On the Dimensionality of Elastic Wave Scattering within Heterogeneous Media

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Abstract - Elastic waves scatter when their wavelength becomes comparable to random spatial fluctuations in the elastic properties of the propagation medium. It is postulated that within the long-wavelength Rayleigh regime, the scattering induced attenuation obeys a $D=1,2,3$ dimensional dependence on wavenumber, k^{D+1} , whilst within the shorter-wavelength stochastic regime, it becomes independent of the dimensions and thus varies as k^2 . These predictions are verified numerically with a recently developed Finite Element method in both 3D, 2D, and 1D, for the example of ultrasonic waves propagating within polycrystalline materials. These findings are thought to be practically useful given the increasing uptake of numerical methods to study highly scattering environments which exhibit multiple scattering, but often remain limited to 2D given computational constraints. It is hoped that these results lay the groundwork for eventually producing computationally efficient 2D simulations which are representative of 3D.

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I. INTRODUCTION

Scattering of elastic waves within heterogeneous media applies to a great number of problems in elastodynamics, including seismology¹ and ultrasonic non-destructive evaluation². For some it enables, for example, the characterisation of the Earth's crust (e.g. Zhao et al.³) whilst for others it hinders, say the detection of defects buried in metallic materials⁴. In the latter case, and within the context of this article, scattering arises when the probing wavelength becomes comparable to the characteristic dimension of random spatial variations in the elastic properties of the medium.

Irrespective of its application, scattering remains a complex phenomenon. A great variety of possible heterogeneities and altering wave behaviour throughout different scattering regimes, restrict analytical models where multiple scattering^{5,6} in particular presents difficulties. Numerical techniques^{7–10} are more flexible and capture both single and multiple scattering, yet are computationally expensive due to the requirement of modelling two length-scales, one corresponding to the wavelength and another to that of the heterogeneity. The continual growth in computational resource however, makes numerical approaches such as the Finite Element (FE) method increasingly attractive^{11–15} to study wave scattering phenomena. Recent such progress¹⁵ has shown FE to be capable of capturing the range of physics required to describe the different scattering regimes.

Even so, its computational cost remains significant; full-scale 3D studies are often unfeasible and are likely to remain so for many practical cases of interest. Hence for the time being, the majority of investigations are limited to 2D^{11–14,16–20} which are not necessarily representative of 3D scattering. At least the implication of a 2D approximation to the scattering problem is not sufficiently understood at present, particularly so across the different scattering regimes. Understanding the dimensional behaviour of scattering therefore becomes important not only for future numerical studies but also for laying the groundwork to achieve more efficient 2D simulations that are usefully representative of 3D.

Scattering behaviour can be studied either in terms of the amplitude loss incurred by the coherent wave field, or the intensity gained by its counterpart, the incoherent scattered wave field. The former constitutes the scattering induced attenuation, usually denoted by the attenuation coefficient, α as an

exponential decay in Equation 1, where U describes the coherent wave amplitude for a plane wave propagating at distance z .

$$U(z) = U_0 e^{-\alpha z} \quad (1)$$

This article treats the scattering induced attenuation and studies its governing dependence on wavelength (or wavenumber) within relatively small yet characteristic numerical models to demonstrate the dimensional behaviour across different scattering regimes in 3D, 2D, and 1D. A range of wavelengths are studied such that the long-wavelength Rayleigh regime and the shorter-wavelength stochastic regime are considered for the example of ultrasonic waves propagating within polycrystalline materials.

The subsequent Section II presents preliminary theories that describe the dimensional dependence of scattering for both regimes. Section III holds the numerical calculations which verify these postulations.

II. THEORETICAL CONSIDERATIONS

Scattering within heterogeneous media, including polycrystalline materials, embodies different regimes – each regime describing a different physical approximation to a particular scattering behaviour. The validity of each region can be classified by three measures of scale¹, foremost of which is the normalised wavenumber, kd , where k is the wavenumber and d is the length scale of the heterogeneity, in this case the average grain size. The two remaining dimensionless numbers are the normalised propagation length, L/d , where L is the propagation distance; and the perturbation index, n , which is a property solely related to the medium, here defined by the degree of elastic variation within the polycrystalline material.

Within the practical confines of ultrasonic NDE, three scattering regimes can be readily identified²¹. Firstly, as a long wavelength approaches dimensional similarity to the heterogeneities, but when k still remains approximately two orders of magnitude smaller than d , the medium ceases to be perceived as a homogenous effective medium and Rayleigh scattering emerges. As the wavelength continues to reduce, Rayleigh scattering transitions into an intermediate scattering regime²¹ which eventually settles into a stochastic scattering region when $kd \sim 1$. Beyond this scope, lies the Geometric-stochastic transition²¹, occurring at $kd \sim 1/n$, where ray theory approximations become applicable and the medium

once again recedes to an, albeit piecewise, homogenous effective medium. Scattering here is subsequently independent of the wavelength for all dimensions; this leaves us to discuss the two aforementioned regimes.

A. Rayleigh scattering

Mason and McSkimmin²² experimentally discovered the fourth order frequency dependence of the scattering induced attenuation for ultrasonic waves within polycrystalline materials, more commonly observed for electromagnetic waves as Rayleigh Scattering²³. This finding established that to an elastic wave, a polycrystalline material appears as a homogenous medium containing randomly distributed scattering spheres²⁴. It is perhaps unsurprising then that in a 2D representation, a scattering sphere would be replaced by a circle, and in 1D by a line. It is thereby recognised that the wavenumber dependence of Rayleigh scattering scales with $D+1$ ²⁵, which is a consequence of the respective Green's functions for a spherical, circular, and a planar scatterer. It therefore seems fair to postulate the same dimensional behaviour should be observed within polycrystalline materials.

We can use the rule of similitude²⁶ to further infer the dimensional dependence on grain size, d , which relates the dependencies of k and d such that the attenuation is proportional to the i -th power of d^i , and the $(i+1)$ -th power of k^{i+1} . The above arguments can be cast into a unified form for D dimensional scattering attenuation, α_R , within the Rayleigh regime.

$$\alpha_R \propto d^D k^{D+1} \quad (2)$$

Whereas it is generally well known that attenuation follows a fourth power dependence on frequency in the Rayleigh regime, it is not well appreciated that this dependence is only of the third order in a 2D representation. Accordingly one should not expect predictions of scattering from inhomogeneities by 2D models to be representative of 3D behaviour either.

B. Stochastic scattering

Once the wavelength becomes dimensionally similar to the grain size, $kd \sim 1$, the attenuation eventually converges to a stochastic asymptote. This was first described by Huntington²⁷ for the ultrasonic

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107 propagation within polycrystalline materials by proposing a phase scrambling mechanism. A similar
 108 approach known as the phase screen approximation²⁸ is used here to derive the attenuation coefficient
 109 of the coherent wave.

110 Let us consider a monochromatic plane wave traversing in the z -direction through a phase screen where
 111 random fluctuations of phase rather than amplitude are imposed on the wave. Such a wave at one $(x, y,$
 112 $z)$ location can be described as an unperturbed wave field U_0 perturbed by a phase perturbation $\delta\theta$.

$$U(x, y, z) = U_0 \exp(i\delta\theta(x, y, z)) \quad (3)$$

113 These changes in phase cause a loss in amplitude when summing the contributions that describe the
 114 coherent wavefront emerging from the screen. This is denoted by $\langle \rangle$ to represent the lateral spatial
 115 average along x, y denoted by:

$$\langle U(x, y, z) \rangle = U_0 \langle \exp(i\delta\theta(x, y, z)) \rangle \quad (4)$$

116 Assuming the phase perturbation obeys a Gaussian distribution, the exponential term can be further
 117 evaluated, as shown by Eckart²⁸.

$$\langle U(x, y, z) \rangle \approx U_0 \exp\left(-\frac{1}{2} \langle \delta\theta^2(x, y, z) \rangle\right) \approx U_0 \exp\left(-\frac{1}{2} \delta\theta_{RMS}^2(z)\right) \quad (5)$$

118 Nagy and Adler²⁹ found that for non-Gaussian distributions, the governing statistical property is still
 119 the r.m.s. phase perturbation, but for loss values above 3 dB the relationship between the logarithmic
 120 loss and $\delta\theta_{RMS}$ is not strictly quadratic. However, by virtue of the central limit theorem, the phase
 121 perturbation over a large number of grains tends to be inherently Gaussian, therefore Eq. (5) is still
 122 applicable although the total loss is well over 3dB, in excess of 10dB. These assumptions can break
 123 down when considering, usually, unnaturally perturbed phase distributions, such as those encountered
 124 by reflections from triangulated periodic surfaces³⁰.

125 By comparison to the definition of the attenuation coefficient, $\exp(-\alpha z)$, we can then write:

$$\alpha \approx \frac{1}{2z} \delta\theta_{RMS}^2(z) \quad (6)$$

126 The phase perturbation in our case relates to a change in the local elastic properties of the medium,
 127 causing a positive or negative fluctuation in wavenumber, δk , away from the mean wavenumber k_0 .

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128 The phase then, after z -direction propagation through N grains, is the summation of all the individual
 129 phases through each n -th grain with an average grain size d .

$$\delta\theta(z) = \sum_n^N \delta k_n d \quad (7)$$

130 This can be rewritten as an effective wavenumber, $\delta k'$, in the form $\delta\theta(z) = \delta k'(z)z$, such that:

$$\delta k'(z) = \frac{1}{z} \sum_n^N \delta k_n d \quad (8)$$

131 In order to evaluate the r.m.s. phase perturbation featured in Equation 5, we can calculate the r.m.s value
 132 of the effective wavenumber, $\delta k'_{RMS}$, by substituting the summation in Equation 8 by its incoherent
 133 sum.

$$\delta k'_{RMS}(z) = \frac{\sqrt{N}}{z} \delta k_{RMS} d = \sqrt{\frac{d}{z}} \delta k_{RMS} \quad (9)$$

134 Which yields:

$$\delta\theta_{RMS}(z) = \sqrt{zd} \delta k_{RMS} \quad (10)$$

135 From Equation 6, we can thus describe the attenuation coefficient in terms of δk_{RMS} .

$$\alpha \approx \frac{d\delta k_{RMS}^2}{2} \quad (11)$$

136 The relevance of this simplistic model lies in the prediction that, as long as the lateral correlation length
 137 of $\delta k_{RMS}(x, y)$ is larger than the wavelength, the scattering-induced loss is proportional to the
 138 propagation distance z in a way that is independent of the dimensionality of the model. This is similar
 139 to Eckart's original finding²⁸ which stated that the losses incurred from acoustic waves reflected from
 140 a rough surface are merely dependent on the properties of its roughness, the r.m.s. height in that case.
 141 In our case, and within our approximations, Eckart's 'roughness' is solely equivalent to the perturbation
 142 in elastic constants.

143 It is therefore expected that, whilst we have seen dimensional dependencies in the Rayleigh regime, this
 144 is not the case for the stochastic regime; the attenuation varies with the second power of frequency in

any representation: 3D, 2D or 1D. Notably in the 1D case, the attenuation follows a second order dependence with frequency throughout both regimes. In summary, regardless of dimensions, the dependence of the attenuation in the stochastic region is described by:

$$\alpha_S \propto dk^2 \quad (12)$$

The above result may seem encouraging for 2D models to approximate 3D scattering behaviour, but it is important to note that despite their shared dimensional dependence, this analysis does not go as far as to say that the absolute scattering and hence also attenuation should be equal.

III. NUMERICAL VERIFICATION

In verification of the preceding predictions, we numerically calculate the wavenumber dependence of the scattering-induced attenuation for plane longitudinal waves propagating through random heterogeneous elastic media in 3D, 2D, and 1D. Waves of millimetre-scale wavelengths with frequencies in the MHz range are modelled to represent typical ultrasonic waves within polycrystalline materials. The perceived attenuation within our models is solely due to scattering, as is the case practically for polycrystalline materials, where other sources of attenuation, through for example absorption, are negligible. The results are expected to be equally valid however for seismic waves³¹ which experience a similar scattering problematic albeit on a different scale.

A. Numerical methodology

The methodology employed here has been previously detailed in¹⁵. The procedure starts by generating a numerical model with a spatial domain of randomly sized and oriented elastic crystals whose average properties are representative of those occurring within polycrystalline morphologies. Voronoi diagrams were relatively recently established for this purpose in various fields including Materials Science^{32–34} and Ultrasonic NDE^{12,14,15}. Generating a Voronoi tessellation requires a set of spatially randomly distributed points, which each serve as a seed for an eventual Voronoi cell, which will in turn represent the geometry for an individual crystallite, or grain. Once such a grain morphology is obtained, in order to emulate polycrystalline material properties, each crystallite is assigned a fixed density but a random crystallographic orientation to determine its elastic properties. When both the seed distribution and

crystallographic orientations are spatially randomised, as is done here, this produces a macroscopically isotropic material with equiaxed grains and no texture. The authors use the software Neper³⁵ for this part of the procedure.

The main obstacle to this numerical approach is the requirement to incorporate two length-scales, one associated with the wavelength and a second with that of the heterogeneity. Namely, it has been shown that to achieve numerical convergence¹⁵, the model mesh must be sampled to satisfy both a minimum spacing of $d/10$ and $\lambda/10$ where λ denotes the wavelength. Depending on the d/λ ratio, this most often results in a mesh sampling which is drastically finer, and thus more computationally expensive, than conventional wave propagation modelling³⁶. Here however, efficient solutions for the explicit time-domain computations are found using the FE solver Pogo³⁷ that exploits parallel processing on graphics processors (GPU).

Once the mesh is generated, symmetry boundary conditions are applied to create a plane longitudinal wave as detailed in¹⁵. Plane waves are desirable as they avoid influences of diffraction, such as those usually associated with sources of finite length, and hence simplify the calculation for attenuation. In the case of a 3D cuboid model exposing six surfaces, a toneburst is applied simultaneously to all of the nodes which lie on one of these surfaces - as a force in the direction normal to the surface. The four surfaces which share an edge with this excitation surface require a rolling boundary condition to approach a plane wave as closely as possible. A perfect plane wave is achieved in the case of a homogeneous medium, but only an approximated plane wave is achieved for the heterogeneous medium; the approximation improves with increasing size of the lateral dimension. The remaining surface which opposes the excitation surface receives the plane wave, hence simulating a pitch-catch configuration. The same method can be extended to 2D and 1D models as illustrated in Figure 1.

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Figure 1: Illustration of numerical models in (a) 1D (b) 2D (c) 3D. For clarity, the illustrations are not representative of the model size.

Model size:	400mm($\times 400$)	10mm $\times$ 200mm	12mm $\times$ 12mm $\times$ 100mm
Grain size:	100 μ m	100 μ m	500 μ m
Centre Freq:	2MHz	2MHz	1MHz
DOF	$2 \times 10^5(\times 400)$	42×10^6	345×10^6

Table 1: Details of FE models used for Rayleigh scattering calculations.

Remaining parameters such as model size also need to be considered to ensure a numerically accurate solution. First in terms of noise, even a numerical measurement in this case contains a contribution of both the desired coherent field and undesired incoherent field. The contribution of the incoherent field however reduces as the lateral extent of the model is increased, due to (coherent) spatial averaging. Secondly, the model must also be of optimal length to ensure the attenuation is within a desirable range for measuring³⁸. Both these constraints impose limitations on the attainable scattering regimes given finite computational resources.

Finally, obtaining a value for attenuation involves calculating the received and sent time-amplitude signals, by ensemble averaging the time-dependent nodal displacements across the send and receive surface. The frequency dependent attenuation can be obtained (for example as shown in³⁸) from the Fourier Transform of each signal.

B. Rayleigh scattering results

The study of attenuation within the Rayleigh regime requires operating at a $kd \ll 1$ length scale. As mentioned previously, relatively long (in the propagation direction) models are therefore preferred in

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order for the grains to significantly reduce the received amplitude. This requirement is more taxing in 3D, and hence a larger grain size (500 μ m), is modelled than in the 1D and 2D models, where smaller grain size (100 μ m) is used. The respective kd values for 3D, 2D, and 1D are 0.5, 0.2, and 0.2. Illustrations and details of each model are shown in Figure 1 and Table 1. The material, Inconel, is described in Table 2.

Material	A	ρ (kg/m ³)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)
Inconel	2.8	8000	234.6	145.4	126.2

Table 2: Material properties used for Rayleigh scattering calculations.

Figure 2 plots the wavenumber dependent attenuation in (a) 1D (b) 2D (c) 3D where errorbars indicate the standard deviation from at least 10 realisations of a random material. The mean wavenumber power law is calculated including its standard deviation, which produces frequency exponents of 1.96, 3.01, and 3.95 for 1D, 2D, and 3D respectively. These values are within satisfactory bounds to the expected integer values of 2, 3, and 4, which thereby confirms the expected k^{D+1} dependence.

A. Stochastic scattering results

Different 3D and 2D models were created to assess attenuation in the stochastic regime; their properties are shown in Table 3. In comparison to the previous section, a broader range of frequencies is now investigated (2-20MHz) and the material used is shown in Table 4.

	2D	2D	3D
Centre frequencies	1-5MHz	6-20MHz	2-20MHz
Model size	30mmx100mm	300mmx10mm	12mmx12mmx10mm
Grain size	500 μ m	500 μ m	500 μ m
DOF	3x10 ⁶	15x10 ⁶	278x10 ⁶

Table 3: Details of FE models used for stochastic scattering calculations.

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Figure 2: Power law calculations for Rayleigh scattering induced attenuation, plotted as normalised attenuation versus normalised wavenumber in (a) 1D (b) 2D (c) 3D.

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Material	ρ (kg/m ³)	C_L^V (m/s)	A	C11 (GPa)	C12 (GPa)	C44 (GPa)
Fictitious	8000	6000	1.5	262.1	136.5	95.3

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Table 4: Material properties used for stochastic scattering calculations.

It is important to note that a question arises at this stage regarding the appropriate grain size distribution to enable an objective comparison of 3D and 2D. In essence, a degree of ambiguity exists when comparing a random distribution of spheres to that of cylinders. Stereology³⁹ is occupied with the inverse problem, namely, how to interpret a 2D measurement of a cross-sectional distribution onto that of the 3D material. Since a 2D slice will not necessarily behave like its 3D parent, the simplest case is assumed here and both media are compared with matching grain size distributions (see Figure 3). This can be interpreted as our 2D model being a slice of a 3D material where every grain is sectioned through its centre and therefore exhibits its largest radius. Whilst this assumption should not influence the wavenumber dependence which is our primary interest, it will affect the absolute attenuation.

Figure 3: Grain size distribution of the 3D and 2D FE models used to investigate stochastic scattering.

The resulting normalised attenuation versus the normalised kd is plotted in Figure 4. Starting from a high kd , it can be seen that within the stochastic region both the 3D and 2D curves remain parallel and exhibit the same gradient. This result confirms the prediction that the wavenumber dependent behaviour maintains dimensional insensitivity within the stochastic regime. An absolute shift in attenuation remains however, in this case in the order of 10 to 20%.

Figure 4: Normalised attenuation against normalised wavenumber for 3D and 2D scattering. Both curves exhibit independent transitional scattering behaviour, characterised by the ‘hump’, before converging to a stochastic asymptote at $kd \sim 8$.

As the wavenumber decreases from the stochastic regime, the attenuation mechanism falls into a transitional regime²¹, here notable in Figure 4 by a characteristic but different ‘hump’ for both the 3D and 2D results. This region constitutes scattering behaviour with rapidly varying dependencies on kd , and also exhibits the largest absolute difference in attenuation between the two models. This is an important observation for numerical modelling, as the transitional behaviour makes it difficult to deploy analytical models here, yet it also shows 2D numerical models have the largest shortcomings within this region.

Finally, at low kd and from the supporting evidence in the previous section, we can observe the 2D attenuation curve failing to attain the steeper slope which is characteristic of Rayleigh scattering in 3D.

Whilst the absolute attenuation is lower in 2D within the stochastic regime, this trend reverses once attenuation approaches the Rayleigh regime. Necessarily the two curves subsequently intersect in-between the Rayleigh and stochastic regime.

IV. CONCLUSION

Our aim was to demonstrate and understand the dimensional behaviour of elastic wave scattering within heterogeneous media. The fundamental dependence of the scattering induced attenuation on wavenumber was postulated for various scattering regimes in 3D, 2D, and 1D. Numerical calculations based on the Finite Element (FE) method simulated scattering from random spatial variations in elastic properties of the medium, such as those experienced by ultrasonic waves propagating within polycrystalline materials. As supported by established theory, it is numerically verified that within the long-wavelength Rayleigh regime, the attenuation is proportional to k^{D+1} where D denotes the dimension. For smaller wavelengths in the stochastic regime however, the calculations show a k^2 dependence regardless of the dimensions. It is hoped that these findings will be useful for future studies of scattering, and that they may lay the groundwork for developing an approach to achieve efficient 2D simulations which are usefully representative of 3D phenomena.

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