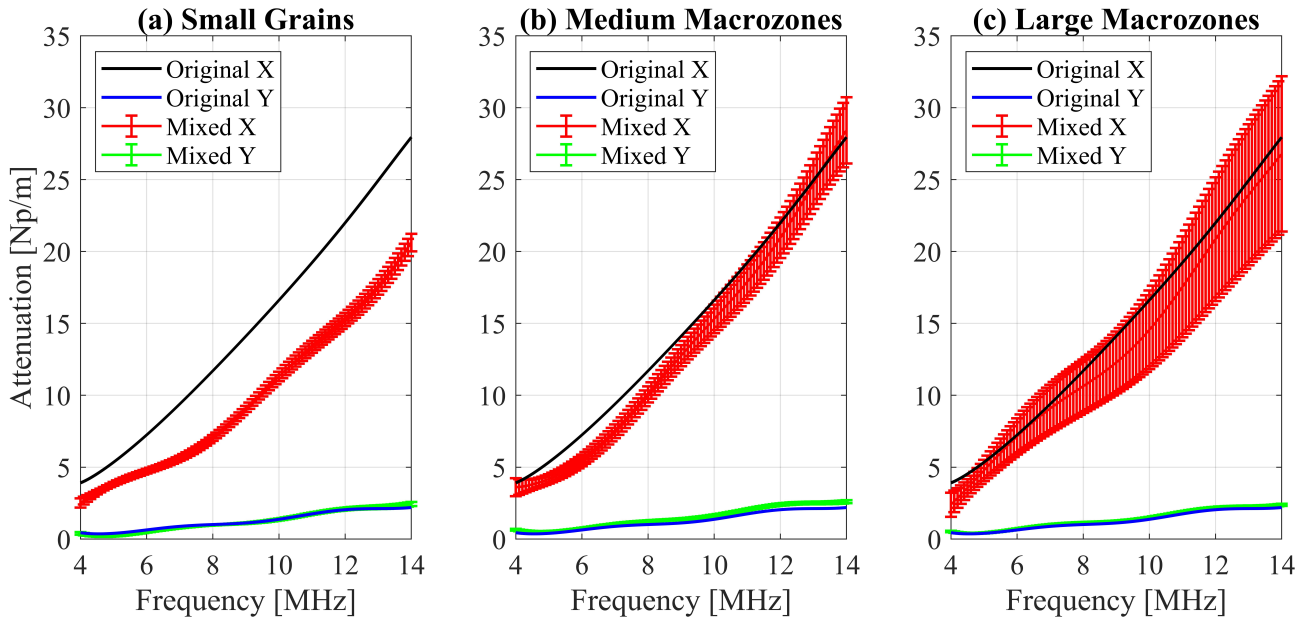


Figure 4.17: Attenuation profiles with the randomisation of feature orientations (mixed) with the sampled Euler angles of the (a) small grains, (b) medium macrozones, and (c) large macrozones only.

4.3.2.3 Misorientation Distribution Function

MDF statistically evaluates the difference in crystal orientations between neighbouring grains in the region of interest, and contains localised spatial information of the orientation contrasts, as opposed to ODF which has no such local information at all. However, the methodology, which involves sampling of Euler angles in the orientation space and reassigning the sampled orientations to grains, loses the localised information in the process and results in the overall MDF of the respective features being rearranged and, in many cases, randomised. This section aims to investigate the effects of the rearranged MDF on attenuation.

Firstly let us revisit the simulation results in Figure 4.17. The large discrepancy of the small grain results indicates that its MDF profile might have led to a higher simulated attenuation, thus prompting a more detailed look at it. For this purpose, a domain containing only the smaller grains is extracted from the EBSD map, as illustrated in Figure 4.18 (a). The macrozones are avoided altogether, since they will tend to dominate the MDF profile due to their larger sizes and having more neighbouring grains. The isolated micrograph contains a list of

grain indices and their respective Euler angles, enabling the computation of the MDF profile shown in Figure 4.18 (b).

In the synthetic model, the sampled Euler angles from the orientation space are randomly assigned to the grain indices, which produces a different MDF profile. To make the obtained MDF profile more holistic and representative, the random assignment process is repeated for 50 realisations of synthesised models, and the results are shown in Figure 4.18 (b). Compared to the original MDF profile, this contains a higher preference of grains with lower misorientation from 0° to 50° , a clear difference is observed in synthetic MDF profile where the dominant distribution clearly shifts towards 50° to 90° after the randomisation procedure.

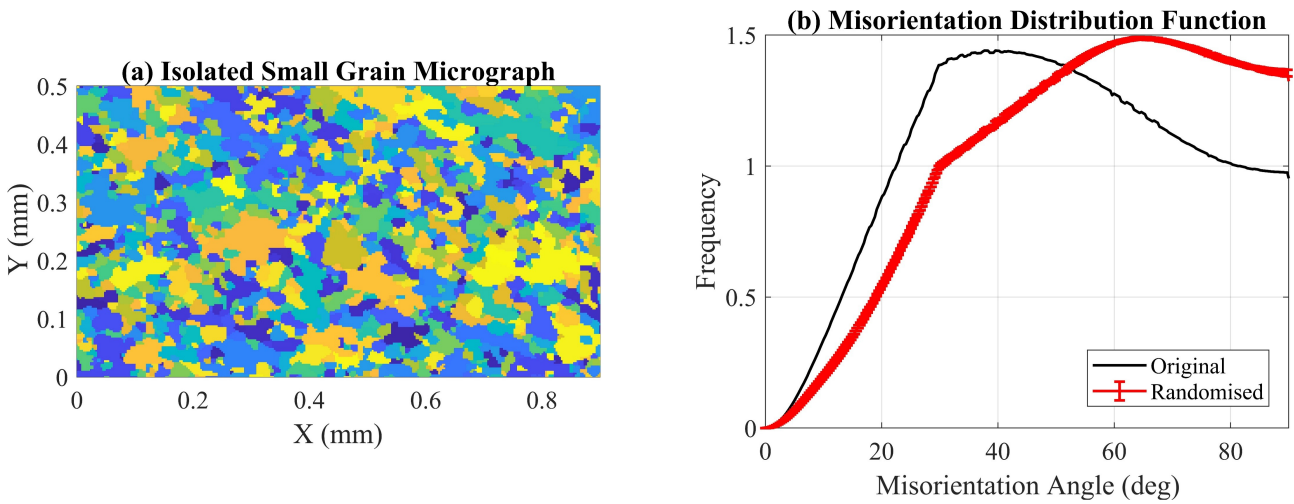


Figure 4.18: (a) A region of small grain features with a dimension of 0.5 by 0.9 mm extracted from the original EBSD micrograph. The colour code represents the grain indices. (b) The micrograph original and randomised MDF profiles.

From a physical standpoint, the dominant $30\text{--}50^\circ$ range in the original MDF profile indicates that the small grain features have reasonably similar C-axis orientations to their neighbours. The angular range is not too distant from the C-axis misorientation threshold applied to classify macrozones, and the correlations of the grain orientations can add to the phase perturbation of the propagation ultrasonic wave and result in higher attenuation, in a similar way compared to the elongated macrozones (albeit with weaker effect). Such correlations are mostly removed in the synthetic grains' randomised sampled Euler angles, therefore the attenuation becomes weaker.

To further illustrate how the randomisation of MDF affects simulated attenuation, the micrograph depicted in Figure 4.18 (a) was incorporated into an FE wave propagation model using identical configurations. As the isolated micrograph is smaller in size, it is replicated and padded on both axes to achieve a final dimension of 10 by 10 mm. The attenuation profiles are then compared in Figure 4.19, revealing that the randomised MDF profile exhibits lower simulated attenuation in both propagating directions. Even though there might have been some influence from the boundaries between padded patches for the original EBSD map (the synthetic model should be affected more weakly given that the MDF is more randomised), the grain morphology remains unchanged and only the crystal orientations vary. This suggests that a substantial portion of the observed attenuation variation can be attributed to differences in the MDF. This agrees with the findings shown in Figure 4.17 (a), where simulated attenuation varied significantly by $\sim 30\%$ due to the replacement of grain orientations by sampled Euler angles, thereby randomizing the overall MDF. It is worth noting that the attenuation values here are lower due to the presence of only small grains in the microstructure

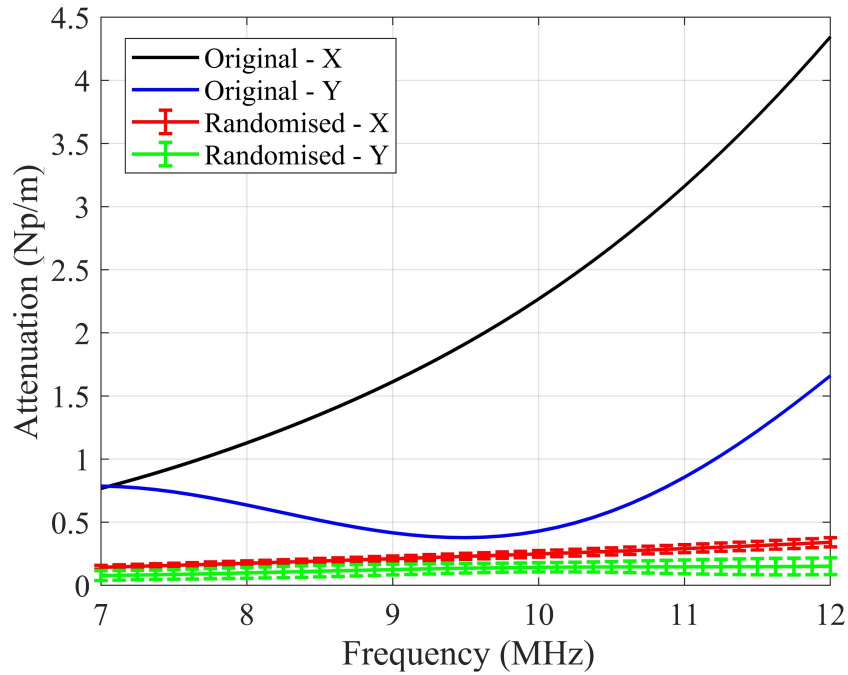


Figure 4.19: Attenuation profiles of the extended micrograph with the original and randomised crystal orientations in both X and Y directions. The randomised results are represented by the mean and standard deviation across 50 realisations.

4.3.3 Discussion

A routine to generate a synthetic microstructural model was established, providing a close resemblance to the reference EBSD data. The EBSD reference data was first processed to extract grain morphological data and crystal orientation information. The grain morphologies were replicated through a triple-segmentation method, and the crystallographic texture was incorporated via sampling in the orientation space. The simulated ultrasound wave speed showed good agreement, whereas the simulated attenuation tended to be underestimated.

Through the investigation, several sources of discrepancies were identified in the simulated attenuation response. The effect of MDF within the small grain features is the most pronounced, leading to a variation in attenuation by $\sim 30\%$, followed by the texture dilution effect and macrozone shapes, each contributing to $\sim 5\%$. It is also worth noting that the study is focused on a more extreme case whereby the sample contains large macrozones with strong texture. Hence, for samples with more regular microstructure, the discrepancies are expected to be smaller.

Resolving some of these contributors proved challenging at this stage, but quantifying their impact allows us to address any discrepancies effectively. For example, the texture dilution effect is inherent to the Euler angle sampling procedure. Likewise, the complex macrozone morphologies cannot be replicated using current polycrystalline generation software [86, 100]. Consequently, this study operates within the present capabilities of the Euler angle sampling and the polycrystalline generation software and accepts the potential error levels of $\sim 5\%$ for ultrasonic attenuation. Since the aim of this study is to develop a synthetic framework that is statistically representative and capable of reproducing dominant physical trends in ultrasonic wave propagation, no explicit accuracy target was imposed. Additionally, considering the significant variability in experimental attenuation values due to grain size distributions [50], an error margin of around 5% can be deemed acceptable which is achieved within this context.

As for the MDF profile, it may be mitigated by swapping grain orientations in an iterative procedure for simple microstructures [101]. However, due to the large size of the micrograph

(10 by 10 mm with a 3 μm step size) and the combination of grains and macrozones with varying MDF properties, replicating the MDF proved challenging. It might be possible to randomly seed some smaller grains and copy their misorientations over, but it is difficult to implement and will require dedicated research in the algorithm, thus is beyond the scope of the chapter. Therefore, an alternative approach involves accounting for the attenuation errors and using them as a reference for comparison with synthetic models. This ensures that the synthetic microstructural model remains representative of the actual features captured in the EBSD map.

This approach is further illustrated in Figure 4.20, where the attenuation profiles are compared. Starting with the original EBSD data, the feature crystal orientations are replaced with sampled Euler angles while keeping the morphology constant. This alteration results in a significant reduction in attenuation, primarily attributed to the removal of MDF within the small grain features. Importantly, this outcome aligns well with the synthetic Neper model, suggesting accurate replication of the overall morphology and texture of the EBSD data. The slight underestimation in attenuation can be attributed to the simplification in the macrozone shapes and boundaries.

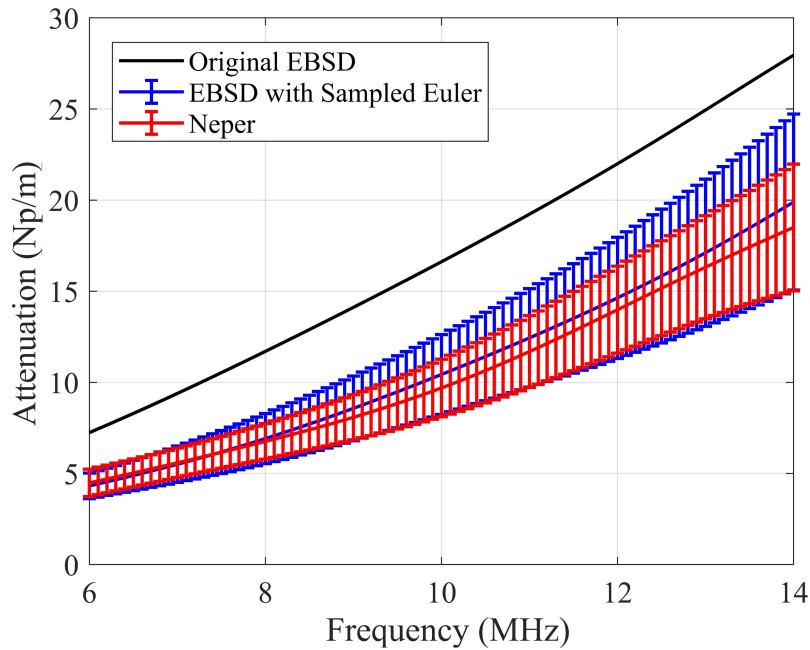


Figure 4.20: Attenuation profile comparing between the original EBSD data, the EBSD with sampled Euler angles, and the synthetic Neper model in X propagation direction. The synthetic attenuation profiles are the average and standard deviation computed across 20 realisations.

The next step involves extending this capability into 3D. This will be challenging, but the work in 2D cases presented in this chapter offers valuable guidance in the synthesis of grain morphologies, and to help minimise potential sources of errors. The formation of synthetic microstructure in 3D would involve orthogonal EBSD scans to determine the overall 3D morphology of the microstructure within the sample of interest. Likewise, the grain and macrozone information extracted from the EBSD maps can be imported into polycrystalline generation software to create synthetic 3D microstructural features that closely resemble those of the reference EBSD data. This allows for the verification of the 3D synthetic models with actual experiments since both are evaluated in three dimensions. Subsequently, the models can be adjusted to accommodate varying sizes and shapes of macrozones. Similar to the work reported in Chapter 3, a parametric investigation can be used to vary the macrozone characteristics to study the full wave-macrozone behaviours.

Backscatter amplitude is an equally important response in ultrasound that needs to be accounted for, but it is not discussed in detail in this study. The reason being that the backscatter response is dependent on the localised contrast between neighbouring grains, which is related to the MDF. Since the variation in MDF was not resolved, the backscatter results are less representative. Moreover, the model configuration also needs to be adjusted for more accurate backscatter simulations. Following [60], a finite-sized transducer is required, coupled with a wide model to eliminate any boundary reflections. This necessitates a larger reference EBSD dataset, which was unavailable during this work. Once the discrepancy in MDF is dealt with, coupled with the new model configuration, the agreement in backscatter response is expected to be improved considerably.

4.4 Conclusion

In this study, a methodology for generating realistic synthetic microstructures based on a 2D EBSD reference dataset was demonstrated. Initially, grain morphology and crystal orientation information were extracted from the EBSD data and fed into the polycrystalline grain

generation software to create synthetic microstructures. Subsequently, the synthetic microstructures were validated and compared to the original EBSD data using TPC calculations and FE simulations of wave propagation.

Both the EBSD and synthetic microstructural models exhibited similar sensitivities to ultrasound attenuation and velocity due to variations in grain morphology and crystal orientations in orthogonal directions. This phenomenon aligns with observations and explanations provided in Chapter 3, who conducted a systematic study using ideal macrozone model configurations. Therefore, the findings presented in this chapter are a step forward towards generating realistic synthetic microstructural features that better represent actual samples for a more accurate and comprehensive analysis.

Several factors contributing to the discrepancies in the simulated attenuation response were identified. In the order of significance, the factors are the presence of MDF, the shape of the macrozones, and the texture dilution effect. While resolving these contributors remains challenging, their impact has been quantified and can be compensated for during the validation process. A potential remedy for the notable MDF effect includes conducting an orientation-randomisation procedure on the reference EBSD data to identify the presence of MDF, followed by a grain-orientation swapping process.

The challenge in understanding the underlying physical interactions between ultrasound and complex material microstructure such as macrozones is the lack of representative samples since they are difficult to control and fully characterise. Hence instead of relying on complex manufacturing processes, this modelling methodology can be adopted to generate realistic and well-defined material microstructures based on EBSD data. Furthermore, by coupling this to the definite wave responses measured in the simulation models, an in-depth systematic study of the wave-macrozone interactions can be conducted to provide a better understanding of the underlying physics behind various mechanisms.

From an industrial perspective, 3D synthetic macrozone microstructure can be constructed to establish quantitative ultrasonic responses, providing a baseline against which potentially harmful macrozones may be identified. In practice, the multi-view measurement approach

described in Chapter 3 can serve as a rapid screening method to flag components exhibiting indications of macrozones. Samples identified through this screening can then be examined using a more detailed measurement methodology informed by the 3D synthetic macrozone models, enabling quantitative characterisation of macrozone attributes and assessment of their potential impact on material performance.

The validation presented in this chapter was performed using a limited number of representative EBSD datasets and corresponding synthetic microstructures, selected to demonstrate the feasibility and sensitivity of the proposed methodology. While this provides confidence in the qualitative trends and relative sensitivities observed, more extensive validation could be achieved by adopting the approach to a wider range of samples exhibiting different macrozone morphologies, volume fractions, and orientations. Such extended validation was beyond the scope of the present study due to the limited availability of suitably characterised samples but represents a clear direction for future work should additional data become available.

Chapter 5

Computational Study of Wave Propagation in the Geometric Regime

5.1 Introduction

From Chapters 3 and 4, it was established that macrozones with strong crystallographic texture and large spatial extent can significantly influence ultrasonic attenuation, backscatter, and velocity. In particular, when macrozone dimensions approach the mm scale and are interrogated at sufficiently high frequencies, the associated scattering behaviour may extend beyond the Rayleigh and stochastic regimes and approach the geometric scattering regime, where the ultrasonic wavelength becomes small relative to characteristic microstructural dimensions.

Despite its relevance to the resolution limits of ultrasonic inspection, the geometric scattering regime remains the least explored of the three classical scattering regimes. The high frequencies required to access this regime lead to rapid attenuation and limited penetration depth, while fully 3D FE models become computationally prohibitive due to the extremely fine meshes required. Consequently, most prior analytical, numerical, and experimental studies have focused on the Rayleigh and stochastic regimes, where attenuation remains moderate and coherent-wave descriptions remain valid.

For completeness, ultrasonic attenuation in polycrystalline materials is commonly classified into three regimes based on the ratio of wavelength λ to grain diameter D [29–31]:

- Rayleigh regime ($\lambda \gg D$): $\alpha \propto D^3 f^4$, dominated by point-like scattering and mode conversion.
- Stochastic regime ($\lambda \approx D$): $\alpha \propto D f^2$, governed by cumulative phase perturbations along the wavefront.
- Geometric regime ($\lambda \ll D$): $\alpha \propto D^{-1} f^0$, arising from multiple reflections and refractions at grain boundaries.

These regimes and their governing mechanisms were reviewed in detail in Chapter 2 and are not repeated here.

A key consideration for numerical modelling of scattering behaviour is dimensionality. Previous studies have demonstrated that attenuation exhibits a clear dimensional dependence in the Rayleigh regime, where the frequency exponent differs between two- and three-dimensional models due to the geometric spreading of scattered energy [40]. In 3D, scattering from point-like grains redistributes energy spherically with a $1/r^2$ dependence, whereas in 2D the spreading is circular and follows a $1/r$ dependence.

However, in the stochastic and geometric regimes, scattering is governed primarily by the effective cross-sectional length of grains and by the number of grain boundaries encountered along the propagation path, respectively [40]. As a result, the detailed dimensionality of the model plays a reduced role in determining qualitative attenuation trends once the Rayleigh regime is exceeded. While absolute attenuation magnitudes may differ between two- and three-dimensional representations, the transition behaviour and frequency scaling in the stochastic and geometric regimes are expected to remain qualitatively comparable.

In light of these considerations, this chapter focuses on investigating ultrasonic wave propagation in the geometric regime using 2D FE models. First, the objective is to assess the validity

of 2D modelling for capturing high-frequency scattering behaviour. Next, to examine the evolution and loss of coherent-wave components as the geometric regime is approached. Finally, to evaluate the influence of propagation distance and material anisotropy on the geometric regime transition. By isolating these effects, the chapter aims to clarify the physical interpretation of attenuation in the geometric regime and establish a foundation for future analytical and experimental investigations.

5.2 Methodology

Since the stochastic and geometric regimes are assumed to be dimensional-independent, 2D FE models were adopted in this study. For a model of equal dimensions using structured mesh, the DOF in 2D is 7500 times smaller than in 3D as compared in the table below. Also, in 3D, increased connectivity between nodes leads to a greater number of non-zero entries in the K-matrix, increasing model size further. Hence, with a 2D setup, it reduces the computational resources needed and enables the generation of multiple models for a systematic in-depth investigation of the wave behaviour in the geometric regime.

Table 5.1: 2D and 3D model DOF

Model Dimension	2D	3D
Model Size (mm)	50×50	$50 \times 50 \times 50$
Mesh Size (mm)	0.01	0.01
Degrees of Freedom	5×10^7	3.75×10^{11}

The FE models were created with a dimension of 50 by 50 mm. A longitudinal excitation source was introduced at the top surface of the model, with symmetrical boundary conditions added on both sides to support plane wave propagation, as illustrated in Figure 5.1. Nodal lines of receivers were added at 10 mm intervals to evaluate the wave profile at varying propagation distances. The excitation frequency was varied from 1 to 100 MHz to cover all three scattering regimes. Structured meshes were used and the mesh size was selected based on the operating frequency to have at least 20 elements per wavelength.

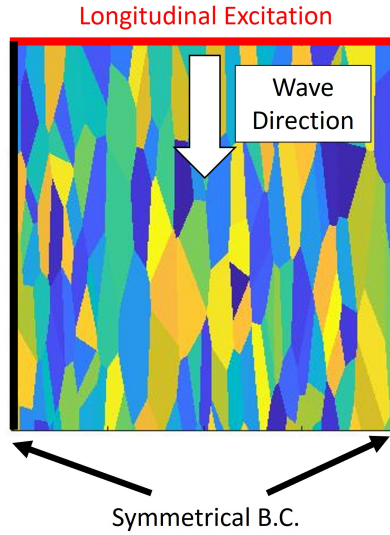


Figure 5.1: A sample 2D FE model setup configuration with elongated grains and symmetrical boundary conditions to support longitudinal plane wave propagation excited from the line of sources located at the top of the model.

Two types of materials—aluminium and lithium—were used to examine the influence of anisotropy. The elastic properties and anisotropy factor of both materials are listed in Table 5.2. aluminium represents a weakly anisotropic material, whereas lithium exhibits one of the strongest single-crystal anisotropy. Since crystal anisotropy affects the velocity mismatch between neighbouring grains which directly impacts wave scattering and attenuation behaviour, the contrast between the two materials provides a useful benchmark for assessing the sensitivity of geometric scattering on crystal anisotropy.

Table 5.2: Single-crystal elastic constants, density, and anisotropy factors used in the simulations.

Material	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	Density (kg/m ³)	A
Aluminium	108	61	28	2700	1.19
Lithium	13	11	8	534	8.00

The synthetic microstructure was generated using Neper software with Voronoi tessellation [86]. A total of 12,250 grains were generated and elongated with an aspect ratio of 5 to enhance the perturbation effects such that the saturation regime can be achieved at lower frequencies [43]. The average grain dimensions are 2.2 by 0.44 mm. The models were solved using Pogo software.

5.3 Results

To achieve statistical convergence, 40 independent random grain orientation realisations were generated at each operating frequency. This number was chosen as a practical compromise between statistical stability and computational cost, and is consistent with prior studies showing convergence of averaged attenuation metrics with a similar number of realisations [42, 43].

Time-domain signals from the 40 realisations were averaged to suppress incoherent contributions while retaining the coherent waveforms. The averaged signals were then Fourier transformed into the frequency domain, and attenuation was calculated using equation 4.1. A sample time-domain signal in the stochastic regime and its respective frequency and attenuation profile are illustrated in Figure 5.2. The attenuation profiles across the 1 to 100 MHz operating frequencies are subsequently stitched together into a single plot that spans across a wide frequency range for ease of comparison.

5.3.1 Dimensionality of Ultrasonic Attenuation

Before expanding the study on the physical effects in the geometric regime, the attenuation profiles are compared across dimensions to ensure that the 2D FE models are representative of 3D wave scattering behaviours. The results are compared in Figure 5.3 and a mismatch is observed in the Rayleigh regime between the 2D and 3D cases. This is corroborated by [40, 85] who showed similar trends in simulation and analytical comparison, indicating that 2D models within the Rayleigh regime tend to overestimate attenuation. Due to the dimensional dependence of the scattering mechanisms, this is an expected outcome and is not a major concern, as the interests of the work lie in the higher operating frequencies.

Within the stochastic regime, where scattering is governed by phase scrambling along the wavefront, the mechanism depends on the length of the grain along the path of propagation and hence is dimensional-independent. As a result, the 2D and 3D profiles within this regime are very similar. The 3D FE simulation concludes at the stochastic regime due to the high

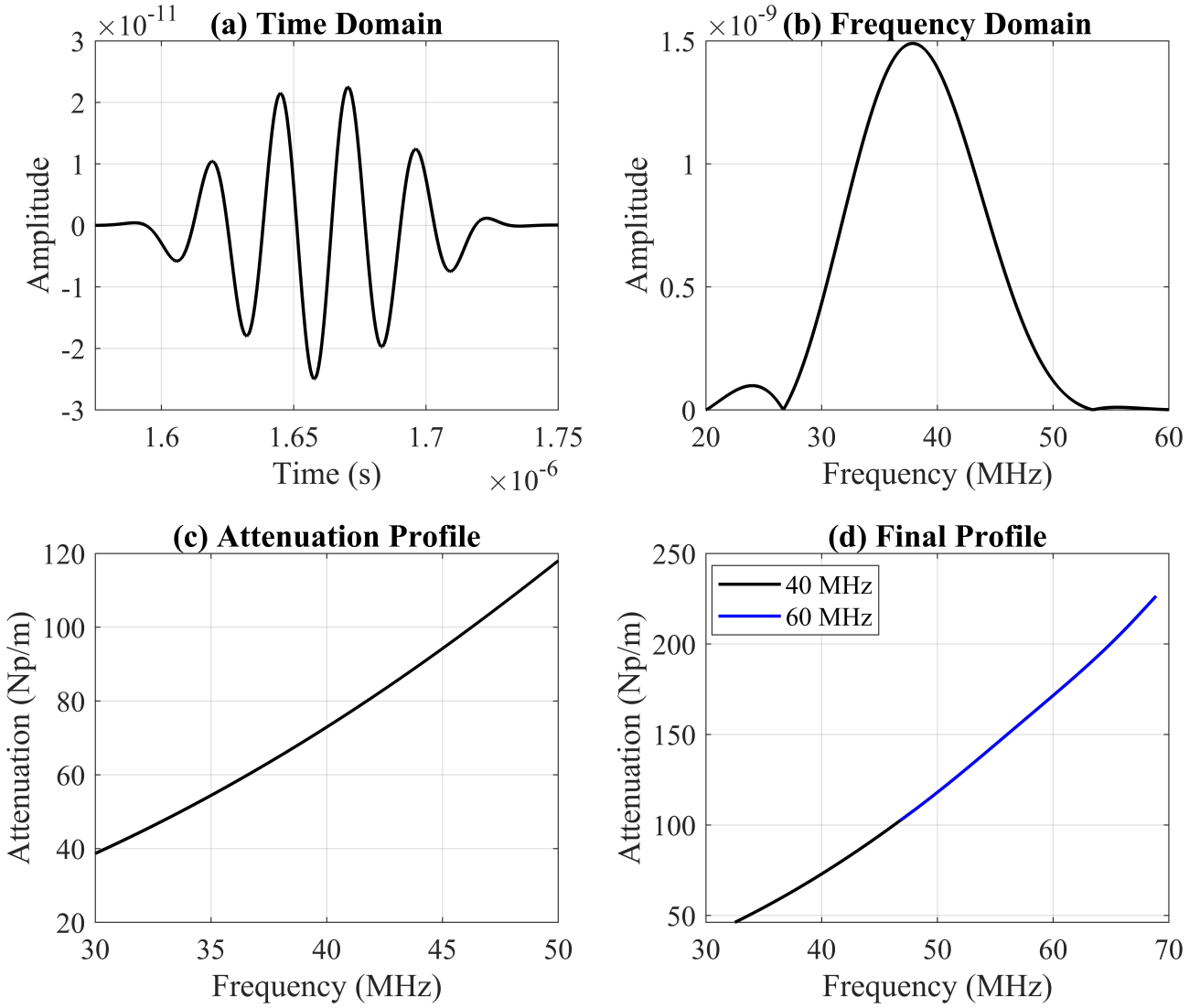


Figure 5.2: A coherent signal at 40 MHz at 10 mm propagation distance in the (a) time and (b) frequency domain. (c) The attenuation profile of the individual coherent signal and (d) the final attenuation profile after stitching the attenuation values at various operating frequencies.

computational resources needed to generate models with large DOF at even higher operating frequencies.

Similarly, attenuation in the geometric regime is theorised to arise from reflections and refractions at grain boundaries. This depends on the number of grain boundaries along the path of propagation and should not be heavily influenced by the dimensionality of the model. Hence, the 2D FE models are deemed sufficient to capture the high-frequency scattering behaviours that are present in actual 3D scenarios.

With further increment in operating frequencies, the 2D FE model first transits into the geometric (saturation) regime, followed by the 3D analytical model. The reason for this discrepancy is attributed to two primary factors, both of which are discussed in greater detail in subsequent sections.

First, propagation distance is not explicitly accounted for in the analytical model, but it is deemed a critical parameter governing the onset of geometric regime in the FE results. The cumulative loss of coherence depends on the total propagation distance, leading to earlier transition at a fixed frequency in finite-length models.

Second, analytical models implicitly assume coherent-wave dominance even within the geometric regime. While this assumption enables closed-form solutions that recover asymptotic attenuation trends, it does not capture the rapid coherence loss and incoherent-dominated scattering observed in the FE simulations.

5.3.2 Coherent and Incoherent Wave Behaviour in the Geometric Regime

In polycrystalline wave propagation theory, the ultrasound response is commonly decomposed into coherent and incoherent components. The coherent wave corresponds to the ensemble-averaged response and represents the deterministic portion of the initially-excited waveform that persists across multiple realisations of the microstructure. The incoherent wave represents

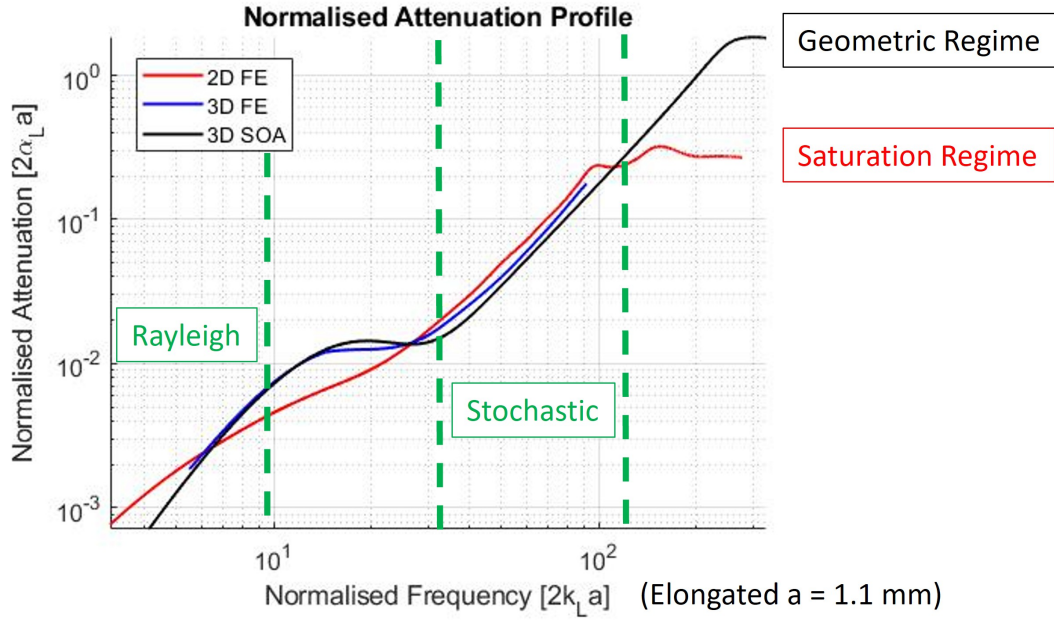


Figure 5.3: Attenuation profiles comparing 2D and 3D FE models with 3D analytical solution across the three scattering regimes for aluminium material.

the microstructure scattering contributions arising from coherent wave interactions with grain boundaries, which are random in phase and vary between different realisations.

At higher operating frequencies and propagation distances, the coherent wave amplitude is expected to decay heavily due to stronger scattering effects. This is evident in Figure 5.4 which shows the original input signal generated at 75 MHz in aluminium. Subsequent waveforms represent the transformation of the input signal after further propagation along the model domain and was exposed to additional scattering. The signal amplitude of the coherent wavefront decreases accordingly, and the trailing incoherent wave energy increases.

Interestingly, when a cosine modulated pulse is used as input, a low-frequency component is observed within the frequency domain in Figure 5.5. This low frequency component arises from a non-zero mean in the time-domain excitation rather than from frequency generation. A symmetric, zero-mean excitation would suppress this effect. Although the impact of this component is usually negligible, since the amplitude of the input pulse and coherent wave is generally much greater.

After significant attenuation due to high-frequency propagation in aluminium, the coherent signal amplitude diminishes and now becomes comparable to the low-frequency component.

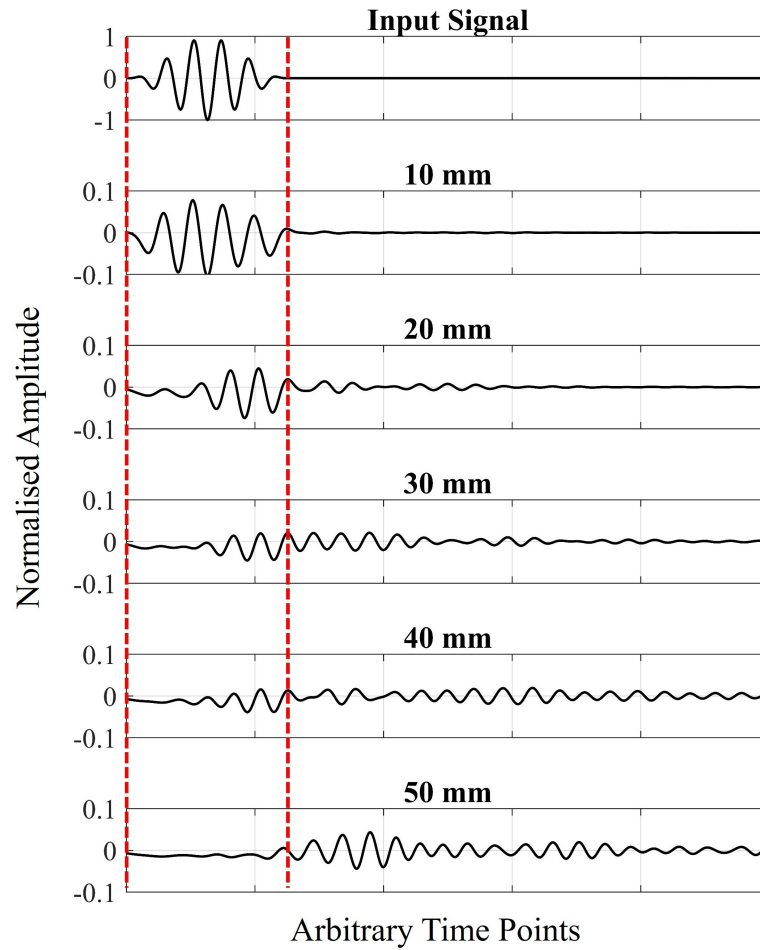


Figure 5.4: Excited and received signals at the corresponding propagation distances with normalised amplitude. The supposed location of the of the coherent signal are marked by the red dotted lines and are aligned for ease of comparison.

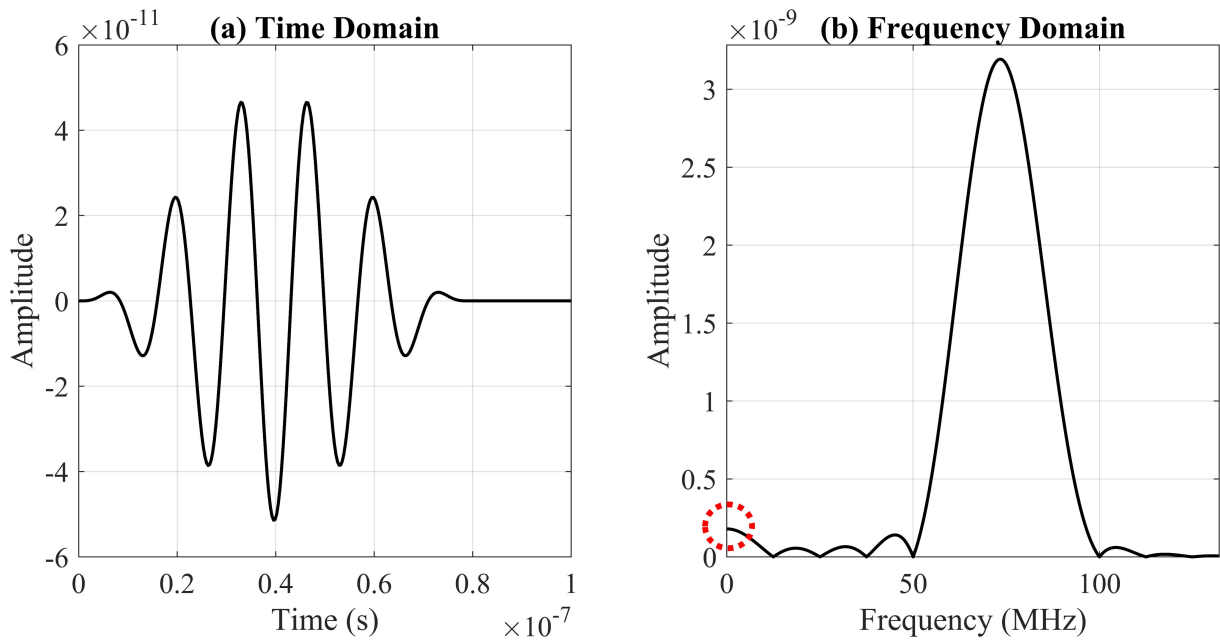


Figure 5.5: Input signal in the (a) time and (b) frequency domain at 75 MHz. The cosine modulated pulse generates a low-frequency component as outlined by the circle.

This creates a form of negative offset in the time domain signal as shown in Figure 5.6 (a), where the signal dips slightly before oscillating about the axis. With the use of this low-frequency component, it enables the identification of the coherent wave location even though the wave had been heavily attenuated. This interpretation relies on the assumption that dispersion effects are negligible, such that the low-frequency component propagates without significant temporal distortion relative to the coherent wave packet.

Before proceeding with the attenuation measurements, the low-frequency component needs to be filtered since it is within the same amplitude range as both the coherent and incoherent signals. Hence, with the application of a high-pass filter, the corresponding time domain signal is compared in Figure 5.6 (a), where the negative offset is removed. This indicates that the coherent wave has been heavily attenuated and has been replaced by scattered and diffracted signals that trail closely behind. A time domain band-pass filter is applied to isolate the coherent and incoherent signals around the region of interest for attenuation computations. The frequency response is illustrated in Figure 5.6 (b) which exhibits a frequency distribution that follows the Gaussian spectrum of the input pulse.

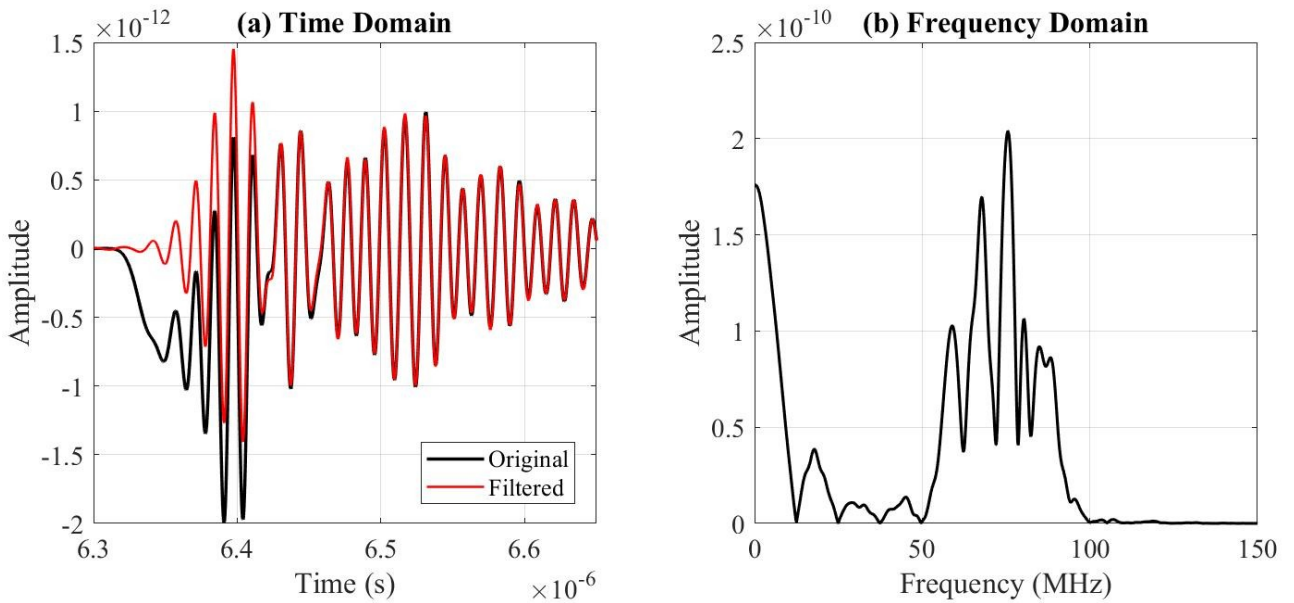


Figure 5.6: Attenuated signal in the (a) time and (b) frequency domain at 75 MHz after propagating through 40 mm distance in aluminium. A negative offset is observed in the time domain which indicates the position of the propagated coherent waveform.

Two types of windows are compared to determine their suitability and effectiveness in evaluating attenuation profiles within the geometric regime. First, a window that is the size of the input coherent signal is evaluated. This window is applied on the propagated signals in the region where the negative offset lies since that indicates the original location of the coherent signal. In this case, the goal is to capture any residuals of the coherent wave while eliminating any possible interference from the scattered signals. This coherent window is selected as it is commonly used in Rayleigh and stochastic attenuation measurements where coherent wave amplitudes are still significant.

The alternative is to extend the window filter to encompass the full trailing scattered signals. During the wave propagation in the geometric regime, the coherent wave gets scattered, diffracted, and refracted which forms the trailing incoherent wave. In the event where the coherent wave cannot be reliably measured due to significant attenuation, the pragmatic approach is to evaluate the incoherent contributions.

The two window types are illustrated in Figure 5.7, with the red line representing the coherent window, and the black line representing the extended incoherent window, for signals of varying propagation distances.

5.3.2.1 Coherent Wave Extraction with Time Domain Averaging

In the Rayleigh and stochastic regimes, the conventional signal processing method is to average the signals across multiple realisations in the time domain, followed by a Fourier transform operation to generate a single attenuation profile [42]. As the coherent wavefront has been heavily attenuated and the incoherent scattered signals are not fully suppressed, the band-pass window filter used to isolate the signal strongly influences the attenuation measurements. A small window surrounding the location of the low-frequency component (negative offset) may introduce artefacts due to the very low amplitude signals in the region. A large window encompassing the incoherent signals may introduce inconsistencies, since the frequency response increases with the size of the window filter.

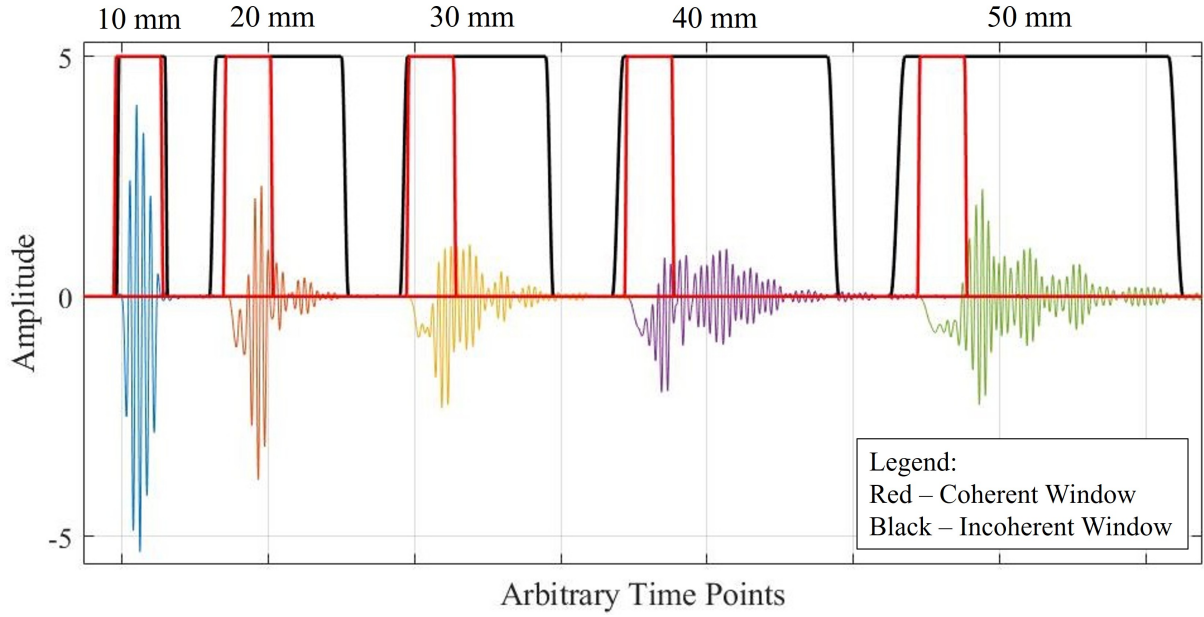


Figure 5.7: Time domain signals at 75 MHz frequency with various propagation distances ranging from 10 mm (left) to 50 mm (right) that are fitted in a single plot for ease of comparison. The coherent window (red) and extended window (black) are used to capture the region of interests.

The attenuation profile for the coherent window filter is shown in Figure 5.8 (a) and slight upward trend in the attenuation profile can be observed. This is in contrast to geometric regime phenomenon where attenuation should plateau. Upon further investigation, it is because the frequency response of the coherent residuals does not yield significant signal amplitude. As the trailing incoherent wave is closely entangled to the coherent wave location, the signals cannot be separated cleanly through windowing. As such, the time-domain filter used intersects with the incoherent waves which introduces artefacts that shows up in the frequency spectrum, particularly since the coherent signal does not hold much weight. This suggests that the coherent window filter is insufficient due to the lack of significant coherent signal response relative to the incoherent counterparts.

To assess the stabilisation of the ensemble averaging procedure and the associated finite-ensemble variability, a convergence study was performed by progressively increasing the number of independent microstructure realisations, N , used in the time-domain averaging. For each

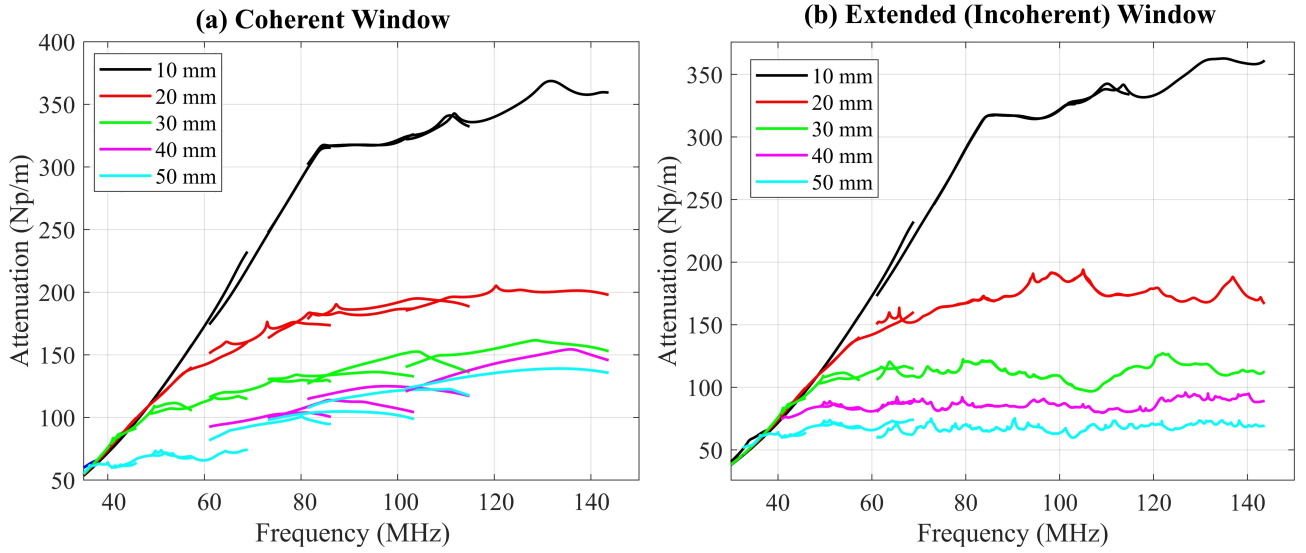


Figure 5.8: Attenuation profiles generated using (a) coherent windows and (b) extended incoherent window, ranging from stochastic to geometric regimes with various propagation distances from 10 to 50 mm.

value of N , an ensemble-averaged waveform was computed as

$$u_N(t) = \frac{1}{N} \sum_{i=1}^N u_i(t), \quad (5.1)$$

where $u_i(t)$ denotes the propagated signal obtained from the i -th independent realisation.

Rather than comparing the ensemble average against a finite-ensemble reference waveform, which would lead to self-referential convergence, stabilisation was quantified using a split-ensemble approach. The full set of $N_{\max} = 40$ independent realisations was randomly partitioned into two disjoint subsets of equal size. For each subset, ensemble-averaged waveforms were computed independently as a function of ensemble size N , and the discrepancy between the two ensemble estimates was evaluated using the normalised L_2 metric

$$E_{\text{split}}(N) = \frac{\|u_A(N, t) - u_B(N, t)\|_2}{\|u_{N_{\max}}(t)\|_2}, \quad (5.2)$$

where u_A and u_B denote the ensemble averages formed from the two subsets. The norm was evaluated over the same coherent analysis window used for attenuation extraction. This random partitioning was repeated 50 times, and the mean and standard deviation of $E_{\text{split}}(N)$ across the 50 repetitions were computed to estimate ensemble-to-ensemble variability.

Figure 5.9 compares the ensemble stabilisation behaviour for representative cases in the stochastic and geometric scattering regimes. In the stochastic regime, the split-ensemble discrepancy decreases rapidly with increasing N , reaching a low residual level after approximately 5–10 realisations, indicating rapid stabilisation of the ensemble-averaged waveform. In contrast, the geometric regime exhibits a substantially slower decay and a markedly higher residual plateau, reflecting persistent ensemble-to-ensemble variability due to the dominance of incoherent scattering. The non-zero residual observed in both cases is a consequence of finite ensemble size and does not indicate a lack of convergence to a well-defined ensemble mean.

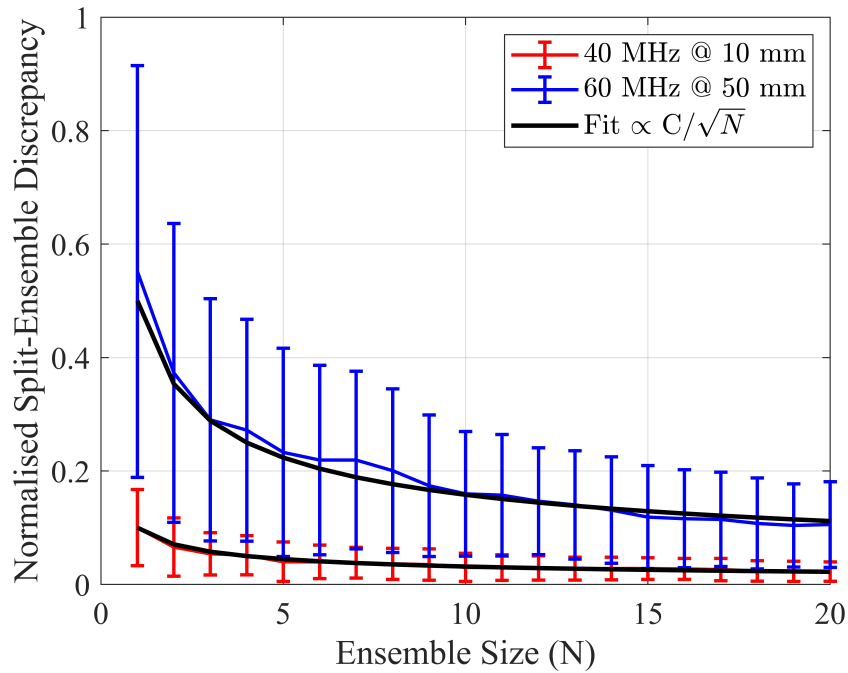


Figure 5.9: Split-ensemble stabilisation of time-domain ensemble averaging with increasing ensemble size N . The normalised L_2 discrepancy between independently averaged waveforms formed from two disjoint subsets of realisations is shown for representative stochastic- and geometric-regime cases. Error bars indicate $\pm$ one standard deviation across 50 random partitions. Black curves indicate reference $C/\sqrt{N}$ scaling ($C=0.1$ and $C=0.5$ for the stochastic and geometric cases, respectively).

The observed decay of the split-ensemble discrepancy with increasing ensemble size is consistent with the $N^{-1/2}$ scaling expected from the central limit theorem, which describes the reduction of variance through averaging of independent realisations. To provide a qualitative reference, curves of the form $C/\sqrt{N}$ are overlaid in Figure 5.9. The proportionality constant C represents the effective amplitude of incoherent fluctuations associated with the scattering process. The fitted values $C \approx 0.5$ for the geometric-regime case and $C \approx 0.1$ for the stochastic-regime

case indicate a substantially larger incoherent contribution in the geometric regime, consistent with its slower stabilisation and higher residual ensemble-to-ensemble variability. Assuming the observed $N^{-1/2}$ scaling persists, the fitted $C/\sqrt{N}$ curves provide a means of extrapolating the expected level of residual ensemble-to-ensemble variability at larger ensemble sizes. These extrapolations should be interpreted as indicative measures of the remaining incoherent component rather than absolute error estimates.

In the geometric regime, a coherent component will still exist in principle at an exponentially small amplitude due to exponential attenuation. Ensemble averaging can, in principle, recover an arbitrarily small coherent mean field. However, in practice, once scattering enters the geometric regime, the coherent component decays so rapidly that it becomes extremely difficult to isolate reliably from incoherent scattered contributions. While this does not alter the physical definition of attenuation as coherent-wave decay, it renders direct measurement of coherent attenuation impractical.

Analytical attenuation models such as the second-order approximation and unified scattering theories describe attenuation in terms of coherent-wave decay and are therefore valid while coherent propagation dominates. These frameworks formally extend into the geometric regime because they are constructed as closed-form perturbative descriptions of mean-field decay and correctly recover asymptotic attenuation trends. However, once scattering enters the geometric regime, phase coherence is rapidly destroyed and wave propagation becomes transport-dominated. In this regime, descriptions based on energy redistribution following coherence loss become more appropriate than coherent-wave attenuation models. Consequently, alternative observables that track energy transport—such as the use of broader time windows and frequency-domain magnitude averaging—offer a pragmatic and experimentally accessible means of characterising wave behaviour in the geometric regime. These approaches do not replace traditional attenuation measurements, but instead provide complementary insight into transport-dominated scattering once coherent propagation is no longer readily observable.

5.3.2.2 Incoherent Energy Extraction with Frequency Domain Averaging

Frequency domain averaging is conducted by first transforming each time domain signal realisation into the frequency domain, after which the magnitude (or power spectrum) of the individual spectra is averaged to produce a single attenuation estimate. This procedure does not attempt to recover phase coherence, but instead estimates the mean transmitted spectral energy which remains well-defined even after coherence is lost. This makes frequency-domain averaging a more appropriate tool for characterising energy loss in the geometric regime, where wave transport is dominated by incoherent scattering rather than coherent propagation—this will be referred to as ‘incoherent attenuation’ throughout the rest of the thesis.

Using the extended window filter to capture the incoherent scattered signals, the incoherent attenuation profiles are illustrated in Figure 5.8 (b) which matches the expectation of frequency independence and plateauing. This highlights the sensitivity of attenuation estimates to both the domain averaging and window selection in the geometric regime. In the geometric regime, the scattered field becomes highly decorrelated in phase after numerous scattering events and further propagation does not preferentially attenuate the scattered field since they only produce random phase and amplitude fluctuations. Consequently, the scattered signal approaches a Gaussian statistical distribution with an envelope that reflects the bandwidth of the input excitation. This leads to an incoherent attenuation profile that is effectively frequency independent which is a characteristic of geometric scattering regime.

Conventionally, attenuation is characterised as a function of propagation distance through an exponential decay law, with the attenuation coefficient itself treated as distance-independent and primarily determined by microstructural morphology. In the Rayleigh and stochastic scattering regimes, the coherent wave remains the dominant carrier of energy, and attenuation directly reflects coherent-wave decay. This relationship remains physically valid in the geometric regime; however, the coherent component becomes increasingly difficult to isolate in practice due to rapid coherence loss and strong incoherent scattering. In the present study, this behaviour is evident in Figure 5.10 at frequencies between 1 to 30 MHz, where the various attenuation profiles representing different propagation distances overlap.

With further increases in operating frequency, the incoherent attenuation profiles in Figure 5.10 diverge, with longer propagation distances exhibiting lower apparent transition frequencies and reduced incoherent attenuation. At first glance, this behaviour appears counter-intuitive as attenuation coefficient is conventionally treated as distance-independent, and one would expect greater energy loss with increasing propagation distance rather than reduced attenuation.

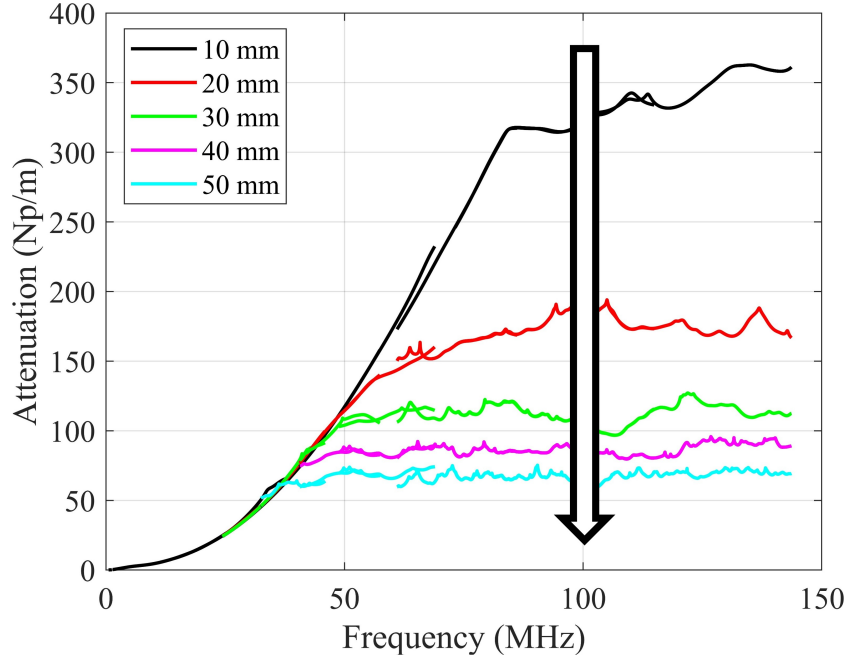


Figure 5.10: Incoherent attenuation profiles with varying propagation distances from 10 to 50 mm covering the Rayleigh to geometric regimes. The profiles overlap within the Rayleigh and stochastic regimes, but diverges once the wave approaches the geometric regime. The vector indicates the drop in the plateau incoherent attenuation with increasing propagation distances.

The underlying hypothesis is that the conventionally calculated attenuation coefficient is intended to describe coherent-wave decay and is therefore not applicable once wave propagation becomes dominated by incoherent scattering in the geometric regime. Under the conventional formulation, illustrated schematically in Figure 5.11, attenuation is extracted from the decay of the coherent wave amplitude with propagation distance. In the example shown, the wave reaches the geometric regime after approximately 10 mm of propagation, beyond which the coherent component has decayed sufficiently for incoherent, multi-path scattering to dominate. Further propagation does not result in additional significant coherent-wave decay but instead redistributes energy through transport-dominated scattering. Consequently, the incoherent attenuation coefficients extracted over longer propagation distances decreases, as highlighted by

the reduced gradients of the blue lines. This behaviour indicates that, in the geometric regime, the incoherent attenuation measurement becomes inversely related to propagation distance, as the overall energy loss is effectively averaged over an increasing path length.

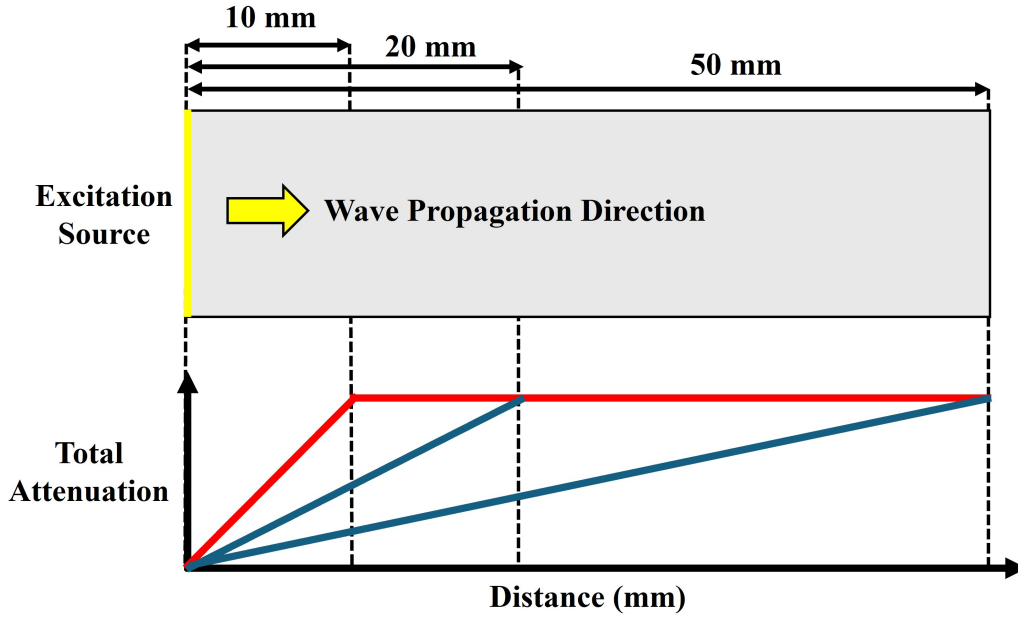


Figure 5.11: Illustration of how calculated incoherent attenuation coefficient (gradient of blue lines) varies with propagation distances in the geometric regime. The initial red line from 0 to 10 mm distance represents the linear accumulation of energy loss and decay of the coherent wave. After the geometric regime is reached, incoherent attenuation extracted over longer propagation distances decreases due to the dominance of incoherent, transport-dominated scattering rather than further coherent-wave decay.

As such, the conventional attenuation formulation remains physically valid into the geometric regime, as it continues to describe the decay of the coherent component. However, once this regime is reached, the coherent wave amplitude becomes exponentially small and increasingly difficult to isolate in practice. Hence, to characterise the cumulative loss of the coherent wave once this transition has occurred, the term ‘Total Attenuation’ is introduced. This quantity represents the total coherent-wave amplitude loss due to scattering and is defined such that it is independent of propagation distance after appropriate normalisation. In the geometric regime, the Total Attenuation may be obtained by multiplying the conventional attenuation coefficient by the corresponding propagation distance to yield:

$$\alpha_{total} = \ln \left(\frac{F}{B} \right) \quad (5.3)$$

where F and B are the front- and back-wall signal amplitudes in the frequency domain, respectively. In this formulation, the propagation distance factor has been explicitly absorbed, allowing direct comparison between incoherent attenuation measurements obtained over different path lengths in the geometric regime.

For example, referring to Figure 5.8 (b), the geometric incoherent attenuation coefficients for 10 and 50 mm propagation distances are approximately 315 and 65 Np/m, respectively. After multiplying each value by their respective distances, the resulting Total Attenuation converges to approximately 3.5 Np for both cases, as shown in Figure 5.12. While this distance compensation causes misalignment within the stochastic regime—where attenuation remains distance-independent by definition—it enables consistent interpretation within the geometric regime. The Total Attenuation therefore provides a convenient diagnostic measure of the cumulative coherent-wave loss, enabling consistent comparison between different propagation distances in the geometric regime. This eliminates ambiguity when comparing samples of identical microstructures but differing thicknesses.

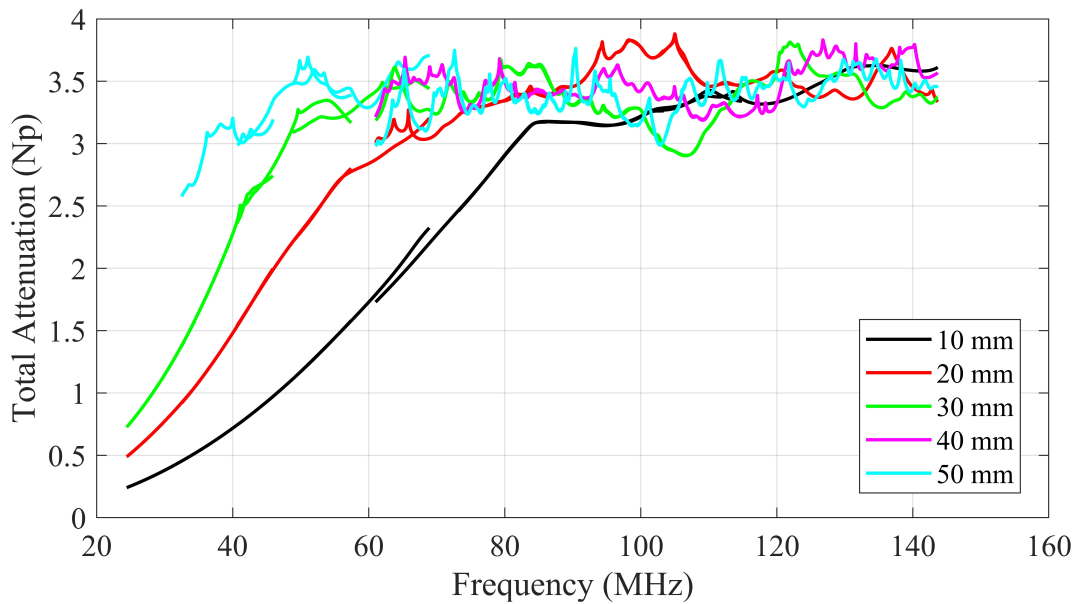


Figure 5.12: Total Attenuation measurement variation with propagation distances ranging from 10 to 50 mm at 75 MHz operating frequency that converges at a value of approximately 3.5 Np in the geometric regime.

5.3.3 Other Parameters Influencing Geometric Transition

Traditionally, geometric regime is defined as the scattering regime where the grain size is much larger than the wavelength. During this scenario, the propagating wave reflects and refracts along the grain boundaries, resulting in scattering and mode-conversions within the medium. This causes the coherent wavefront to be heavily attenuated, with the leftover scattered signals that are projected on the incoherent attenuation profile as a plateau.

5.3.3.1 Propagation Distance

From the previous investigations, with grain size and operating frequency kept constant, propagation distance also affected the transition frequency towards the geometric regime. To further examine this phenomenon, propagation distances ranging from 2.5 to 2000 mm were modelled, and the corresponding transition frequencies were plotted as a function of distance as shown in Figure 5.13. At a propagation distance of 2 m, the wave transits into the geometric regime at 15 MHz and this translates to a wavelength of approximately 0.4 mm. Compared to the characteristic grain dimension of 2.2 mm, this operating condition would conventionally be associated with the Rayleigh or stochastic scattering regimes. This observation therefore demonstrates that wavelength-to-grain-size ratios alone are insufficient to predict the observable transition to the geometric regime.

This is an important finding, as propagation distance is typically not treated as an explicit variable in 3D scattering analytical models. In such models, attenuation is formulated as a distance-independent coefficient that characterises the local rate of coherent energy loss per unit length. However, while the attenuation coefficient itself is distance-independent, the cumulative loss of coherence and redistribution of energy into the incoherent scattered counterparts depend on the total propagation distance. The propagation distance itself does not alter the intrinsic scattering regimes, but the accumulation of scattering events either in the Rayleigh or stochastic regimes over long propagation distances can result in coherence loss and the transition towards geometric regime.

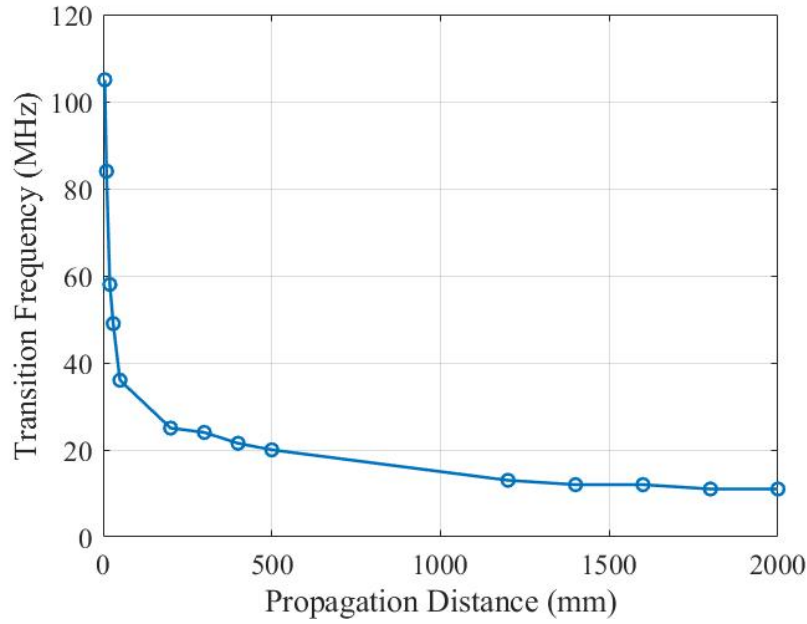


Figure 5.13: Geometric transition frequency as a function of propagation distance in aluminium.

5.3.3.2 Material Anisotropy

The comparison between aluminium and lithium demonstrated the amplifying role of anisotropy on scattering. As shown in Figure 5.14, lithium exhibited an earlier transition towards geometric regime at a lower frequency, with a larger plateau attenuation value. This was attributed to the very high anisotropy factor of lithium ($A = 8$) as opposed to aluminium ($A = 1.19$), resulting in large velocity mismatches between neighbouring grains, causing stronger scattering effects at the boundaries.

In strongly anisotropic materials, the propagation velocity varies significantly with direction, leading to a larger spread of group velocities within a polycrystalline aggregate. As ultrasonic wave traversed through such materials, neighbouring grains often present mismatched acoustic impedance, enhancing reflection and refraction at each boundary. This not only increases the amplitude of scattered components, but also introduces phase discontinuities that accelerate coherence loss. Additionally, anisotropy also promotes mode-conversions between longitudinal and shear waves at grain interfaces, further redistributing the energy across multiple propagation paths. These combined effects explained the transition into the geometric regime at lower frequency and the higher overall attenuation observed in lithium.

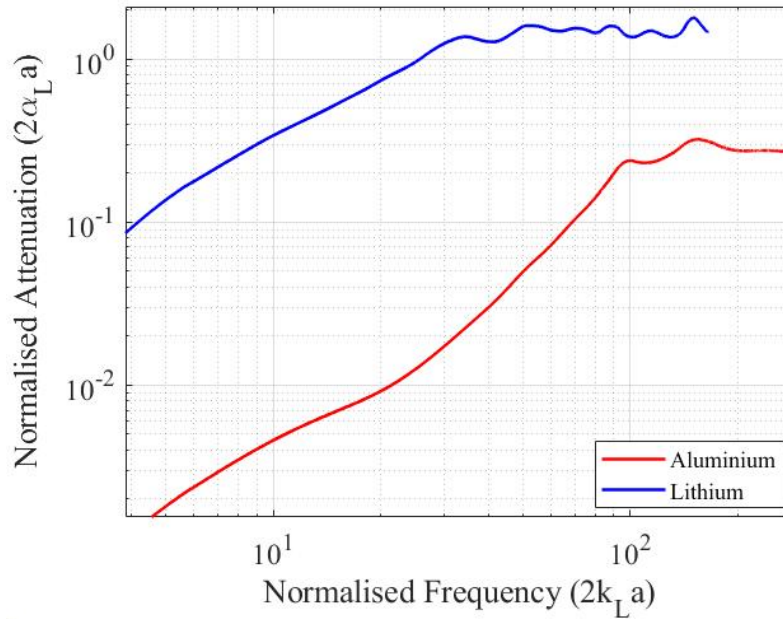


Figure 5.14: Normalised attenuation profile for both aluminium and lithium materials with 10 mm propagation distance and a frequency range from 1 to 100 MHz.

Furthermore, the attenuation profile of lithium is steeper per unit propagation distance, and the trailing scattered signals carry a larger proportion of the transmitted energy. This implies that strongly anisotropic materials will suffer from more rapid coherence loss, limiting the practical penetration depth of high-frequency ultrasonic inspections. In contrast, weakly anisotropic materials such as aluminium retain partial coherence over longer distances, making them more amenable to experimental investigation in the geometric regime.

5.4 Discussion

As an ultrasonic wave propagates through a statistically homogeneous polycrystalline medium, spatial fluctuations in elastic stiffness and wave speed introduce random phase perturbations along the propagation path. In unified scattering theory and radiative transport formulations, the total wavefield is commonly decomposed into a coherent (mean) component and an incoherent (fluctuating) component [102, 103].

Let $u(L, \omega)$ denote the complex wavefield at propagation distance L . The coherent field is defined as the ensemble average:

$$u_c(L, \omega) = \langle u(L, \omega) \rangle, \quad (5.4)$$

which represents the phase-preserving component of the wave. In random scattering media, the coherent field decays exponentially with propagation distance:

$$\langle u(L, \omega) \rangle = u_0(\omega) \exp[-\alpha_s(\omega)L], \quad (5.5)$$

where $\alpha_s(\omega)$ is the scattering-induced attenuation coefficient [32, 102]. According to unified scattering theory and SOA formulations for statistically homogeneous polycrystals, the coherent-field attenuation in the stochastic scattering regime exhibits a quadratic dependence on frequency:

$$\alpha_s(\omega) \propto \omega^2, \quad (5.6)$$

reflecting the cumulative effect of random phase perturbations introduced by elastic property fluctuations along the propagation path [32, 37]. The inverse of the extinction coefficient defines a characteristic coherence (or extinction) length,

$$L_c(\omega) = \frac{1}{\alpha_s(\omega)}, \quad (5.7)$$

which represents the distance over which phase coherence with the incident wave is preserved. As emphasised by Weaver and subsequent authors, this extinction length governs the decay of the ensemble-averaged (coherent) field [34, 102]. Combining the SOA frequency scaling with the definition of the extinction length yields:

$$L_c(\omega) \propto \omega^{-2} \propto \frac{1}{f_G^2}, \quad (5.8)$$

where f_G denotes the geometric transition frequency. This relation implies that the geometric transition is inherently distance-dependent—for a given propagation distance L , increasing

frequency reduces the coherence length until $L \sim L_c$, beyond which the coherent component becomes negligible and the observed response is dominated by incoherent, multiply scattered contributions.

Figure 5.15 shows the inverse-squared transition frequency plotted against propagation distance for the numerical results. The approximately linear relationship confirms the predicted scaling $(1/f_G^2) \propto L$, consistent with a coherence-length-controlled transition. Slight deviations at short and longer distances are likely attributed to discrete frequency resolution and the threshold-based definition of transition frequency. Overall, the linear trend demonstrates that the onset of the geometric regime is governed by cumulative coherence loss over distance rather than by a local wavelength-to-grain-size criterion alone.

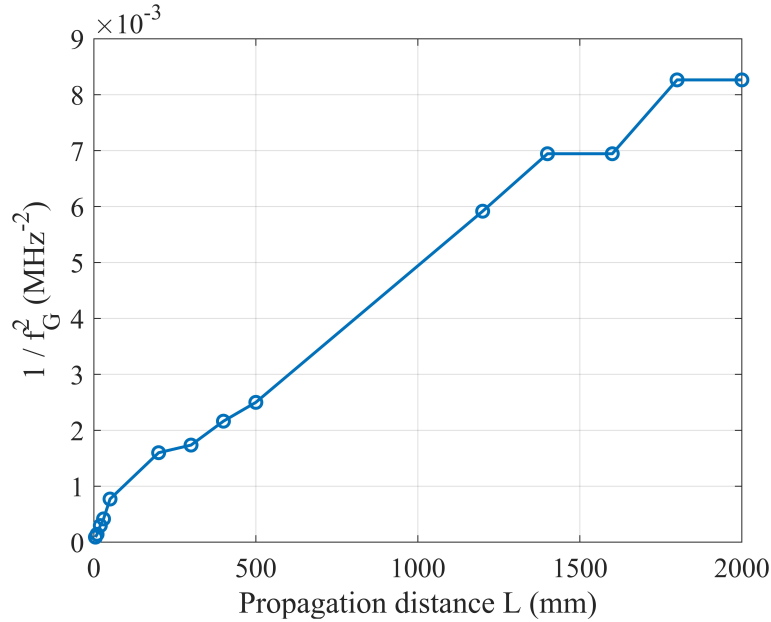


Figure 5.15: Linearised representation of the distance-dependent geometric transition frequency, plotted as $1/f_G^2$ versus propagation distance L . The approximately linear trend supports the predicted scaling derived from the coherence-length argument.

In this representation, the slope of the $(1/f_G^2) \propto L$ relationship reflects the strength of coherent-wave attenuation, which depends on microstructural scattering strength (e.g., grain morphology, texture and material anisotropy). A non-zero intercept can be interpreted as an effective offset distance, capturing near-field effects and finite windowing associated with the practical identification of the transition frequency.

With this coherence-length interpretation in mind, it becomes clear that conventional scattering regime classifications based solely on grain-size-to-wavelength ratios are incomplete, as they do not account for cumulative coherence loss with propagation distance or the influence of material anisotropy. To provide an operational definition of the geometric regime that explicitly incorporates these effects, the coherence fraction is introduced as

$$\eta(L, \omega) = \frac{I_c(L, \omega)}{\langle I(L, \omega) \rangle} = \frac{|\langle u(L, \omega) \rangle|^2}{\langle |u(L, \omega)|^2 \rangle}, \quad (5.9)$$

which measures the fraction of transmitted energy that remains phase-coherent after a propagation distance L . Here, $\langle \cdot \rangle$ denotes an ensemble average over independent microstructural realisations. The numerator represents the coherent intensity obtained from ensemble averaging of the complex field, while the denominator represents the total transmitted spectral energy obtained by averaging the intensity across realisations. The coherence fraction η therefore quantifies the relative contribution of coherent energy to the total wavefield.

From the numerical models, representative signals approaching the geometric regime are extracted to evaluate the coherence fraction and determine a practical threshold for the onset of incoherent-dominant scattering behaviour. The propagated signals are isolated using an extended time window and processed using time-ensemble averaging and frequency-domain magnitude averaging to extract the coherent and incoherent contributions, respectively. The ratio of the coherent to total spectral response at the geometric transition frequency is evaluated and shown in Figure 5.16. The results indicate that the onset of geometric behaviour occurs when the coherent spectral amplitude falls to approximately 20–30% of the mean spectral magnitude, corresponding to a coherent energy fraction of $\eta \sim 0.05$ – 0.1 .

Based on these observations, the scattering regimes may be characterised by the following observable signatures:

- Rayleigh regime: $\eta > \eta_{\text{crit}}$ and $p \approx 4$,
- Stochastic regime: $\eta > \eta_{\text{crit}}$ and $p \approx 2$,
- Geometric regime: $\eta \ll \eta_{\text{crit}}$ and $p \approx 0$,

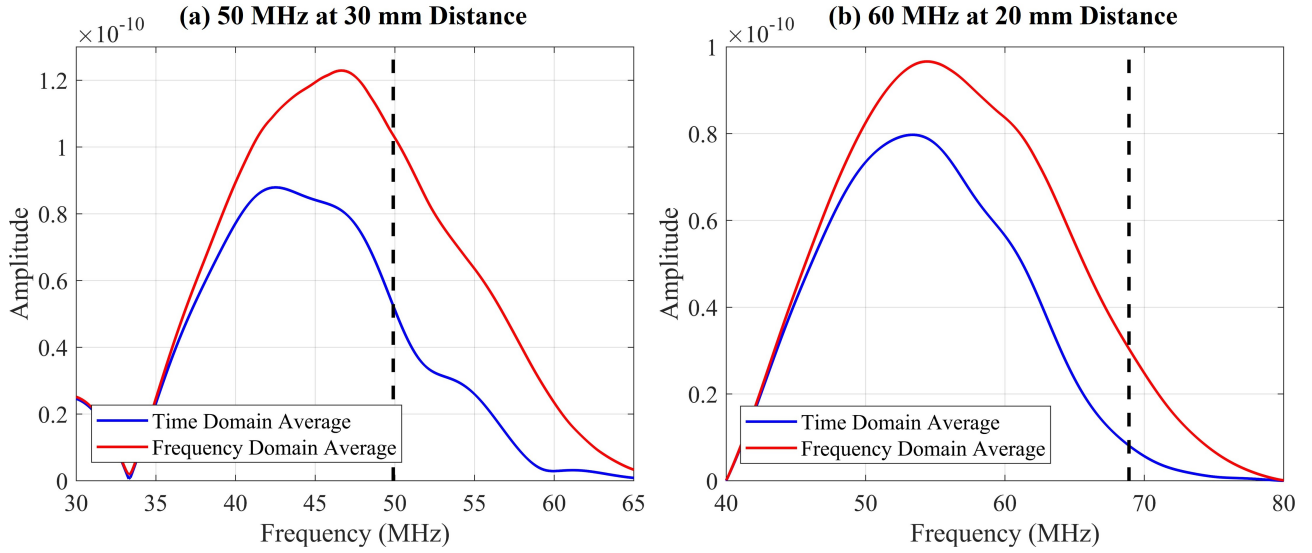


Figure 5.16: Frequency response of time-domain and frequency-domain averaged signals for (a) 50 MHz with 30 mm propagation distance and (b) 60 MHz with 20 mm propagation distance. The black dotted line indicates the geometric transition frequency with an approximate magnitude fraction of 0.25 in both cases.

where $\eta_{\text{crit}} \sim 0.05\text{--}0.1$ is a practical coherence threshold below which the coherent component no longer dominates the transmitted field, and p denotes the local frequency dependence of attenuation. Once this threshold is crossed, wave propagation becomes incoherent-dominated and attenuation is no longer governed by coherent-wave decay. As a consequence, the attenuation profile naturally approaches frequency independence ($p \approx 0$), which should be interpreted as an outcome of coherence loss rather than an independent defining criterion.

5.5 Conclusion

This work used ensembles of finite element simulations to investigate ultrasonic wave propagation and scattering in the high-frequency geometric regime. By adopting 2D models, it enabled systematic parameter studies across frequency, propagation distance, and material anisotropy while retaining the essential scattering trends beyond the Rayleigh regime.

The results show that, at sufficiently high frequencies, the coherent component becomes small within a short near-field region and the transmitted response becomes dominated by multiply scattered energy. Under these conditions, the incoherent attenuation extraction based

on coherent-wave decay becomes distance dependent and can yield counter-intuitive trends, including reduced apparent incoherent attenuation and lower apparent transition frequencies for longer propagation distances. A coherence-length interpretation captures this behaviour and predicts a distance-dependent transition frequency scaling of the form $(1/f_G^2) \propto L$, demonstrating that the onset of geometric behaviour is governed by both propagation distance and scattering strength rather than by wavelength-to-grain-size ratios alone.

Signal processing was also found to be critical in the geometric regime. Narrow time windows targeting residual coherent arrivals, combined with time-domain ensemble averaging, are prone to artefacts from the incoherent components which have not been fully suppressed once coherent energy becomes negligible. In contrast, extended time windows that capture the redistributed forward-propagating energy, together with frequency-domain magnitude averaging, provide stable attenuation estimates that exhibit the expected plateauing behaviour. These findings motivate a shift from coherent-wave attenuation concepts toward a distance-aware, incoherent-dominant interpretations in the geometric regime.

Finally, material anisotropy was shown to markedly accelerate coherence loss: the strongly anisotropic lithium models transition into geometric behaviour at lower frequencies and exhibit higher plateau attenuation than weakly anisotropic aluminium, reflecting increased velocity mismatch and stronger boundary scattering. This implies that practical application of geometric regime techniques will depend not only on grain size and wavelength ratios but also on crystallographic texture and anisotropy.

Overall, this study provides a computational basis for interpreting high-frequency scattering in polycrystals and proposes distance-aware, operational criteria for identifying the geometric regime based on coherent energy fraction and frequency-scaling behaviour. Future work should focus on extending these findings to 3D using parallelised solvers, developing analytical models to quantify connections to transport parameters such as mean free paths, and validate the predicted distance dependence experimentally. Such efforts will be essential to fully define the potential of the geometric regime and to determine its role in establishing the ultimate resolution limits of ultrasonic nondestructive evaluation.

It should also be noted that the geometric scattering behaviour investigated here is examined under idealised boundary conditions that retain both coherent and incoherent energy within the domain. These boundary conditions do not alter the intrinsic attenuation of the coherent wave, but they do influence the observable signal content by preventing additional losses associated with beam divergence, finite transducer aperture, and coupling effects that are present in practical ultrasonic inspections. As a result, the transition into the geometric regime identified in this study should be interpreted as a conservative upper bound on the persistence of coherent ultrasonic information. Consequently, if coherent responses become unobservable under these idealised conditions, they are unlikely to be recoverable in real inspection scenarios.

Chapter 6

Conclusion

6.1 Thesis Review

This thesis has examined the complex interactions between ultrasonic waves and Ti-64 microstructure embedded with macrozones. Macrozones have been shown as a potential cause to the onset of CDF, resulting in premature fatigue failure of aircraft engine components. Traditional characterisation methods such as EBSD, while effective, are destructive, time-consuming, surface-limited, and impractical for in-service inspections.

Ultrasonic testing, with the underlying elastodynamic principles, demonstrated promise in evaluating such complex microstructures, with the added advantage of being non-destructive, cost-effective, and having applicability to real components. This thesis explored how ultrasound responses such as attenuation, backscatter, and velocity varies in the presence of macrozones. Across the chapters, the work integrated FE models, experimental validation, and synthetic microstructure generation to form a coherent framework for linking ultrasound responses with underlying material microstructure.

Chapter 2 laid the theoretical groundwork, reviewing microstructural features and their relation to elastic wave propagation, wave scattering mechanisms, and prior macrozone studies.

Chapter 3 provided a parametric FE study of wave–macrozone interactions, showing how size, shape, and orientation of macrozones influence attenuation, backscatter, and velocity, which were validated experimentally.

Chapter 4 advanced this by introducing a synthetic microstructure methodology directly informed by EBSD datasets, enabling generation of representative digital twins. This bridged modelling and experiment, providing a scalable way to explore realistic morphologies.

Chapter 5 advanced the analysis into the geometric scattering regime, revealing distance-dependent coherence loss, transport-dominated attenuation behaviour, and the amplifying role of anisotropy. This led to a reinterpretation of attenuation measurements at high frequency and the introduction of a distance-aware Total Attenuation concept.

Together, these contributions move beyond isolated case studies to present an integrated strategy: from simplified parametric insight, through synthetic microstructural realism, to frontier investigations at the resolution limit. The novelty lies not only in individual findings—such as distance-dependent regime transitions or anisotropy-induced amplification—but also in combining modelling, experiment, and synthetic data into a framework that can be translated toward industry practice.

6.2 Key Contributions

The main contributions of this research can be summarised as follows:

1. Parametric Investigation of Wave–Macrozone Interactions

Using 2D FE models, systematic studies revealed the influence of macrozone size, shape, and orientation on ultrasonic responses. These results were experimentally validated, providing a strong foundation for linking measurable ultrasonic parameters to underlying microstructural features.

This investigation was intentionally limited to 2D models and idealised macrozone configurations, which prioritised physical interpretability over full quantitative fidelity.

2. Synthetic Microstructure Methodology

A novel workflow was developed to generate representative synthetic Ti-64 microstructure embedded with macrozones directly from EBSD datasets. By integrating grain statistics, orientation distribution function, and feature segmentation, the methodology successfully reproduced realistic microstructures whose ultrasonic responses could be studied in detail. This approach offers a powerful tool for bridging the gap between modelling and experimental characterisation.

At this stage, the approach remains 2D and does not fully capture 3D macrozone connectivity or MDF within individual features.

3. Extension into the Geometric Scattering Regime

This thesis extended FE modelling into the geometric scattering regime, an area rarely explored due to computational and interpretational challenges. The results demonstrate that the observable transition into geometric behaviour is governed not only by wavelength-to-grain-size ratios, but also by cumulative coherence loss with propagation distance. A convergence analysis showed that ensemble averaging rapidly suppresses incoherent fluctuations in the Rayleigh and stochastic regimes, but becomes ineffective once coherence collapses in the geometric regime. This motivated a shift from coherent-wave attenuation concepts to transport-dominated interpretations and the introduction of a Total Attenuation metric that captures cumulative coherent-wave loss independent of propagation distance.

These findings were obtained under idealised boundary conditions and limited averaging, and further validation is required to establish quantitative convergence criteria under experimental conditions.

4. Framework for Non-Destructive Evaluation of Macrozones

Collectively, the results demonstrate that ultrasonic testing, supported by FE modelling and synthetic dataset generation, can form the basis of a structured framework for detecting and characterising macrozones in Ti-64 alloys.

In this framework, bulk ultrasonic measurements (attenuation, velocity, and backscatter) are first used as a rapid screening tool to identify components exhibiting anisotropic or anomalous responses. These observations are then interpreted using parametric FE models to infer the likely macrozone characteristics responsible for the measured behaviour. Synthetic microstructures informed by EBSD statistics are subsequently employed to refine this interpretation and establish physically consistent bounds on macrozone size, morphology, and orientation.

This staged approach provides industry with a practical pathway to move from raw ultrasonic signals to informed microstructural assessment, supporting decision-making in manufacturing qualification and in-service inspection to mitigate CDF risks.

6.3 Industrial Impact

The outcomes of this research are directly relevant to the aerospace industry, where the detection and management of macrozones in Ti-64 components is critical to mitigate the risks of CDF. Current industrial practice relies heavily on destructive microstructural characterisation and conservative life-management strategies, which are costly and limited in their ability to assess spatially heterogeneous features in-service.

The framework developed in this thesis demonstrates how ultrasonic measurements, when interpreted using physically informed FE models and representative synthetic microstructures, can provide insight into macrozone morphology, orientation, and spatial extent without sectioning or material removal. In particular, the combination of directional attenuation, backscatter analysis, and synthetic microstructure modelling offers a pathway towards identifying potentially harmful macrozones early in the manufacturing process or during service inspections.

From an industrial standpoint, the proposed methodology supports a tiered inspection strategy. Rapid bulk ultrasonic screening may first be used to flag components exhibiting anomalous anisotropic responses, followed by more targeted directional or phased-array measurements informed by synthetic modelling. This approach has the potential to reduce unnecessary in-

spection frequency, improve confidence in life assessments, and lower the risk of undetected CDF-critical microstructures in safety-critical components such as compressor discs and fan blades.

While further development is required before industrial deployment, particularly in terms of three-dimensional modelling and quantitative inversion, the work presented here establishes a scientifically grounded basis upon which such inspection methodologies can be built.

6.4 Future Work

While this study has advanced the understanding of wave-microstructure interactions, further research is warranted to strengthen its industrial applicability. The following directions directly address the methodological limitations identified in the preceding chapters and outline the steps required to transition the proposed framework towards quantitative and industrial deployment.

1. Extending the FE models into 3D for more accurate representation of macrozones in actual samples and to enable direct quantitative comparison to experimental results. Particularly within the Rayleigh regime where dimensionality affects the attenuation profile, this is an important aspect for consideration. Instead of a full-factorial parametric study, selected cases can be used instead to target specific macrozone characteristics that are potential triggers of CDF.
2. Refining synthetic microstructure generation to better capture complex morphologies and texture distributions. This includes feeding grain size and morphological distributions into Neper to streamline the microstructure generation procedure. This also enables the adaption of the methodology to other complex microstructures. The methodology can also be further developed into 3D which would require orthogonal EBSD sectorial scans to determine the complete morphology of the microstructure. This information is then fed into Neper to generate a 3D synthetic microstructure for more quantitative analysis.

3. Develop inversion algorithms to directly retrieve macrozone characteristics from ultrasonic signals, enabling practical non-destructive evaluation in manufacturing and in-service inspections. With the use of backscatter signals, macrozone-generated hotspots were detected. This methodology can be refined further with the use of phased arrays for sectorial and orthogonal scans. This, coupled with the directional backscatter inversion algorithms could provide more accurate characterisation of macrozones. For instance, the use of phased arrays to acquire sectorial scans provides multi-angle backscatter data from a single surface. The resulting directional backscatter patterns add independent constraints, reducing single-view ambiguity and enabling more accurate inversion of macrozone orientation and extent.
4. Expand upon the work in the geometric regime by incorporating the effects of propagation distances in the analytical solution. This could help redefine the geometric regime since it may also be achieved at comparable grain size to wavelength ratio with enough propagation distance. The FE model and analytical solutions can be validated with experimental scans by propagating low frequency ultrasonic waves repeatedly through an actual aluminium sample.

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Publications and Conference Presentations

Journal Publications

1. W. Y. Yeoh, B. Lan, and M. J. S. Lowe, “Representative microstructures for two-dimensional computational studies of ultrasonic wave propagation in titanium alloys,” *Proc. Roy. Soc. A*, 2025, Art. no. 20240776, DOI: 10.1098/rspa.2024.0776.
2. W. Y. Yeoh, B. Lan, and M. J. S. Lowe, “Investigation of the influence of macrozones in titanium alloys,” *Proc. Roy. Soc. A*, vol. 479, 2023, Art. no. 20230176, DOI: 10.1098/rspa.2023.0176.
3. L. Katch, W. Y. Yeoh, O. Touzanov, M. Pacheco, B. Lan, A. P. Argüelles, “Shear Wave Ultrasound Inspection of Flaws in Silicon Wafers,” *IEEE Trans. Ultrason., Ferroelectr., Freq. Control*, 2023. DOI: 10.1109/TUFFC.2023.3321254
4. Gillespie, J., W. Y. Yeoh, C. Zhao, N. D. Parab, T. Sun, A. D. Rollett, B. Lan, C. M. Kube, “In situ characterization of laser-generated melt pools using synchronized ultrasound and high-speed X-ray imaging,” *J. Acoust. Soc. Am.*, vol. 150, no. 4, pp. 2409–2420, 2021. DOI: 10.1121/10.0006386.

Conference Presentations

1. W. Y. Yeoh, B. Lan, and M. J. S. Lowe, “2D finite element modelling for ultrasonic attenuation measurement in polycrystalline media,” in *Proc. ASME 48th Annu. Rev. Prog. Quant. Nondestruct. Eval. (QNDE 2021)*, Online Conf., 2021.
2. W. Y. Yeoh, B. Lan, and M. J. S. Lowe, “Characterisation of macrozones in titanium alloys using ultrasonic testing,” in *Proc. ASME 49th Annu. Rev. Prog. Quant. Nondestruct. Eval. (QNDE 2022)*, San Diego, CA, USA, 2022.
3. W. Y. Yeoh, B. Lan, and M. J. S. Lowe, “Characterisation of macrozones in titanium alloys using ultrasonic testing,” in *Proc. Br. Inst. Non-Destruct. Test. (BINDT) Annu. Conf.*, Telford, U.K., 2022.
4. W. Y. Yeoh, B. Lan, and M. J. S. Lowe, “Generation of realistic synthetic macrozones for elastic wave finite element models,” in *Proc. ASNT Res. Symp.*, Columbus, OH, USA, 2023.