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# Comparison of ultrasonic attenuation within two- and three-dimensional polycrystalline media

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## Abstract

An analytical approach to develop explicit formulas of attenuation coefficient in both 2D and 3D cases is proposed. It results in a better understanding of the grain scattering mechanisms within a polycrystalline material and the grain size effects on the attenuation of an ultrasonic wave. It is based on the Stanke and Kino's model and uses the Born approximation. An explicit formula is deduced for untextured polycrystals with equiaxed grains of cubic symmetry and allows a rigorous comparison of the attenuation coefficient between both 2D and 3D cases. It confirms that the attenuation in the Rayleigh region is higher in 2D simulation than in 3D one, while very similar coefficients are obtained in the stochastic region for both cases. The study of the explicit formula allows the decomposition of the attenuation coefficient into various scattering-induced components, which leads to a better understanding of different grain scattering mechanisms. The reflection/transmission at grain boundaries between wave modes of a same type mainly explains a same attenuation coefficient in the stochastic region for both 2D and 3D modelings. The conversion at grain boundaries between different types of wave modes provides some explanations for a higher attenuation value given by the 2D modeling in the Rayleigh region. The effect of the grain size on the attenuation coefficient is then predicted by the 2D analytical calculation and by the FE simulation. The analytical-numerical comparison validates the numerical calculations and the approach suggests a way of using the 2D FE calculations to predict the evolution of the attenuation coefficient with the wave frequency in 3D.

*Keywords:* Finite element modeling; Ultrasonic attenuation; Grain scattering; Grain size effect; 2D/3D analytical modeling; Polycrystalline material

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## 1. Introduction

For on-line quality control both in laboratory and in industry, the amplitude attenuation of ultrasonic waves provides continuous and non-destructive information on polycrystalline microstructure [1–3]. It mainly results from scattering by grain boundaries delineating domains with different elastic properties, which, in the case of a single-phase polycrystal, are linked to crystallographic orientation. Depending on the ratio of the wavelength  $\lambda$  to the mean grain size  $d$ , three regions are usually defined: (1) the *Rayleigh scattering region* for  $\lambda \gg d$ ; (2) the *stochastic scattering region* for  $\lambda \approx d$ ; (3) the *diffusion scattering region* for  $\lambda \ll d$ . The limits between the three regions depend upon the material properties and generally cannot be strictly specified [4, 5].

Early models for the attenuation were limited to the single-scattering approximation, assuming that ultrasonic waves scatter at each grain boundary independently [6–8]. This assumption is only valid for weak scattering. It may break down for strong scattering materials or at relatively high frequencies. Stanke and Kino [4] proposed a unified theory valid in all frequency regions by using the second-order Keller approximation [9]. Their approach took some degree of multiple scattering into account by writing the scattered field as an averaged field which has been scattered at grain boundaries. The unified theory resulted in a highly non-linear equation in the 3D case (see Eq.(101) and Eq.(102) in [4]). Instead of the perturbation theory used by Stanke and Kino, Weaver relied on the Dyson’s equation to account for multiple-scattering through the self-energy operator [10]. When Born approximation is used, both Weaver’s and Stanke and Kino’s models gave rise to the same solution for the attenuation coefficients [11]. Extension of these two seminal models to polycrystalline materials with crystallographically textures [12], elongated grains [13], or a distribution of grain sizes [14] was investigated in the 3D case using the Born approximation. Though these ideas can be easily extended to the 2D case, it appears, to our knowledge, that no explicit formulas of attenuation coefficient were developed for the 2D case.

Some works indicate that a 2D approach is not fully representative of 3D scattering, particularly in the Rayleigh region and for the transition between the different scattering regions [15, 16]. For example, a scattering strengthening is observed in the Rayleigh region for 2D simulations. Consequently, a 2D theoretical model would be imperative for a further understanding of the dimensional behavior of ultrasonic scattering-induced attenuation. On another level, the numerical modeling is necessary to complement the analytical one [15, 17–20], and 2D finite element (FE) simulations are advantageous in their relative simplicity and efficiency compared to 3D ones while retaining the key concepts. A 2D theoretical model is thus of great significance to bring a better understanding of the limits of 2D calculations and to develop more efficient 2D simulations that can be representative of 3D phenomena.

43 In the following, Section 2 starts from the Stanke and Kino’s model to give  
44 an explicit solution to the eigenvalue problem of the acoustic tensor. The Born  
45 approximation makes possible to obtain an explicit formula for the ultrasonic  
46 attenuation coefficient expressed as a simple integral form of the dyadic Green’s  
47 tensor and a spatial correlation function for both 2D and 3D cases. Section  
48 3 presents a quantitative comparison of attenuation coefficients calculated in  
49 2D and 3D cases for an untextured and single-phase polycrystal with equiaxed  
50 grains of cubic symmetry. The contribution of different scattering mechanisms  
51 to the attenuation is also discussed to provide a physical interpretation to differ-  
52 ences observed between the 2D and 3D cases. Finally, in Section 4, an example  
53 is given by the analysis of the effect of the grain size on the attenuation in a  
54  $\beta$ -titanium polycrystal. 2D analytical predictions are compared with numerical  
55 results obtained by FE simulations.

## 56 **2. Explicit formula of attenuation in single-phase untextured poly-** 57 **crystals**

58 Considering a polycrystalline heterogeneous domain  $\Omega \subset \mathbb{R}^{dim}$  ( $dim = 2, 3$ )  
59 with boundary  $\partial\Omega$  and defined by a position-dependent elastic tensor  $\mathbf{C}(\mathbf{x})$   
60 and a uniform density  $\rho$ . Let us assume that there is no source term, the time  
61 harmonic elastic wave equation inside  $\Omega$  reads as:

$$\mathbf{L}(\mathbf{u}(\mathbf{x}, \omega)) \equiv \rho\omega^2\mathbf{u}(\mathbf{x}, \omega) + \nabla_{\mathbf{x}} \cdot (\mathbf{C}(\mathbf{x}) : \boldsymbol{\varepsilon}_{\mathbf{x}}(\mathbf{u}(\mathbf{x}, \omega))) = \mathbf{0} \quad (1)$$

62 In (1),  $\mathbf{u}(\mathbf{x}, \omega)$  denotes the Fourier transform with respect to time of the dis-  
63 placement field  $\mathbf{u}(\mathbf{x}, t)$ ,  $\nabla_{\mathbf{x}}$  the usual space gradient operator and  $\boldsymbol{\varepsilon}_{\mathbf{x}}(\mathbf{u}(\mathbf{x}, \omega)) =$   
64  $\nabla_{\mathbf{x}} \otimes_s \mathbf{u}(\mathbf{x}, \omega)$  the infinitesimal strain tensor. Herein, tensors and vectors are  
65 denoted using bold letters. Otherwise,  $\omega$  in  $\mathbf{u}(\mathbf{x}, \omega)$  will be omitted in the  
66 following for the sake of simplicity.

67 Herein, the theoretical study is developed within the framework of the uni-  
68 fied theory proposed by Stanke and Kino [4] following a general formulation  
69 established by Karal and Keller [9]. The objective is to develop an explicit  
70 model of  $\langle \mathbf{u}(\mathbf{x}) \rangle$  the expected wave of an ensemble of possible inhomogeneous  
71 media, with  $\langle \cdot \rangle$  denoting an ensemble average. For a particular inhomogeneous  
72 medium of the ensemble, its inhomogeneity degree can be quantified by consid-  
73 ering the deviation of  $\mathbf{C}(\mathbf{x})$  its elastic tensor from  $\mathbf{C}^0$  the one of an equivalent  
74 homogeneous medium:  $\delta\mathbf{C}(\mathbf{x}) = \mathbf{C}(\mathbf{x}) - \mathbf{C}^0$ . Former work proved the equival-  
75 ent homogeneous medium was to be chosen as the Voigt-averaged material of  
76 the ensemble [4, 10]. In the following, both the subscript and the superscript  
77 “0” always indicate fields or variables related to the equivalent homogeneous  
78 medium.

79 Following procedure described in [4, 9, 21], single-phase, untextured and  
80 weakly scattering polycrystals are considered. The untextured assumption leads

81 to  $\langle \delta \mathbf{C}(\mathbf{x}) \rangle = \mathbf{0}$  and that of weak scattering means that the relative inhomogeneity degree  $\epsilon$  is much less than 1.  $\epsilon$  is defined by  $\epsilon^2 = \langle (k(\mathbf{x}) - k_0)^2 \rangle / k_0^2$  with  
 82  $\mathbf{k}$  the wave vector and  $k = |\mathbf{k}|$  the propagation constant. Using the second-  
 83 order Keller approximation, the following explicit equation for  $\langle \mathbf{u}(\mathbf{x}) \rangle$  accurate  
 84 to order of  $\epsilon^2$  can be obtained:

$$\mathbf{L}^0(\langle \mathbf{u}(\mathbf{x}) \rangle) - \langle \mathbf{L}^1(\int_{\Omega} \mathbf{G}^T(\mathbf{x}'; \mathbf{x}) \cdot \mathbf{L}^1(\langle \mathbf{u}(\mathbf{x}') \rangle) d\mathbf{x}') \rangle = 0 \quad (2)$$

where  $\mathbf{L}^0$  and  $\mathbf{L}^1$  are respectively the homogeneous and perturbation operators defined by:

$$\mathbf{L}^0(\mathbf{u}(\mathbf{x})) = \rho \omega^2 \mathbf{u}(\mathbf{x}) + \nabla_{\mathbf{x}} \cdot (\mathbf{C}^0 : \boldsymbol{\varepsilon}(\mathbf{u}(\mathbf{x}))) \quad (3a)$$

$$\mathbf{L}^1(\mathbf{u}(\mathbf{x})) = \nabla_{\mathbf{x}} \cdot (\delta \mathbf{C}(\mathbf{x}) : \boldsymbol{\varepsilon}_{\mathbf{x}}(\mathbf{u}(\mathbf{x}))) \quad (3b)$$

86 In (2),  $\mathbf{G}(\mathbf{x}'; \mathbf{x})$  is the dyadic Green function tensor defined by  $\mathbf{G}(\mathbf{x}'; \mathbf{x}) =$   
 87  $\mathbf{e}_m \otimes \mathbf{g}_m(\mathbf{x}'; \mathbf{x})$ ,  $\mathbf{e}_m$  is a unit vector of an orthonormal basis  $\{\mathbf{e}_m\}_{m=1, \dots, dim}$ , and  
 88  $\mathbf{g}_m(\mathbf{x}'; \mathbf{x})$  is the solution of the following time harmonic elastic wave problem  
 89 defined in the infinite equivalent homogeneous medium submitted to  $\delta(\mathbf{x} -$   
 90  $\mathbf{x}')\mathbf{e}_m$ , a point load at  $\mathbf{x}'$  oriented in the  $\mathbf{e}_m$  direction:

$$\mathbf{L}^0(\mathbf{g}_m(\mathbf{x}'; \mathbf{x})) + \delta(\mathbf{x} - \mathbf{x}')\mathbf{e}_m = \mathbf{0}. \quad (4)$$

91 To simplify the second term on the right-hand side of equation (2), several  
 92 assumptions were proposed in [4, 21]. Firstly, the elastic tensor variation and  
 93 the characteristic function of grains are assumed to vary independently. Sec-  
 94 ondly, the elastic tensor is assumed to vary independently from grain to grain.  
 95 Furthermore, by taking into account the single-phase assumption and the fact  
 96 that the deviation of elastic tensor  $\delta \mathbf{C}(\mathbf{x})$  in each grain, denoted as  $\delta \mathbf{C}^g$  in the  
 97 following, is constant, the two-point autocorrelation function of elastic tensors  
 98 consequently becomes:

$$\langle \delta \mathbf{C}(\mathbf{x}) \otimes \delta \mathbf{C}(\mathbf{x}') \rangle = \langle \delta \mathbf{C}^g \otimes \delta \mathbf{C}^g \rangle W(\mathbf{r}) \quad (5)$$

99 where  $W(\mathbf{r})$ , with  $\mathbf{r} = \mathbf{x} - \mathbf{x}'$ , denotes the spatial correlation function of two  
 100 points  $\mathbf{x}$  and  $\mathbf{x}'$  describing the possibility that they are in the same grain, and  
 101  $\langle \delta \mathbf{C}^g \otimes \delta \mathbf{C}^g \rangle$  the average over all crystallographic orientations [20]. Finally, the  
 102 problem (2) can be written in the following way:

$$\mathbf{L}^0(\langle \mathbf{u}(\mathbf{x}) \rangle) - \langle \delta \mathbf{C}^g \otimes \delta \mathbf{C}^g \rangle \overset{(2 \dots 8) \leftarrow}{\widehat{\cdot}} \mathbf{Q}(\langle \mathbf{u} \rangle; \mathbf{x}) = 0 \quad (6)$$

103 with  $\mathbf{Q}(\langle \mathbf{u} \rangle; \mathbf{x})$  a 7-th order tensor defined by:

$$Q_{jklm'n'p'q'}(\langle \mathbf{u} \rangle; \mathbf{x}) = \frac{\partial}{\partial x_j} \left( \int_{\Omega} \frac{\partial G_{m'k}(\mathbf{x} - \mathbf{x}')}{\partial x_l} \frac{\partial}{\partial x_{n'}} (W(\mathbf{x} - \mathbf{x}') \frac{\partial \langle u_{p'}(\mathbf{x}') \rangle}{\partial x_{q'}}) d\mathbf{x}' \right) \quad (7)$$

104 In (6), the product operator  $\overbrace{\quad}^{(2\cdots 8)\leftarrow}$  indicates that the tensor contraction is ap-  
 105 plied between the indices from 2 to 8 of the tensor  $\langle \delta \mathbf{C}^g \otimes \delta \mathbf{C}^g \rangle$  and the indices  
 106 of  $\mathbf{Q}(\langle \mathbf{u} \rangle; \mathbf{x})$ . Otherwise, the farfield assumption allows replacing  $\mathbf{G}(\mathbf{x}'; \mathbf{x})$  by  
 107  $\mathbf{G}(\mathbf{0}; \mathbf{x} - \mathbf{x}') \equiv \mathbf{G}(\mathbf{x} - \mathbf{x}')$ .

108 Now, the basic idea is to find the solution of the problem (6) assuming that  
 109 it has the form of a plane wave:

$$\langle \mathbf{u}(\mathbf{x}) \rangle = \mathbf{U} e^{ik\hat{\mathbf{k}} \cdot \mathbf{x}} \quad (8)$$

110 with  $\hat{\mathbf{k}}$  a unit vector defining the propagation direction and  $\mathbf{U}$  the polarization  
 111 vector. For any angular frequency  $\omega$ , the propagation constant  $k$  is searched  
 112 under the form  $k = \omega/v + i\alpha$  with  $v$  the wave velocity and  $\alpha$  the attenua-  
 113 tion coefficient. The wave scattering due to elastic tensor perturbations can be  
 114 quantified by analyzing the wave constant  $k$ . Indeed, the difference between  
 115 the real part of  $k$  and the real wave constant  $k_0$  in the equivalent homogeneous  
 116 medium gives the phase velocity deviation from the latter, and its imaginary  
 117 part quantifies the attenuation.

118 Putting the plane wave form (8) of the average field solution  $\langle \mathbf{u}(\mathbf{x}) \rangle$  in (6),  
 119 the following eigenvalue problem of the wave constant  $k$  for the perturbed acous-  
 120 tic tensor  $\Gamma(k\hat{\mathbf{k}})$  can be obtained [4]:

$$\underbrace{\left( \underbrace{\mathbf{C}^0 : (\hat{\mathbf{k}} \otimes_s \mathbf{U})}_{\Gamma^0(\hat{\mathbf{k}}) \cdot \mathbf{U}} \right) \cdot \hat{\mathbf{k}} - \left( (\delta \mathbf{C}^g \otimes \delta \mathbf{C}^g) \overbrace{\quad}^{(3\cdots 6)\leftarrow} \mathbf{P}(k\hat{\mathbf{k}}) : (\hat{\mathbf{k}} \otimes_s \mathbf{U}) \right) \cdot \hat{\mathbf{k}}} = \rho \omega^2 k^{-2} \mathbf{U} \quad (9)$$

$$\Gamma(k\hat{\mathbf{k}}) \cdot \mathbf{U} = \Gamma^0(\hat{\mathbf{k}}) \cdot \mathbf{U} + \delta \Gamma(k\hat{\mathbf{k}}) \cdot \mathbf{U}$$

121 with:

$$P_{klmn}(k\hat{\mathbf{k}}) = \int_{\mathbb{R}^{dim}} G_{km}(\mathbf{r}) \frac{\partial^2}{\partial r_n \partial r_l} (W(\mathbf{r}) e^{ik\hat{\mathbf{k}} \cdot \mathbf{r}}) d\mathbf{r} \quad (10)$$

122 We recall that in the equivalent homogeneous medium we have:  $\Gamma^0(\hat{\mathbf{k}}) \cdot \mathbf{U}_\beta^0 =$   
 123  $\rho \omega^2 k_{0\beta}^{-2} \mathbf{U}_\beta^0$  ( $\beta = L, T$ ), with  $\mathbf{U}_L^0 \parallel \hat{\mathbf{k}}$  and  $\mathbf{U}_T^0 \perp \hat{\mathbf{k}}$ .  $k_{0\beta}$  denotes the wave  
 124 constant in the equivalent homogeneous medium for the longitudinal wave with  
 125  $\beta = L$  or for the transverse wave with  $\beta = T$ . A sketch showing in the 3D case  
 126 the orthonormal basis  $\{\mathbf{e}_m\}_{m=1,\dots,3}$ , the unit vector of propagation direction  $\hat{\mathbf{k}}$   
 127 and the polarization vectors  $\mathbf{U}_\beta^0$  is presented in Figure 1.

128 Otherwise, the expression of the dyadic Green function in an isotropic and  
 129 homogeneous elastic medium is well known [22, 23]:

$$\mathbf{G}(\mathbf{r}) = \frac{1}{4\pi\rho\omega^2} \left( \nabla_{\mathbf{r}} (\nabla_{\mathbf{r}} (A(k_{0T}r) - A(k_{0L}r))) + k_{0T}^2 A(k_{0T}r) \mathbf{I} \right) \quad (11)$$

130 with  $r = |\mathbf{r}|$ ,  $\mathbf{I}$  the identity tensor, and the function  $A(\cdot)$  is space dimension  
 131 dependent and is defined by:

$$A^{3D}(k_{0\beta}r) = \frac{e^{ik_{0\beta}r}}{r}, \quad A^{2D}(k_{0\beta}r) = i\pi H_0^{(1)}(k_{0\beta}r) \quad (12)$$

132 In (12),  $H_0^{(1)}(\cdot)$  denotes Hankel function of the first kind. It is worth noticing  
 133 that, in the case of a 2D problem defined for example in the plane  $Ox_1x_3$ ,  
 134 it expresses the outward-propagating cylindrical wave solution, assumed to be  
 135 uniform along the  $\mathbf{e}_2$  direction.

136 The eigenvalue problem (9) is highly nonlinear and its solving is not trivial.  
 137 However, Stanke and Kino has carried out analytical development of (9) for un-  
 138 textured single-phase polycrystalline media with equiaxed grains in the 3D case  
 139 (see Eq.(101) and Eq.(102) in [4]). Then they applied the Born approximation  
 140 to finally obtain explicit formulas for the attenuation coefficient.

141 Unfortunately, the approach proposed by Stanke and Kino cannot be applied  
 142 to the 2D case due to Hankel function of the first kind involved in the 2D Green  
 143 function. To get around this difficulty, our main idea is to assume that, in the  
 144 case of weakly scattering media,  $\mathbf{U}$  the wave mode of the average field solution  
 145 can be approximated by the same type of pure wave mode, *i.e.*  $\mathbf{U}_\beta^0 \parallel \hat{\mathbf{k}}$  (for  
 146  $\beta = L$ ) or  $\mathbf{U}_\beta^0 \perp \hat{\mathbf{k}}$  (for  $\beta = T$ ). Then, by applying the scalar product with  $\mathbf{U}_\beta^0$   
 147 to both side of (9), the following equation for the propagation constant  $k_\beta$  with  
 148 the wave propagation direction  $\hat{\mathbf{k}} = \mathbf{e}_j$  is obtained:

$$k_\beta^2 - k_{0\beta}^2 = k_\beta^2 \frac{\langle \delta C_{j^\beta jkl} \delta C_{mnj^\beta j} \rangle P_{klmn}(\mathbf{k}_\beta \mathbf{e}_j)}{C_{j^\beta j j^\beta j}^0} \quad (13)$$

149 We note that herein the Einstein summation convention is systematically used.  
 150 In (13), the indice  $j^\beta$  indicates the polarization direction of a  $\beta$ -type wave that  
 151 propagates in the  $\mathbf{e}_j$  direction. For example, for  $\beta = L$  and  $j = 3$ , we have  
 152  $j^\beta = 3$ , while for  $\beta = T$  and  $j = 3$ , if the transverse wave is polarized in the  
 153 space direction  $\mathbf{e}_1$ , we have  $j^\beta = 1$ .

154 Now, the use of the Born approximation leads to the assumption that  $k_\beta^2 -$   
 155  $k_{0\beta}^2 \approx 2k_{0\beta}(k_\beta - k_{0\beta})$  and  $k_\beta \approx k_{0\beta}$  on the left and right hand sides of (13),  
 156 respectively. The following explicit formula is finally established for both 2D  
 157 and 3D cases:

$$k_\beta = k_{0\beta} + \frac{k_{0\beta}}{2C_{j^\beta j j^\beta j}^0} \langle \delta C_{j^\beta jkl} \delta C_{mnj^\beta j} \rangle P_{klmn}(\mathbf{k}_{0\beta} \mathbf{e}_j) \quad (14)$$

158 In the 2D case, even if any analytical derivation of (14) seems impossible due to  
 159 the complexity of Hankel function, it is very interesting as it can be numerically  
 160 evaluated by using softwares such as Matlab (see Appendix A1). Hence, both  
 161 propagation velocity variation and attenuation can then be calculated using

162 (14). However, in the following, we are only interested in the study of the  
 163 explicit formula of the attenuation coefficient:

$$\alpha^\beta = \text{Im} \left( \frac{k_{0\beta}}{2C_{j^\beta j^\beta j^\beta}^0} \langle \delta C_{j^\beta j^\beta j^\beta} \delta C_{mnj^\beta j^\beta} \rangle P_{klmn}(k_{0\beta} \mathbf{e}_j) \right) \quad (15)$$

164 where  $\text{Im}(\cdot)$  specifies the imaginary part.

165 Moreover, other interesting explicit formulas can be derived after the cal-  
 166 culation of derivatives in the Green function and their decomposition into two  
 167 parts,  $\mathbf{G}^\beta(\mathbf{r})$  (for  $\beta = L, T$ ), related to the longitudinal and transverse waves  
 168 respectively:

$$\mathbf{G}^\beta(\mathbf{r}) = \frac{(1 - c(\beta))}{4\pi\rho\omega^2} (A_{rr}(k_{0\beta}r) \hat{\mathbf{r}} \otimes \hat{\mathbf{r}} - A_{\mathbf{I}}(k_{0\beta}r) \mathbf{I}) \quad (16)$$

In (16),  $\hat{\mathbf{r}}$  denotes the unit vector along the  $\mathbf{r}$  direction,  $c(\beta)$  is a constant equal  
 to 0 for  $\beta = L$  and to 2 for  $\beta = T$ , and the functions  $A_{rr}$  and  $A_{\mathbf{I}}$  are space  
 dimension dependent and are defined by:

$$\begin{aligned} A_{rr}^{3D}(k_{0\beta}r) &= \frac{e^{ik_{0\beta}r}}{r^3} (3 - 3ik_{0\beta}r - k_{0\beta}^2 r^2) \\ A_{\mathbf{I}}^{3D}(k_{0\beta}r) &= \frac{e^{ik_{0\beta}r}}{r^3} \left( 1 - ik_{0\beta}r - \frac{c(\beta)}{2} k_{0\beta}^2 r^2 \right) \end{aligned} \quad (17a)$$

$$\begin{aligned} A_{rr}^{2D}(k_{0\beta}r) &= i\pi \left( \frac{k_{0\beta}}{r} H_1^{(1)}(k_{0\beta}r) - \frac{1}{2} k_{0\beta}^2 (H_0^{(1)}(k_{0\beta}r) - H_2^{(1)}(k_{0\beta}r)) \right) \\ A_{\mathbf{I}}^{2D}(k_{0\beta}r) &= i\pi \left( \frac{k_{0\beta}}{r} H_1^{(1)}(k_{0\beta}r) - \frac{c(\beta)}{2} k_{0\beta}^2 H_0^{(1)}(k_{0\beta}r) \right) \end{aligned} \quad (17b)$$

169 Then, both longitudinal and transverse wave attenuation coefficients,  $\alpha^L$   
 170 and  $\alpha^T$  are expressed as the sum of two terms, one induced by scattering into  
 171 a same type of wave, and the other generated by mode conversion [10]:

$$\alpha^L = \alpha^{LL} + \alpha^{LT}, \quad \alpha^T = \alpha^{TL} + \alpha^{TT} \quad (18)$$

172 with

$$\alpha^{\beta\gamma} = \text{Im} \left( \frac{k_{0\beta} \langle \delta C_{j^\beta j^\beta j^\beta} \delta C_{mnj^\beta j^\beta} \rangle}{2C_{j^\beta j^\beta j^\beta}^0} \int_{\Omega} G_{km}^\gamma(\mathbf{r}) \frac{\partial^2}{\partial r_n \partial r_l} (W(\mathbf{r}) e^{ik_{0\beta} \mathbf{e}_j \cdot \mathbf{r}}) d\mathbf{r} \right) \quad (19)$$

173 The indices  $\beta\gamma = LT, TL$  indicate terms related to wave scattering due to  
 174 mode conversion between different types of waves at grains boundaries, whereas  
 175  $\beta\gamma = LL, TT$  indicate terms related to wave scattering due to mode reflection  
 176 and transmission of a same type of wave at grain boundaries.

177 We note that the effect of the crystallographic orientation on the attenuation  
 178 is evaluated, accurately to order of  $\epsilon^2$ , through the term  $\langle \delta C_{j^\beta j^\beta j^\beta} \delta C_{mnj^\beta j^\beta} \rangle$ .



179 Otherwise, the influence of grain size and shape is measured by the two-point  
 180 spatial correlation function  $W(\mathbf{r})$ . As there is no further hypotheses imposed to  
 181  $W(\mathbf{r})$ , the use of the explicit formulas (15) and (18) is not restricted only to the  
 182 case of equiaxed grains. Nevertheless, those explicit formulas are valid only in  
 183 the limit of frequencies below the geometric scattering domain since the Born  
 184 approximation is made.

185 It is obvious that the explicit formulas make possible detailed analyses of  
 186 different involved terms, which is helpful to understand the different scattering  
 187 mechanisms represented by these terms and to provide an analytical interpretation  
 188 for the scattering phenomenon in various frequency domains. To do this,  
 189 the formula (19) of  $\alpha^{\beta\gamma}$  is written as the sum of different terms in the following  
 190 way:

$$\alpha^{\beta\gamma} = \sum_{k,l,m,n} \alpha_{klmn}^{\beta\gamma} \quad (20)$$

191 with

$$\alpha_{klmn}^{\beta\gamma} \equiv \text{Im} \left( \frac{k_{0\beta} \langle \delta C_{j^\beta jkl} \delta C_{mnj^\beta j} \rangle}{2C_{j^\beta j^\beta j}^0} \int_{\Omega} G_{km}^{\gamma}(\mathbf{r}) \frac{\partial^2}{\partial r_n \partial r_l} (W(\mathbf{r}) e^{ik_{0\beta} \mathbf{e}_j \cdot \mathbf{r}}) d\mathbf{r} \right) \quad (21)$$

192 Note that, in (21) the indices  $k$ ,  $l$ ,  $m$ , and  $n$  appearing only once in the left-hand  
 193 term, their repetition in the right-hand term does not imply summation. It is  
 194 worth noticing that, due to the symmetries of the elastic tensor and the dyadic  
 195 Green's tensor,  $\alpha_{klmn}^{\beta\gamma}$  shows the following inherent symmetry:

$$\alpha_{pqpp}^{\beta\gamma} = \alpha_{pppq}^{\beta\gamma} \quad (22)$$

196 Furthermore, it can be shown that the non-zero components are:

$$\langle \delta C_{j^\beta jkl} \delta C_{mnj^\beta j} \rangle \neq 0 \Rightarrow \alpha_{klmn}^{\beta\gamma} \neq 0, \text{ if } \begin{cases} k = l \text{ and } m = n \\ k \neq l \text{ and } mn = kl \text{ or } lk \end{cases} \quad (23)$$

197 Consequently, there exist only six independent components contributing to  $\alpha^{\beta\gamma}$   
 198 in the 2D case, while in the 3D case, there are fourteen contributing components  
 199 for each set of  $\alpha^{LL}$  and  $\alpha^{LT}$ , and fifteen contributing components for each set of  
 200  $\alpha^{TT}$  and  $\alpha^{TL}$ . We note that, in the 2D case under the plane strain assumption,  
 201 the elastic constants associated with  $\mathbf{e}_2$  direction are not involved.

202 It is worth noticing that the explicit formulas developed in the present work  
 203 can be applied to polycrystalline materials containing crystallites of any sym-  
 204 metry class, provided that the average correlation functions of elastic tensor  
 205  $\langle \delta \mathbf{C}^g \otimes \delta \mathbf{C}^g \rangle$  are calculated [24]. In the following, the  $\beta$ -titanium metal is taken  
 206 as an example for analytical calculations. The choice is dictated by the increas-  
 207 ing interest for titanium alloys due to their superior combination of properties.  
 208 Final parts are frequently obtained by hot forming so that ultrasonic investi-  
 209 gation is a suitable tool to follow microstructure evolutions during the process.

210 For the  $\beta$ -titanium, its inhomogeneity degrees  $\epsilon_\beta$ , defined in [4] with respect to  
 211 the wave propagation constants, ranks between the aluminum low anisotropy [4]  
 212 and the higher anisotropy of Inconel 600 [25]. Though the influence of the in-  
 213 homogeneity degrees on the attenuation coefficient is beyond the scope of this  
 214 work, a comparison is presented in Appendix A2 between three different ma-  
 215 terials, which confirms that the results obtained for  $\beta$ -titanium are valid and  
 216 could be extended. The attenuation coefficients  $\alpha$ ,  $\alpha^{\beta\gamma}$  and their different non-  
 217 zero contributing terms  $\alpha_{klmn}^{\beta\gamma}$  have been calculated, in order to highlight some  
 218 common and different features between 2D and 3D scattering phenomena.

### 219 3. Main common and different features between 2D and 3D attenu- 220 ation phenomena

221 The material properties of the considered  $\beta$ -titanium polycrystalline material  
 222 are given in Table I. Its degree of anisotropy for longitudinal waves,  $\epsilon_L = 2.74\%$ ,  
 223 is twice larger than the one of aluminum but still very low compared to unity  
 224 [4] and its average correlation functions of elastic tensor  $\langle \delta C_{j\beta jkl} \delta C_{mnj\beta j} \rangle$  are  
 225 given by Table 2 in [26]. Due to the equiaxed grain assumption,  $W(\mathbf{r}) = W(r)$   
 226 depends only on the scalar variable  $r$ . In the present work, as often proposed  
 227 in the relative literature [27],  $W(r)$  is approximated by an exponential function  
 $W(r) = e^{-2r/d}$ , with  $d$  the grain size.

	$C_{1111}$ (GPa)	$C_{1122}$ (GPa)	$C_{2323}$ (GPa)	$\epsilon_L$ (%)	$\epsilon_T$ (%)	$\rho$ (kg/m <sup>3</sup> )
Single Crystallite in cubic axes	134.0	110.0	36.0	2.74	8.73	4428
Equivalent homogeneous medium	153.0	100.0	26.5	0.0	0.0	4428

Table I: Elastic properties of a BCC  $\beta$ -titanium metal [28].

228

229 In the following, as usually done to obtain a master curve for attenuation  
 230 vs. frequency, which is independent on the grain size,  $\alpha d$  the attenuation per  
 231 crystallite is drawn with respect to  $x_{0\beta}$  the normalized frequency using the base-  
 232 10 logarithmic scale.  $x_{0\beta} = 2\pi d/\lambda_\beta = 2\pi f d/v_{0\beta}$  is the ratio of the grain size  $d$   
 233 to the wavelength  $\lambda_\beta$ , with  $v_{0\beta}$  the wave velocity in the equivalent homogeneous  
 234 medium.

235 First of all, the explicit formula of the attenuation (15) is validated for  
 236 longitudinal waves in the 3D case by comparison with the model of Stanke and  
 237 Kino. Figure 2 shows that the explicit formula (15) slightly underestimates the  
 238 attenuation compared to the Stank-Kino's model and the relative difference in  
 239 attenuation coefficient between both models is less than 0.8%. Therefore, we

240 can use the proposed explicit formulas to get further analytical comparisons  
 241 between the 2D and 3D cases.

### 242 3.1. Asymptotic and the transition behaviors of Rayleigh and stochastic regions

243 It has been shown, in the preceding section, that the scattering-induced at-  
 244 tenuation results from wave mode conversion and wave mode reflection/transmission,  
 245 which can be measured by  $\alpha^{\beta\gamma}$  with  $\beta \neq \gamma$  and  $\alpha^{\beta\beta}$  respectively. Originally pro-  
 246 posed in 3D within the framework of the Weaver's model [13], these two mech-  
 247 anisms are highlighted within the framework of the Stanke and Kino's model in  
 248 3D and extended in 2D in the present work. A particular attention is therefore  
 249 paid to the behavior of the  $\beta\gamma$  and  $\beta\beta$  attenuation components in the 2D case  
 250 and compared to the 3D case within the different scattering regions.

251 Both cases of longitudinal and transverse waves are considered and the cor-  
 252 responding master curves of attenuation per crystallite coefficient,  $\log_{10}(\alpha d)$  vs.  
 253  $\log_{10}(x_0)$ , are presented in Figures 3(a) and (b), respectively. Otherwise, to  
 254 better quantify comparisons between the 2D and 3D cases, curves of the ratio  
 255  $\alpha^{\beta,3D}/\alpha^{\beta,2D}$  and of the slope of the master curves are also plotted and analyzed  
 256 (Figure 4). We recall that the limits between the Rayleigh and stochastic regions  
 257 cannot be strictly pinpointed. In Figures 3 and 4, the Rayleigh region is asymp-  
 258 totically located in the lowest frequency range, corresponding to the smallest  
 259 values of  $x_{0\beta}$ , while the stochastic one corresponds to the high frequency range  
 260 and the large  $x_{0\beta}$  values. The 2D and 3D cases are to be compared in the follow-  
 261 ing, including for the scattering mechanisms in the Rayleigh and the stochastic  
 262 regions, the slope variations of the master curves, the frequency dependence of  
 263 attenuation in different regions and the attenuation levels.

264 Concerning the scattering mechanism in the stochastic region, a same be-  
 265 havior is observed whatever the propagating wave type and whatever the space  
 266 dimension: the scattering is mainly controlled by the reflection/transmission  
 267 of the same type of wave mode. For example,  $\alpha^{LL}$  the attenuation due to  
 268 longitudinal-to-longitudinal wave scattering contributes to more than 94% of  
 269 the total attenuation for  $(x_{0L}, \log_{10} x_{0L}) = (31.6, 1.5)$ , which corresponds to the  
 270 upper range of the stochastic region (Figure 3(a)). The contribution of  $\alpha^{LT}$  or  
 271  $\alpha^{TL}$  the attenuation due to wave mode conversion is much less significant (by  
 272 two or three orders of magnitude).

273 But, in the Rayleigh region, the scattering phenomenon differs between lon-  
 274 gitudinal and transverse waves:

- 275 • For the longitudinal waves, the scattering mechanism is governed by the  
 276 conversion between longitudinal and transverse wave modes. For exam-  
 277 ple,  $\alpha^{LT}$  the attenuation due to longitudinal-to-transverse wave scatter-  
 278 ing makes a contribution of more than 96% to the total attenuation for

279  $(x_{0L}, \log_{10} x_{0L}) = (0.08, -1.1)$  (Figure 3(a)). The attenuation  $\alpha^{LT}$  due  
 280 to the wave mode conversion is higher by almost two orders of magni-  
 281 tude than  $\alpha^{LL}$ . However, when frequencies increase, this contribution de-  
 282 creases and becomes independent on frequency beyond  $(x_{0L}, \log_{10} x_{0L}) \approx$   
 283  $(4.2, 0.6)$ , due to the transition from Rayleigh to stochastic regions.

- 284 • For the transverse waves, conversely, the attenuation  $\alpha^{TT}$  due to transverse-  
 285 to-transverse scattering is at least two orders of magnitude higher than  
 286  $\alpha^{TL}$  coming from the wave mode conversion (Figure 3(b)).

287 As a consequence, it can be noticed that, the transition between the Rayleigh  
 288 region and the stochastic one is different between the two cases of longitudinal  
 289 and transverse waves. It is due to the fact that a same scattering mechanism  
 290 is active whatever the frequency region in the case of the transverse waves,  
 291 while two different scattering mechanisms are active depending on the involved  
 292 frequency domain in the case of longitudinal waves. Accordingly, in the case of  
 293 transverse waves, a monotonically decreasing slope of the master  $\log_{10}(\alpha d)$  vs.  
 294  $\log_{10}(x_0)$  curves is observed (right axis of Figure 4(b)). While, in the case of  
 295 longitudinal waves, an inflection point exists for the master curve and indicates  
 296 the Rayleigh-to-stochastic transition (right axis of Figure 4(a)). Moreover, it is  
 297 reasonable to state that the transition starts at lower frequencies in the 2D case  
 298 than in the 3D case, according to the inflection points obtained in both cases  
 299 shown in Figure 4(a).

300 Comparison in the frequency dependence of the attenuation per crystallite  
 301 coefficient, i.e. the exponent  $n$  value, between 2D and 3D cases is further made  
 302 based on the slope of the master curves. Previous studies in the 3D case sug-  
 303 gested that the scattering-induced attenuation per crystallite coefficient  $\alpha d$  was  
 304 proportional to  $x_{0\beta}^n$ , with a specific asymptotic value of the exponent  $n$  depen-  
 305 dent on the scattering region:  $n = 4$  in the Rayleigh region and  $n = 2$  in the  
 306 stochastic region [4]. In the 2D case, Figures 4(a) and (b) (right axis in blue)  
 307 show a different frequency dependence of the attenuation per crystallite in the  
 308 Rayleigh region:  $n = 3$  for the both cases of longitudinal and transverse waves.  
 309 This result confirms the classic argument already obtained in the 3D case [4, 13]  
 310 that the Rayleigh scattering region is dependent on the volume of grain as in  
 311 the 2D case the grain volume is reduced to its surface. On the other hand, the  
 312 exponent  $n$  is equal to 2 in the stochastic region for both 2D and 3D cases. How-  
 313 ever, the evolution of the exponent  $n$  from the Rayleigh region to the stochastic  
 314 one differs between the two cases of longitudinal and transverse waves: for the  
 315 longitudinal waves, the exponent decreases at first, then increases and tends to  
 316 2, while for the transverse waves, it decreases continuously tends to 2 for the  
 317 3D case and to a value very close to 2 in the 2D case.

318 As far as the comparison in the attenuation level between 2D and 3D is  
 319 concerned, the attenuation differs mostly in the Rayleigh region for both lon-  
 320 gitudinal and transverse waves: the attenuation coefficient obtained in the 3D

321 case is about one order of magnitude less than the one obtained in the 2D  
322 case. The difference between the 2D and 3D attenuation values decrease as the  
323 frequency increases. But, such difference is inverted within or after the Rayleigh-  
324 to-stochastic transition domain: the 3D attenuation coefficient becomes larger  
325 than the 2D one. For example, in the case of longitudinal waves a maximum  
326 ratio  $\alpha^{L,3D}/\alpha^{L,2D}$  equal to 1.75 is obtained, which occurs within the Rayleigh-  
327 to-stochastic transition domain and is dependent on the inhomogeneity degree  
328  $\epsilon$  of the material (left axis of Figure 4(a)). In the case of transverse waves, the  
329 ratio  $\alpha^{T,3D}/\alpha^{T,2D}$  is an monotonic increasing function, which tends towards 1.5  
330 in the stochastic region (left axis of Figure 4(b)).

### 331 3.2. Analytical interpretation of dominant scattering mechanisms

332 Now, the non-zero components of the attenuation coefficient  $\alpha_{klmn}^{\beta\gamma}$  defined  
333 in Section 2, which describe scattering contributions at grain boundary into all  
334 directions, are separately presented and analyzed. The propagation direction is  
335 taken to be the  $\mathbf{e}_3$  direction, *i.e.*  $j = 3$  in (15) and (19), without loss of general-  
336 ity. We note that in the 3D case the assumption of macroscopically untextured  
337 media leads to an equivalence of the directions  $\mathbf{e}_1$  and  $\mathbf{e}_2$  with respect to the  
338 propagation direction  $\mathbf{e}_3$ . This implies more particularly for the longitudinal  
339 waves that there is equality between some corresponding components  $\alpha_{klmn}^{\beta\gamma}$ ,  
340 e.g.  $\alpha_{1313}^{LT} = \alpha_{2323}^{LT}$ .

341 The case of longitudinal waves is firstly analyzed.

- 342 • In the stochastic scattering region, which corresponds to the frequency  
343 range  $x_{0L} \in ]5, 35[$  for the considered polycrystals, it has been shown that  
344  $\alpha^{LL}$  due to  $L$ -wave mode reflection/transmission is predominant. All the  
345 non-zero components  $\alpha_{klmn}^{LL}$  are plotted in Figure 5 and among them, it  
346 is obvious that  $\alpha_{3333}^{LL}$  makes the dominant contribution to  $\alpha^{LL}$ . Detailed  
347 analysis of the equations given in Section 2, *e.g.* (2), (3), (19) and (20),  
348 show that among the different components contributing to  $\alpha^{LL}$ , only  $\alpha_{3333}^{LL}$   
349 is due to a “pure”  $L$ -wave mode reflection/transmission in the sense that  
350 it involves only longitudinal wave modes propagating and polarized in the  
351  $\mathbf{e}_3$  direction. Therefore, this result is in agreement with the fact that the  
352 stochastic scattering can be regarded as a one-dimensional phenomenon  
353 linked to only the averaged grain length along the wave propagation di-  
354 rection. This analysis of the components of  $\alpha^{LL}$  provides an analytical  
355 interpretation for first power dependence of attenuation on grain size and  
356 a similar attenuation level in the stochastic domain for longitudinal waves  
357 for both the 2D and 3D models.
- 358 • In the Rayleigh scattering region that corresponds to the frequency range  
359  $x_{0L} \in ]0, 0.6[$  for the considered polycrystals, it has been shown that  $\alpha^{LT}$   
360 due to wave mode conversion is predominant. Indeed, as can be seen from

361 Figure 3,  $\alpha^{LT}$  increases and gradually becomes insensitive to frequency,  
 362 making a negligible contribution in the stochastic scattering region. All  
 363 the non-zero components  $\alpha_{klmn}^{LT}$  are therefore plotted only in the Rayleigh  
 364 scattering in Figure 6 and it is obvious that their contributions to  $\alpha^{LT}$   
 365 are comparable. In other words, it is important to take into account all  
 366 possible mechanisms. Taking the 2D case as an example, the longitudinal  
 367 wave mode propagating and polarized in the  $\mathbf{e}_3$  direction can, due to  
 368  $\delta\mathbf{C}$ , result in a mode (stress vector) propagating in the  $\mathbf{e}_n$  direction and  
 369 polarized in the  $\mathbf{e}_m$  direction. It gives rise to a mode propagating in the  
 370  $\mathbf{e}_l$  direction and polarized in the  $\mathbf{e}_k$  direction, which finally contributes to  
 371 a transverse wave mode. This result confirms that the Rayleigh scattering  
 372 involves all space directions and provides an analytical interpretation of  
 373 its dependency on the grain volume (or surface) in the 3D (or 2D) case.  
 374 However, we note that, for example in the 2D case, the two most important  
 375 contributions are given by  $\alpha_{1313}^{LT}$  and  $\alpha_{3131}^{LT}$ .

- 376 • Another interesting result is that all the components  $\alpha_{nmnn}^{LT}$  with  $m \neq n$   
 377 are negative, which correspond to an amplification instead of an atten-  
 378 uation. Detailed analysis of such components shows that it results from  
 379 the partial derivative term  $\partial^2/\partial r_n \partial r_m (W(r)e^{ik_0L\mathbf{e}_3 \cdot \mathbf{r}})$  which works out  
 380 to be negative when  $m \neq n$ . However, this cannot explain completely why  
 381  $\alpha_{nmnn}^{LT}$  is negative. Indeed, according to the definition of the tensor  $\mathbf{P}$   
 382 (10), when  $m \neq n$ , the negative partial derivative term leads to  $P_{nmnn} < 0$   
 383 and  $P_{mmnn} < 0$ . But, because of the fact that,  $\langle \delta C_{33mn} \delta C_{nm33} \rangle > 0$ , and  
 384  $\langle \delta C_{33mm} \delta C_{nn33} \rangle < 0$  when  $m \neq n$  [26], only  $\alpha_{nmnn}^{LT}$  is negative. One  
 385 plausible interpretation is  $\alpha_{nmnn}^{LT}$  (or  $\alpha_{mmnn}^{LT}$ ) expresses an intermediate  
 386 mode conversion between two modes, one propagating in the  $\mathbf{e}_n$  direction  
 387 and polarized in the  $\mathbf{e}_m$  (or  $\mathbf{e}_n$ ) direction and the other propagating in the  
 388  $\mathbf{e}_m$  direction and polarized in the  $\mathbf{e}_n$  (or  $\mathbf{e}_m$ ) direction. Therefore, when  
 389 the correlation between the corresponding elastic constants is positive in  
 390 the case with  $n \neq m$ , the attenuation in the  $\mathbf{e}_n$  direction gives rise to an  
 391 amplification in the perpendicular  $\mathbf{e}_m$  direction.

392 Then, the case of transverse waves is analyzed. It has been shown that  $\alpha^{TT}$   
 393 due to  $T$ -wave mode reflection/transmission is predominant in both the Rayleigh  
 394 and the stochastic scattering regions. All the non-zero components  $\alpha_{klmn}^{TT}$  are  
 395 plotted in Figure 7, with an enlarged view at low frequencies in the Rayleigh  
 396 region  $x_{0T} \in ]0.2, 0.6[$ . Analyses similar to the case of longitudinal waves are  
 397 obtained.

- 398 • In the Rayleigh region, each component makes a comparable contribution  
 399 to  $\alpha^{TT}$ , which confirms that the Rayleigh scattering involves all space  
 400 directions and provides an analytical interpretation of its dependency on  
 401 the grain volume (or surface) in the 3D (or 2D) case.
- 402 • In the stochastic region, only the component  $\alpha_{1313}^{TT}$  in the 2D case and

403 only the components  $\alpha_{1313}^{TT}$  and  $\alpha_{2323}^{TT}$  in the 3D case make significant  
 404 contributions. More particularly, the contribution of  $\alpha_{1313}^{TT}$  is dominant  
 405 and expresses, according to the analysis presented above, a “pure” T-  
 406 wave mode reflection/transmission involving only transverse wave modes  
 407 propagating in the  $\mathbf{e}_3$  direction and polarized in the  $\mathbf{e}_1$  direction. Once  
 408 again, the stochastic scattering for transverse waves can be considered as  
 409 a one-dimension phenomenon depending only on the average grain length  
 410 in the propagation direction. Otherwise, in the 3D case,  $\alpha_{2323}^{TT}$  gives also  
 411 an important contribution. However, quantitative comparison shows a  
 412 comparable magnitude of  $\alpha_{1313}^{TT}$  between the 2D and 3D cases, so the  
 413 contribution in the 3D case of  $\alpha_{2323}^{TT}$ , *i.e.* the third direction  $\mathbf{e}_2$  ignored  
 414 by 2D models, leads to  $\alpha^{T,3D} > \alpha^{T,2D}$  in the stochastic region, with the  
 415 ratio  $\alpha^{T,3D}/\alpha^{T,2D}$  tends to a value larger than 1.5 (Figure 4(b)).

416 From above discussions, main common and different features between both  
 417 2D and 3D cases of the grain scattering induced attenuation are analyzed, such  
 418 as a decrease in the frequency and grain size dependence and an increase in the  
 419 attenuation levels in the Rayleigh region for both longitudinal and transverse  
 420 waves propagating within a 2D polycrystal medium. However, in essence, the  
 421 scattering mechanisms are the same in 2D and 3D cases, *i.e.*, the Rayleigh  
 422 scattering is dependent on the volume of grains, while the stochastic scattering  
 423 is dependent only on the grain length along the wave propagation direction.  
 424 From this point of view, the attenuation in an infinite 3D space can be deduced  
 425 according to more efficient 2D simulations given that the Born approximation  
 426 is valid.

## 427 4. Numerical validation and analysis

### 428 4.1. Computational model

429 To study the effect of the grain size on the grain scattering-induced atten-  
 430 uation, 2D FE simulations were performed using an in-house software OOFE  
 431 (Object Oriented Finite Element program) [29]. It is an implicit solver based  
 432 on a time-discontinuous space-time Galerkin method [30, 31]. The details of the  
 433 FE modeling, such as the use of structured and unstructured meshes, compari-  
 434 son of symmetry and periodic boundary conditions, and the mesh convergence,  
 435 have been described elsewhere [15, 16, 20, 25, 32, 33]. Here, only the necessary  
 436 steps to numerically model a plane wave propagation within an anisotropic het-  
 437 erogeneous polycrystalline medium are discussed. The same material is taken  
 438 as for the analytical calculation.

439 A polycrystalline medium is generated by a Voronoï tessellation, as achieved  
 440 for example in [15, 32, 34–38], which has been shown to represent closely a  
 441 realistic polycrystalline microstructure. Three different mean grain sizes were

442 considered: 34, 80, and 160 $\mu\text{m}$ . We chose a rectangular sample of dimension  
443  $W \times H$  (x-coordinates  $\times$  y-coordinates) (Figure 8), with  $H = 10.16\text{mm}$ . For  
444 the two largest grain sizes,  $W = 20.32\text{mm}$ , while  $W = 5.08\text{mm}$  for the smallest  
445 grain size of 34 $\mu\text{m}$  to reduce the memory required for the calculation. Details  
446 of FE model are depicted in Table II. The grain diameter follows a Gaussian  
447 distribution with a constant standard deviation equal to about 0.1 whatever the  
448 grain size. To obtain an untextured polycrystal, crystallographic orientation for  
449 each grain defined by the Euler angle  $\theta(\varphi_1, \phi, \varphi_2)$ , which gives the orientation  
450 of the cubic axes of each grain with respect to the specimen Cartesian basis,  
451 is randomly chosen:  $\varphi_1 = \text{random}[0, 2\pi[$ ,  $\phi = \arccos(\text{random}[-1, 1])$  and  $\varphi_2 =$   
452  $\text{random}[0, 2\pi[$ .

Mean grain size $\bar{D}$	34 $\mu\text{m}$	80 $\mu\text{m}$	160 $\mu\text{m}$
Center frequencies	4-16MHz	4-16MHz	4-16MHz
Dimension(mm) ( $W \times H$ )	5.08 $\times$ 10.16	20.32 $\times$ 10.16	20.32 $\times$ 10.16
Grains in each sample	53656	38758	11427
No. of samples	5	7	23

Table II: Details of numerical FE model.

453 Discretization size used both in the time and space is of great importance  
454 for the accuracy of the numerical results. For numerical simulation of wave  
455 propagation in homogeneous media, it is generally recommended to have at  
456 least 15 elements included in the shortest wavelength of interest. However, in  
457 polycrystalline media, denser elements are required when the grain size is of  
458 an order of magnitude much smaller than the shortest wavelength [15, 18, 20,  
459 39]. Investigations indicate that numerical calculations of ultrasonic attenuation  
460 and/or scattering converge at a smaller  $d/h$  value for a sample with a smaller  
461 grain size [15, 20, 39]. In the present work, the ratio of grain size to element  
462 size,  $d/h$ , has been set to be approximately 6.0 for samples with the grain sizes  
463 of 34 and 80 $\mu\text{m}$ , and to be around 12.0 for the grain size of 160 $\mu\text{m}$ , which  
464 corresponds to more than 30 elements per shortest wavelength. The calculation  
465 of the attenuation coefficient converges for an acceptable threshold of 5.5% for  
466 all the considered grain sizes. Once the element size is defined, the accuracy  
467 of time integration of the implicit solver is guaranteed given that the time step  
468  $\Delta t$  is no more than the smallest transit time of the wave through any of the  
469 elements:  $\Delta t \leq h_{min}/\max_{\theta}(v_L)$ , where  $h_{min}$  is the smallest element size [18].

470 For simulating a scenario of a longitudinal plane wave in an infinite domain  
471 as assumed in the analytical model, a uniformly distributed pressure loading  
472  $p(\mathbf{x}, t)\mathbf{e}_y$  is imposed to all the nodes on the emitter line, in this case the  $y = Y0$   
473 line in Figure 8, with  $\mathbf{e}_y$  denoting the unit vector in the  $y$  direction. To simulate  
474 a broadband ultrasonic incident signal representing an ablative laser pulse, the  
475 amplitude of the pressure loading is the sum of two Ricker signals varying in  
476 time, whose frequency content is centered to 5MHz and 10MHz respectively.



477 For such an external loading, the valid frequency domain is limited to a range  
478 from 4 to 16MHz, this leads to a range from  $375\mu\text{m}$  to 1.5mm for wavelengths.  
479 Hence, the Rayleigh region and the Rayleigh-to-stochastic transition domain  
480 are covered with respect to the considered grain sizes. Symmetry boundary  
481 condition is used to accommodate the desired plane wave mode, *i.e.*, vanishing  
482 nodal displacements (and thus also velocities and accelerations) in the direction  
483 normal to the two lines that are parallel to the wave propagation direction,  
484 namely  $x = X0$  and  $x = X1$  in Figure 8. The displacement and velocity of all  
485 the nodes on the emitter line  $y = Y0$  and the receiver line  $y = Y1$  are recorded.

486 To reduce the gap between the numerical simulation involving a finite number  
487 of grains and the analytical models, multiple realizations of microstructures  
488 with randomly generated crystallographic orientations but with the same  
489 Voronoi-type grain morphology are calculated. The number of realizations is  
490 set to be 5, 7 and 23 for the three grain sizes of 34, 80 and  $160\mu\text{m}$ , respectively,  
491 resulting in roughly the same number of grains considered for each grain size.  
492 The attenuation for each grain size is then calculated by averaging over the  
493 corresponding realizations.

#### 494 4.2. Numerical results and comparison with the theoretical model

495 The averaged numerical results (represented as solid circles) and the minimum  
496 and maximum limits (represented as bars) of attenuation are plotted as  
497 a function of frequency in Figure 9. In the low frequency region [4, 13]MHz,  
498 the attenuation coefficient increases continuously as frequency for a given grain  
499 size, and increases as grain size at a given frequency. By contrast, in the higher  
500 frequency region [12, 16]MHz, a similar evolution tendency is observed only for  
501 samples with both grain sizes of 34 and  $80\mu\text{m}$ . Indeed, by comparing the grain  
502 size to the wavelength in this frequency region, the Rayleigh scattering behavior  
503 is mainly found for the two smallest grain sizes, whereas the Rayleigh-to-stochastic  
504 scattering transition behavior is found for the largest grain size  
505 of  $160\mu\text{m}$ , which reduces greatly the power dependence of attenuation on frequency.  
506 However, the results for the largest grain size of  $160\mu\text{m}$  is shown to be  
507 non-monotonic in the high frequency region [15, 16]MHz, which is not expected  
508 by the classical Stanke-Kino theory considering only one single mean grain size.  
509 It can be probably attributed to the distribution of grain sizes [25] and will be  
510 discussed in the end of this section.

511 Figure 10(a) presents, using the base-10 logarithmic scale and for the 2D  
512 case, master curves, calculated analytically and numerically, of  $\alpha d$  the attenuation  
513 coefficient per crystallite versus  $x_0$  the normalized frequency. The FE  
514 calculations for the three different grain sizes are well superimposed on the analytical  
515 master curve. The reduction of frequency dependence of attenuation  
516 in the Rayleigh region, from the exponent  $n = 4$  for the 3D case to  $n = 3$  for  
517 the 2D case, is quantitatively confirmed for frequency range  $(x_{0L}, \log_{10} x_{0L}) <$

518 (0.6, -0.22) by the numerical results. Afterwards, for the Rayleigh-to-stochastic  
 519 transition, the first concave hump is roughly recovered for frequencies  $x_0 > 0.6$   
 520 by the numerical results. Nevertheless, rigorous comparison shows that the nu-  
 521 merically estimated transition region is more pronounced than the analytically  
 522 predicted one. Specifically, the attenuation level becomes slightly larger in the  
 523 region  $0.6 < x_0 < 2.4$  (corresponding to  $-0.22 < \log_{10}(x_{0L}) < 0.38$ ).

524 As discussed in Section 2, the inverse exponential two-point correlation func-  
 525 tion under the assumption of Poisson-distributed cord length is used for the  
 526 feasibility of the analytical deviation. However, a series of studies have proved  
 527 that this form of correlation function failed to consider effects of a complete  
 528 grain-size distribution on ultrasonic attenuation [14, 25, 33]. In the FE mod-  
 529 eling presented here, a relative small distribution width of grain sizes was gen-  
 530 erated, which would give rise to a strong deviation of the spatial correlation  
 531 function model from the exponential form, and accordingly lead to the dis-  
 532 agreement between the classical analytical model and our numerical models.  
 533 It has been demonstrated [25], that the attenuation behavior in the transition  
 534 region strongly depends on the grain morphology and grain size distribution, as  
 535 it is dominated by the mode conversion component  $\alpha^{LT}$ .

536 Thanks to  $\alpha^{L,3D}/\alpha^{L,2D}$  (Eq. 15) the analytically identified ratio of atten-  
 537 uation coefficient between 3D and 2D models, 3D estimations can be deduced  
 538 by 2D simulations. Comparison between the deduced 3D results for different  
 539 grain sizes and the analytical prediction is plotted in Figure 10(b), which shows  
 540 an acceptable agreement. It is demonstrated that more efficient 2D simulations  
 541 can be conducted to be representative for the 3D case on condition that the  
 542 Born approximation is valid.

## 543 5. Conclusions

544 In this paper, the grain scattering-induced attenuation coefficient has been  
 545 expressed in an explicit integral form of the dyadic Green's tensor and a spatial  
 546 correlation function, applicable for ultrasonic waves propagating in both 2D  
 547 and 3D polycrystalline media. Especially, the explicit formula in 2D allowed  
 548 the Stanke and Kino's master curve of the effect of grain size on attenuation to  
 549 be drawn and compared with the 3D original.

550 Several different and common features for the 2D and 3D attenuation phe-  
 551 nomena were observed and discussed. In the Rayleigh region, the attenuation  
 552 of the 2D model shows a reduction of the frequency and grain size dependence,  
 553 which results in a higher attenuation level compared to the 3D model. Con-  
 554 versely, in the stochastic region, a same frequency and grain size dependence is  
 555 obtained for both 2D and 3D cases. As far as the attenuation level is concerned  
 556 within or after the Rayleigh-to-stochastic transition domain, the difference be-

557 tween the 2D and 3D cases is inverted. For the longitudinal waves, the attenua-  
558 tion in 3D becomes higher than in 2D and the ratio of attenuation between the  
559 two cases reaches a maximum value (equal to 1.75 for the studied polycrystal)  
560 within the Rayleigh-to-stochastic transition domain, then it decreases and tends  
561 to the value of 1. For the transverse waves, the ratio of attenuation between  
562 the 3D and 2D cases is an monotonic increasing function of frequency from the  
563 Rayleigh region to the stochastic region (which tends to the value of 1.5 for the  
564 studied polycrystal).

565 Two levels of decomposition of the attenuation coefficient in different scattering-  
566 induced coefficients were proposed and allowed a better understanding of the  
567 scattering mechanisms leading to wave attenuation in a polycrystal. For the  
568 stochastic region, the dominating scattering mechanism is the reflection / trans-  
569 mission between a same type of wave modes, whatever the space dimension and  
570 the type of waves. Detailed analysis, owing to the second level of decomposition  
571 of the mode reflection / transmission contribution, provided an analytical in-  
572 terpretation of the fact that the attenuation is only controlled by the averaged  
573 grain length along the wave propagation direction. It gave also an explana-  
574 tion for a higher attenuation coefficient of the transverse wave in 3D than in  
575 2D in the stochastic region. For the Rayleigh region, the dominating scatter-  
576 ing mechanism differs between the longitudinal waves and the transverse ones,  
577 which is the longitudinal/transverse conversion for the longitudinal waves and  
578 the transverse-to-transverse reflection/transmission for the transverses waves.  
579 However, detailed analysis based on the second level of decomposition allowed a  
580 good explanation of the fact that attenuation in Rayleigh region mainly depends  
581 on the grain volume.

582 2D FE simulations were performed in an untextured body-centered-cubic  
583 (bcc) titanium polycrystal with equiaxed grains. A Voronoi-type grain mi-  
584 crostructure with a narrow Gaussian distribution of sizes was studied. Several  
585 average grain sizes were considered and they were chosen to cover the Rayleigh  
586 and the Rayleigh-to-stochastic transition regions. A good agreement was found  
587 in the Rayleigh region between the numerical simulations and the analytical pre-  
588 dictions which validates the FE modeling. Nevertheless, an oscillatory behavior  
589 was found in the transition region due to the influence of grain size distribution,  
590 which was not considered by the exponential form of spatial correlation func-  
591 tion used in the analytical deviation. 3D numerical estimations were deduced  
592 from 2D FE simulations thanks to the ratio of analytical attenuation coefficient  
593 between the 3D and the 2D modelings. These results are expected to be useful  
594 for achieving efficient 2D simulations that could be representative of 3D.

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602 **Appendix A1. Numerical calculation of the explicit formulas of the**  
 603 **attenuation coefficients**

604 Detailed equations and numerical procedure developed to evaluate the at-  
 605 tenuation coefficients defined by (18) are hereafter presented.

606 Given the material properties, a mean grain size  $d$  and the normalized fre-  
 607 quency region of interest, the objective is to calculate all the contributing terms  
 608  $\alpha_{klmn}^{\beta\gamma}$  ( $\beta, \gamma = L, T$ ), which are mainly defined using two second order symmetric  
 609 tensors  $\mathbf{G}^\beta(\mathbf{r})$  and  $\mathbf{D}^\beta(\mathbf{r})$ . The Green function tensor  $\mathbf{G}^\beta(\mathbf{r})$  is given by (16).  
 610 Otherwise, assuming that the ultrasonic wave propagates in the  $\mathbf{e}_3$  direction and  
 611 the spatial correlation function has an inverse exponential form  $W(\mathbf{r}) = e^{-r/a}$ ,  
 612 with  $a = d/2$ , it can be shown that the second derivative tensor  $\mathbf{D}^\beta(\mathbf{r})$  reads  
 613 as:

$$\begin{aligned} \mathbf{D}^\beta(\mathbf{r}) &\equiv \nabla_{\mathbf{r}}(\nabla_{\mathbf{r}}(W(\mathbf{r})e^{ik_{0\beta}\mathbf{e}_3 \cdot \mathbf{r}})) \\ &= e^{ik_{0\beta}r\mathbf{e}_3 \cdot \hat{\mathbf{r}} - r/a} \left( \left( \frac{1}{ra} + \frac{1}{a^2} \right) \hat{\mathbf{r}} \otimes \hat{\mathbf{r}} - \frac{1}{ra} \mathbf{I} - k_{0\beta}^2 \mathbf{e}_3 \otimes \mathbf{e}_3 - \frac{2ik_{0\beta}}{a} \hat{\mathbf{r}} \otimes_s \mathbf{e}_3 \right) \end{aligned} \quad (24)$$

614 with  $\hat{\mathbf{r}}$  the unit vector defining the direction of  $\mathbf{r}$ .

For convenience of calculation, the Cartesian coordinates  $(r_1, r_3)$  for the 2D  
 case (resp.  $(r_1, r_2, r_3)$  for the 3D case) are converted into the polar coordinates  
 $(r, \theta)$  (resp. the spherical coordinate  $(r, \theta, \varphi)$ ). Then, the equation (19) to be  
 calculated finally becomes:

$$\alpha^{\beta\gamma, 2D} = \text{Im} \left( \frac{k_{0\beta} \langle \delta C_{j^\beta j^\beta j^\beta j^\beta} \delta C_{mnj^\beta j^\beta} \rangle}{2C_{j^\beta j^\beta j^\beta j^\beta}^0} \int_{r=0}^{\infty} \int_{\theta=0}^{2\pi} G_{km}^\gamma(r, \theta) D_{ln}^\beta(r, \theta) r \, d\theta \, dr \right) \quad (25a)$$

$$\alpha^{\beta\gamma, 3D} = \text{Im} \left( \frac{k_{0\beta} \langle \delta C_{j^\beta j^\beta j^\beta j^\beta} \delta C_{mnj^\beta j^\beta} \rangle}{2C_{j^\beta j^\beta j^\beta j^\beta}^0} \int_{r=0}^{\infty} \int_{\varphi=0}^{\pi} \int_{\theta=0}^{2\pi} G_{km}^\gamma(r, \theta, \varphi) D_{ln}^\beta(r, \theta, \varphi) r^2 \sin\varphi \, d\theta \, d\varphi \, dr \right) \quad (25b)$$

615 In (25), the two-points autocorrelation function of elastic constants  $\langle \delta C_{j\beta jkl} \delta C_{mnj\beta j} \rangle$   
616 are given by Eq.(100) in [4]. Taking an overall consideration of the symmetry  
617 properties of the tensors  $\delta \mathbf{C}$ ,  $\mathbf{G}(\mathbf{r})$  and  $\mathbf{D}(\mathbf{r})$ , it is found that only six compo-  
618 nents  $\alpha_{klmn}^{\beta\gamma}$  have to be calculated in the 2D case, while in the 3D case, there  
619 are fourteen components to calculate for  $\alpha^{LL}$  and  $\alpha^{LT}$  and fifteen for  $\alpha^{TT}$ .

620 Two integration methods are developed and compared.

621 The first method calculate numerically the double and triple integrals defined  
622 by (25). In this case, MATLAB functions “integral2” and “integral3” are used.  
623 In order to guarantee the precision of numerical integration and to determine a  
624 pertinent interval of integration for the variable  $r \in [0, \infty]$ , the variation of the  
625 integrands defined in (25) within the infinite interval  $[0, \infty]$  of the variable  $r$  is  
626 analyzed. Figure 11 illustrates the variation in the 2D case. Given values of  $\theta$   
627 and  $x_0$ , the integrands decrease very rapidly in the region  $r \ll d$  and become very  
628 close to zero when  $r \gg d$ . According to this analysis, the interval of integration  
629 for  $r$  is chosen equal to  $[0.0001d, 100d]$ , which is furthermore subdivided into  
630 five subintervals:  $[0.0001d, 0.1d] \cup [0.1d, 0.25d] \cup [0.25d, d] \cup [d, 10d] \cup [10d, 100d]$ .  
631 In each subinterval, the MATLAB 2D or 3D integral functions are applied with  
632 the default relative and absolute error tolerances. We remark that this method  
633 applied to the 3D explicit formula is very time consuming and to speed up the  
634 calculation in higher frequency region, it is possible to relax both relative and  
635 absolute error tolerances.

636 The second method calculates firstly and analytically all the integrals with  
637 respect to  $\theta$  in the 2D case (resp. to  $(\theta, \varphi)$  in the 3D case). Then the inte-  
638 grals with respect to  $r$  are performed numerically, using for exemple MATLAB  
639 function “integral”.

640 In the 2D case, after the analytical development of the integrals with respect  
641 to  $\theta$ , the ~~six~~ **five** integrands  $\eta_{kmln}^{\beta\gamma}$  useful for the calculation of  $\alpha_{klmn}^{\beta\gamma}$ , without

642 the part  $\frac{\langle \delta C_{j^\beta j k l} \delta C_{m n j^\beta j} \rangle (1 - c(\gamma))}{2C_{j^\beta j j^\beta j}^0} \frac{1 - c(\gamma)}{4\pi\rho\omega^2}$ , can be expressed as follows:

$$\begin{aligned}
\frac{\eta_{3333}^{\beta\gamma}(r)}{k_{0\beta} r e^{-r/a}} &= A_{rr}(k_{0\gamma} r) \left( \left( \frac{1}{ra} + \frac{1}{a^2} \right) \hbar_{C4}^{2D}(k_{0\beta} r) - \frac{2ik_{0\beta}}{a} \hbar_{C3}^{2D}(k_{0\beta} r) - \left( k_{0\beta}^2 + \frac{1}{ra} \right) \hbar_{C2}^{2D}(k_{0\beta} r) \right) \\
&\quad - A_{\mathbf{I}}(k_{0\gamma} r) \left( \left( \frac{1}{ra} + \frac{1}{a^2} \right) \hbar_{C2}^{2D}(k_{0\beta} r) - \frac{2ik_{0\beta}}{a} \hbar_{C1}^{2D}(k_{0\beta} r) - \left( k_{0\beta}^2 + \frac{1}{ra} \right) \hbar_{S0}^{2D}(k_{0\beta} r) \right) \\
\frac{\eta_{1111}^{\beta\gamma}(r)}{k_{0\beta} r e^{-r/a}} &= A_{rr}(k_{0\gamma} r) \left( \left( \frac{1}{ra} + \frac{1}{a^2} \right) \hbar_{S4}^{2D}(k_{0\beta} r) - \frac{1}{ra} \hbar_{S2}^{2D}(k_{0\beta} r) \right) \\
&\quad - A_{\mathbf{I}}(k_{0\gamma} r) \left( \left( \frac{1}{ra} + \frac{1}{a^2} \right) \hbar_{S2}^{2D}(k_{0\beta} r) - \frac{1}{ra} \hbar_{S0}^{2D}(k_{0\beta} r) \right) \\
\frac{\eta_{1313}^{\beta\gamma}(r)}{k_{0\beta} r e^{-r/a}} &= A_{rr}(k_{0\gamma} r) \left( \left( \frac{1}{ra} + \frac{1}{a^2} \right) \hbar_{S2C2}^{2D}(k_{0\beta} r) - \frac{ik_{0\beta}}{a} \hbar_{S2C1}^{2D}(k_{0\beta} r) \right) \\
\frac{\eta_{1133}^{\beta\gamma}(r)}{k_{0\beta} r e^{-r/a}} &= A_{rr}(k_{0\gamma} r) \left( \left( \frac{1}{ra} + \frac{1}{a^2} \right) \hbar_{S2C2}^{2D}(k_{0\beta} r) - \frac{2ik_{0\beta}}{a} \hbar_{S2C1}^{2D}(k_{0\beta} r) - \left( k_{0\beta}^2 + \frac{1}{ra} \right) \hbar_{S2}^{2D}(k_{0\beta} r) \right) \\
&\quad - A_{\mathbf{I}}(k_{0\gamma} r) \left( \left( \frac{1}{ra} + \frac{1}{a^2} \right) \hbar_{C2}^{2D}(k_{0\beta} r) - \frac{2ik_{0\beta}}{a} \hbar_{C1}^{2D}(k_{0\beta} r) - \left( k_{0\beta}^2 + \frac{1}{ra} \right) \hbar_{S0}^{2D}(k_{0\beta} r) \right) \\
\frac{\eta_{3311}^{\beta\gamma}(r)}{k_{0\beta} r e^{-r/a}} &= A_{rr}(k_{0\gamma} r) \left( \left( \frac{1}{ra} + \frac{1}{a^2} \right) \hbar_{S2C2}^{2D}(k_{0\beta} r) - \frac{1}{ra} \hbar_{C2}^{2D}(k_{0\beta} r) \right) \\
&\quad - A_{\mathbf{I}}(k_{0\gamma} r) \left( \left( \frac{1}{ra} + \frac{1}{a^2} \right) \hbar_{S2}^{2D}(k_{0\beta} r) - \frac{1}{ra} \hbar_{S0}^{2D}(k_{0\beta} r) \right)
\end{aligned} \tag{26}$$

643 We remark that  $\eta_{3131}^{\beta\gamma}(r) = \eta_{1331}^{\beta\gamma}(r) = \eta_{3113}^{\beta\gamma}(r) = \eta_{1313}^{\beta\gamma}(r)$ .  $\hbar^{2D}$  functions in (26)

644 are defined using Bessel functions of the first kind  $J_\nu$  in the following way:

$$\begin{aligned}
\hbar_{S_0^2}^{2D}(y) &= \int_{\theta=0}^{2\pi} e^{iy \cos \theta} d\theta = 2\pi J_0(y) \\
\hbar_{C_1^2}^{2D}(y) &= \int_{\theta=0}^{2\pi} e^{iy \cos \theta} \cos \theta d\theta = 2i\pi J_1(y) \\
\hbar_{C_2^2}^{2D}(y) &= \int_{\theta=0}^{2\pi} e^{iy \cos \theta} \cos^2 \theta d\theta = 2\pi(y^{-1} J_1(y) - J_2(y)) \\
\hbar_{C_3^2}^{2D}(y) &= \int_{\theta=0}^{2\pi} e^{iy \cos \theta} \cos^3 \theta d\theta = 2i\pi(3y^{-1} J_2(y) - J_3(y)) \\
\hbar_{C_4^2}^{2D}(y) &= \int_{\theta=0}^{2\pi} e^{iy \cos \theta} \cos^4 \theta d\theta = 2\pi(-1 + 3y^{-2}) J_2(y) \tag{27} \\
\hbar_{S_2^2}^{2D}(y) &= \int_{\theta=0}^{2\pi} e^{iy \cos \theta} \sin^2 \theta d\theta = 2\pi y^{-1} J_1(y) \\
\hbar_{S_4^2}^{2D}(y) &= \int_{\theta=0}^{2\pi} e^{iy \cos \theta} \sin^4 \theta d\theta = 6\pi y^{-2} J_2(y) \\
\hbar_{S_2C_1^2}^{2D}(y) &= \int_{\theta=0}^{2\pi} e^{iy \cos \theta} \sin^2 \theta \cos \theta d\theta = 2i\pi y^{-1} J_2(y) \\
\hbar_{S_2C_2^2}^{2D}(y) &= \int_{\theta=0}^{2\pi} e^{iy \cos \theta} \sin^2 \theta \cos^2 \theta d\theta = 2\pi(y^{-1} J_1(y) - 3y^{-2} J_2(y))
\end{aligned}$$

645 In the 3D case, after the analytical development of the integrals with respect  
646 to  $\theta$  and  $\varphi$ , the fifteen integrands  $\eta_{kmln}^{\beta\gamma}$  useful for the calculation of  $\alpha_{klmn}^{\beta\gamma}$ ,

647 without the part  $\frac{\langle \delta C_{j^\beta jkl} \delta C_{mnj^\beta j} \rangle (1 - c(\gamma))}{2C_{j^\beta jj^\beta j}^0} \frac{1}{4\pi\rho\omega^2}$ , can be expressed as follows:

$$\begin{aligned}
\frac{\eta_{3333}^{\beta\gamma}(r)}{k_{0\beta}r^2e^{-r/a}} &= 2\pi A_{rr}(k_{0\gamma}r) \left( \left( \frac{1}{ra} + \frac{1}{a^2} \right) \hbar_{C4S1}^{3D}(k_{0\beta}r) - \frac{2ik_{0\beta}}{a} \hbar_{C3S1}^{3D}(k_{0\beta}r) - \left( k_{0\beta}^2 + \frac{1}{ra} \right) \hbar_{C2S1}^{3D}(k_{0\beta}r) \right) \\
&\quad - 2\pi A_{\mathbf{I}}(k_{0\gamma}r) \left( \left( \frac{1}{ra} + \frac{1}{a^2} \right) \hbar_{C2S1}^{3D}(k_{0\beta}r) - \frac{2ik_{0\beta}}{a} \hbar_{C1S1}^{3D}(k_{0\beta}r) - \left( k_{0\beta}^2 + \frac{1}{ra} \right) \hbar_{S1}^{3D}(k_{0\beta}r) \right) \\
\frac{\eta_{1111}^{\beta\gamma}(r)}{k_{0\beta}r^2e^{-r/a}} &= A_{rr}(k_{0\gamma}r) \left( \frac{3\pi}{4} \left( \frac{1}{ra} + \frac{1}{a^2} \right) \hbar_{S5}^{3D}(k_{0\beta}r) - \pi \frac{1}{ra} \hbar_{S3}^{3D}(k_{0\beta}r) \right) \\
&\quad - A_{\mathbf{I}}(k_{0\gamma}r) \left( \pi \left( \frac{1}{ra} + \frac{1}{a^2} \right) \hbar_{S3}^{3D}(k_{0\beta}r) - 2\pi \frac{1}{ra} \hbar_{S1}^{3D}(k_{0\beta}r) \right) \\
\frac{\eta_{1122}^{\beta\gamma}(r)}{k_{0\beta}r^2e^{-r/a}} &= A_{rr}(k_{0\gamma}r) \left( \frac{\pi}{4} \left( \frac{1}{ra} + \frac{1}{a^2} \right) \hbar_{S5}^{3D}(k_{0\beta}r) - \pi \frac{1}{ra} \hbar_{S3}^{3D}(k_{0\beta}r) \right) \\
&\quad - A_{\mathbf{I}}(k_{0\gamma}r) \left( \pi \left( \frac{1}{ra} + \frac{1}{a^2} \right) \hbar_{S3}^{3D}(k_{0\beta}r) - 2\pi \frac{1}{ra} \hbar_{S1}^{3D}(k_{0\beta}r) \right) \\
\frac{\eta_{1212}^{\beta\gamma}(r)}{k_{0\beta}r^2e^{-r/a}} &= \frac{\pi}{4} A_{rr}(k_{0\gamma}r) \left( \frac{1}{ra} + \frac{1}{a^2} \right) \hbar_{S5}^{3D}(k_{0\beta}r) \\
\frac{\eta_{1313}^{\beta\gamma}(r)}{k_{0\beta}r^2e^{-r/a}} &= \pi A_{rr}(k_{0\gamma}r) \left( \left( \frac{1}{ra} + \frac{1}{a^2} \right) \hbar_{S3C2}^{3D}(k_{0\beta}r) - \frac{ik_{0\beta}}{a} \hbar_{S3C1}^{3D}(k_{0\beta}r) \right) \\
\frac{\eta_{1133}^{\beta\gamma}(r)}{k_{0\beta}r^2e^{-r/a}} &= \pi A_{rr}(k_{0\gamma}r) \left( \left( \frac{1}{ra} + \frac{1}{a^2} \right) \hbar_{S3C2}^{3D}(k_{0\beta}r) - \frac{2ik_{0\beta}}{a} \hbar_{S3C1}^{3D}(k_{0\beta}r) - \left( k_{0\beta}^2 + \frac{1}{ra} \right) \hbar_{S3}^{3D}(k_{0\beta}r) \right) \\
&\quad - 2\pi A_{\mathbf{I}}(k_{0\gamma}r) \left( \left( \frac{1}{ra} + \frac{1}{a^2} \right) \hbar_{S1C2}^{3D}(k_{0\beta}r) - \frac{2ik_{0\beta}}{a} \hbar_{S1C1}^{3D}(k_{0\beta}r) - \left( k_{0\beta}^2 + \frac{1}{ra} \right) \hbar_{S1}^{3D}(k_{0\beta}r) \right) \\
\frac{\eta_{3311}^{\beta\gamma}(r)}{k_{0\beta}re^{-r/a}} &= A_{rr}(k_{0\gamma}r) \left( \pi \left( \frac{1}{ra} + \frac{1}{a^2} \right) \hbar_{S3C2}^{3D}(k_{0\beta}r) - 2\pi \frac{1}{ra} \hbar_{S1C2}^{3D}(k_{0\beta}r) \right) \\
&\quad - A_{\mathbf{I}}(k_{0\gamma}r) \left( \pi \left( \frac{1}{ra} + \frac{1}{a^2} \right) \hbar_{S3}^{3D}(k_{0\beta}r) - 2\pi \frac{1}{ra} \hbar_{S1}^{3D}(k_{0\beta}r) \right)
\end{aligned} \tag{28}$$

648 We remark that  $\eta_{2222}^{\beta\gamma}(r) = \eta_{1111}^{\beta\gamma}(r)$ ,  $\eta_{2211}^{\beta\gamma}(r) = \eta_{1122}^{\beta\gamma}(r)$ ,  $\eta_{1221}^{\beta\gamma}(r) = \eta_{2112}^{\beta\gamma}(r) =$   
649  $\eta_{2121}^{\beta\gamma}(r) = \eta_{1212}^{\beta\gamma}(r)$ , and  $\eta_{3n3n}^{\beta\gamma}(r) = \eta_{n33n}^{\beta\gamma}(r) = \eta_{3nn3}^{\beta\gamma}(r) = \eta_{n3n3}^{\beta\gamma}(r)$  for  $n = 1, 2$ ,  
650 and  $\eta_{3131}^{\beta\gamma}(r) = \eta_{3232}^{\beta\gamma}(r)$ .  $\hbar^{3D}$  functions in (28) are defined in the following way:



$$\begin{aligned}
\hbar_{S1}^{3D}(y) &= \int_{\varphi=0}^{\pi} e^{iy \cos \varphi} \sin \varphi \, d\varphi = 2y^{-1} \sin(y) \\
\hbar_{S3}^{3D}(y) &= \int_{\varphi=0}^{\pi} e^{iy \cos \varphi} \sin^3 \varphi \, d\varphi = 4(-y^{-2} \cos(y) + y^{-3} \sin(y)) \\
\hbar_{S5}^{3D}(y) &= \int_{\varphi=0}^{\pi} e^{iy \cos \varphi} \sin^5 \varphi \, d\varphi = -16(3y^{-4} \cos(y) + (-3 + y^2)y^{-5} \sin(y)) \\
\hbar_{C1S1}^{3D}(y) &= \int_{\varphi=0}^{\pi} e^{iy \cos \varphi} \cos \varphi \sin \varphi \, d\varphi = 2i(-y^{-1} \cos(y) + y^{-2} \sin(y)) \\
\hbar_{C2S1}^{3D}(y) &= \int_{\varphi=0}^{\pi} e^{iy \cos \varphi} \cos^2 \varphi \sin \varphi \, d\varphi = 2(2y^{-2} \cos(y) + (-2 + y^2)y^{-3} \sin(y)) \\
\hbar_{C3S1}^{3D}(y) &= \int_{\varphi=0}^{\pi} e^{iy \cos \varphi} \cos^3 \varphi \sin \varphi \, d\varphi = 2i((6 - y^2)y^{-3} \cos(y) + 3(-2 + y^2)y^{-4} \sin(y)) \\
\hbar_{C4S1}^{3D}(y) &= \int_{\varphi=0}^{\pi} e^{iy \cos \varphi} \cos^4 \varphi \sin \varphi \, d\varphi = 2(4(-6 + y^2)y^{-4} \cos(y) + (24 - 12y^2 + y^4)y^{-5} \sin(y)) \\
\hbar_{S3C1}^{3D}(y) &= \int_{\varphi=0}^{\pi} e^{iy \cos \varphi} \sin^3 \varphi \cos \varphi \, d\varphi = -4i(3y^{-3} \cos(y) + (-3 + y^2)y^{-4} \sin(y)) \\
\hbar_{S4C1}^{3D}(y) &= \int_{\varphi=0}^{\pi} e^{iy \cos \varphi} \sin^4 \varphi \cos \varphi \, d\varphi = -4((-12 + y^2)y^{-4} \cos(y) - (-12 + 5y^2)y^{-5} \sin(y))
\end{aligned} \tag{29}$$

652 Figure 12 presents, for both 2D and 3D cases, the integrands  $f_{klmn}^L(r) =$   
653  $f_{klmn}^{LL}(r) + f_{klmn}^{LT}(r)$ , defined in (25) and after analytical integration with respect  
654 to  $\theta$  in 2D and to  $(\theta, \varphi)$  in 3D, plotted at three different frequencies, in order to  
655 illustrate how they evolve with respect to  $r$ .

656 For both 2D and 3D cases, the two developed integration methods give  
657 almost the same results. For example, the relative difference between them in  
658 2D is less than 0.0006% for both longitudinal and transverse waves. As expected,  
659 the second method is shown to be much more stable and rapid than the first  
660 one, especially in the 3D case. Specifically, it takes about 30 minutes for 2D  
661 analysis and a few hours for 3D analysis by using the first method, while both  
662 2D and 3D numerical analysis can be finished within one minute by using the

663 second method.

664 **Appendix A2. Effects of anisotropy and inhomogeneity degrees of a**  
665 **polycrystalline material on the attenuation level**

666 In order to have a preliminary understanding on the effects of anisotropy and  
667 inhomogeneity degrees of a polycrystalline material on the attenuation level, we  
668 compare here the attenuation coefficient of the following three materials with  
669 cubic-symmetry: the  $\beta$ -titanium considered in the present work, an Inconel 600  
670 studied in [25], and a fictitious material defined in [33]. The characteristics of  
671 these materials are presented in Table III.

672 In our work we use  $\epsilon_\beta$  ( $\beta = L, T$ ) to define the inhomogeneity degrees of  
673 respectively the longitudinal and the transverse wave propagation constants in  
674 a polycrystalline material. They come from the work by Stanke and Kino [4]  
675 and are defined as follows:

$$\begin{aligned} \epsilon_L &= \sqrt{\frac{4}{525} \frac{C_{11} - C_{12} - 2C_{44}}{C_{11}^0}} = \sqrt{\frac{4}{525}} (1 - A) \frac{C_{11} - C_{12}}{C_{11}^0} \\ \epsilon_T &= \sqrt{\frac{3}{700} \frac{C_{11} - C_{12} - 2C_{44}}{C_{44}^0}} = \sqrt{\frac{3}{700}} (1 - A) \frac{C_{11} - C_{12}}{C_{44}^0} \end{aligned} \quad (30)$$

676  
677  
678 In (30),  $A$  denotes a degree of elastic anisotropy for crystals of cubic symmetry  
679 defined by Zener [40, 41] as:

$$A = \frac{C_{44}}{C_{11} - C_{12}} \quad (31)$$

680  
681  
682 A comparison between the longitudinal wave attenuation coefficients is pre-  
683 sented in Figure 13 for the three materials, calculated both in 2D and in 3D.  
684 Firstly, the overall evolution of these curves are very similar for both 2D and  
685 3D cases, which validate our discussion for the only titanium. To go in more de-  
686 tail, in the Rayleigh region, both anisotropy and inhomogeneity degrees  $A$  and  
687  $\epsilon_L$  have an insignificant effect on the attenuation coefficient. Maybe a higher  
688 anisotropy degree  $A$  leads to a slightly higher attenuation of the longitudinal  
689 wave. This is consistent with our conclusion that the Rayleigh scattering de-  
690 pends on the grain volume, involving all space directions, so the anisotropy  
691 degree of crystallite is the pertinent parameter to consider. On another hand,  
692 in the stochastic region, the higher the inhomogeneity degree  $\epsilon_L$ , the higher  
693 the longitudinal attenuation level. This was expected taking into account de-  
694 pendency of the stochastic scattering for the longitudinal waves on the average

695 grain length along the propagation direction. So the inhomogeneity degree of  
the propagation constant significantly influences the attenuation level.

Materials	$C_{11}$ (GPa)	$C_{12}$ (GPa)	$C_{44}$ (GPa)	$A$	$\epsilon_L$ (%)	$\epsilon_T$ (%)	$\rho$ (kg/m <sup>3</sup> )
$\beta$ -titanium: Single crystallite in cubic axes	134.0	110.0	36.0	3.00	2.74	8.73	4428
$\beta$ -titanium: Voigt-averaged homogeneous medium	150.0	100.0	26.5	0	0	0	4428
Inconel600 [25]: Single crystallite in cubic axes	234.6	145.4	126.2	2.83	4.8	15.23	8260
Inconel600 [25]: Voigt-averaged homogeneous medium	300.0	112.8	93.6	0	0	0	8260
Fictitious material [33]: Single crystallite in cubic axes	237.1	149.0	107.8	2.40	3.87	10.15	8000
Fictitious material [33]: Voigt-averaged homogeneous medium	288.1	123.5	82.3	0	0	0	8000

Table III: Elastic properties for three different polycrystalline materials with cubic symmetry.

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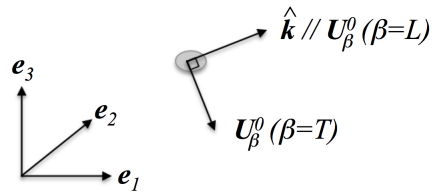


Figure 1: Sketch showing in the 3D case the unit vector of propagation direction  $\hat{\mathbf{k}}$  and the polarization vectors  $\mathbf{U}_\beta^0$  within the orthonormal basis  $\{\mathbf{e}_m\}_{m=1,\dots,3}$ .

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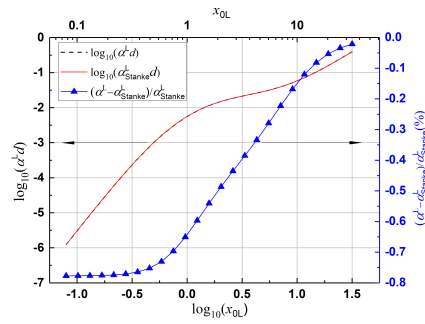


Figure 2: Comparison in 3D between the longitudinal wave attenuation coefficient  $\alpha_{\text{Stanke}}^L$  by Stanke and Kino [4] and  $\alpha^L$  calculated with the explicit formula (15).

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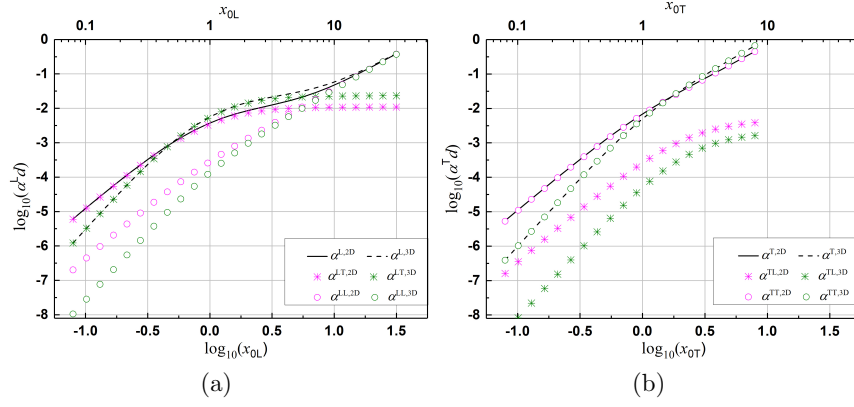


Figure 3: Evolution of  $\alpha d$  the attenuation per crystallite with respect to  $x_0$  the normalized frequency for (a) longitudinal waves and (b) transverse waves, respectively, in a  $\beta$ -titanium polycrystal: comparison between 2D and 3D calculations, and contribution of the scattering modes to the attenuation.

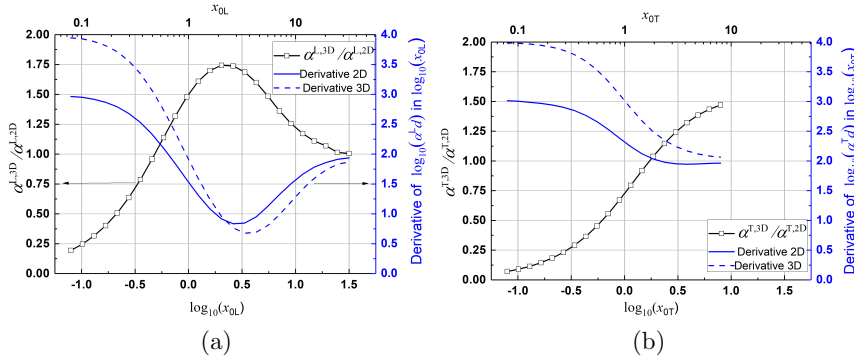


Figure 4: Evolution of the ratio of attenuation coefficients calculated in 3D and 2D (left axis in black) and the derivative of  $\log_{10}(\alpha d)$  w.r.t.  $\log_{10}(x_0)$ , *i.e.* the exponent  $n$  value (right axis in blue), for (a) longitudinal waves and (b) transverse waves, respectively, in a  $\beta$ -titanium polycrystal.

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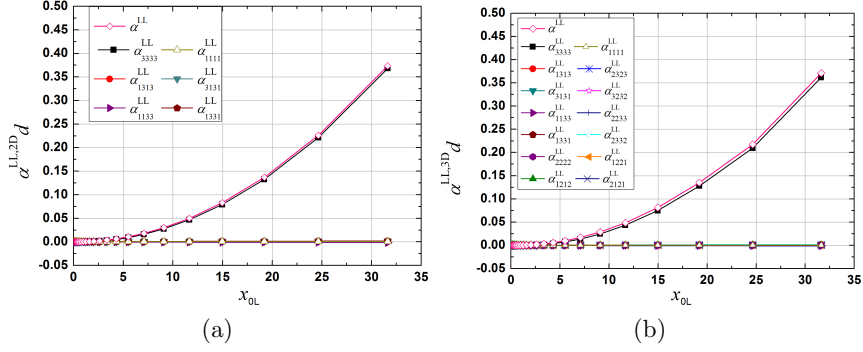


Figure 5: Evolution of the longitudinal-to-longitudinal wave scattering-induced attenuation,  $\alpha_{klmn}^{LL}$ , w.r.t. the normalized frequency in (a) 2D and (b) 3D case.

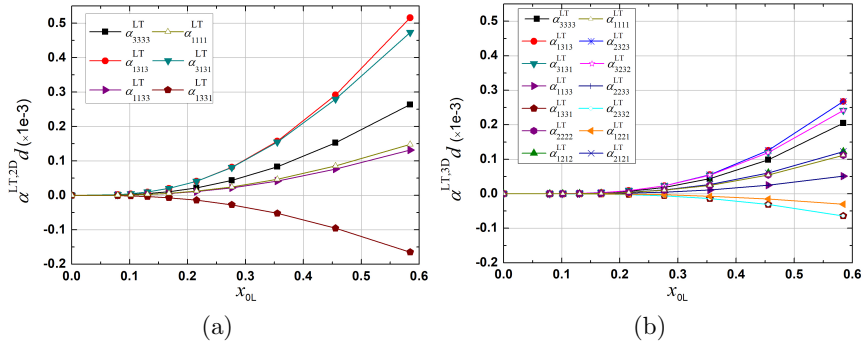


Figure 6: Evolution of the longitudinal-to-transverse wave scattering-induced attenuation,  $\alpha_{klmn}^{LT}$ , w.r.t. the normalized frequency in (a) 2D and (b) 3D case.

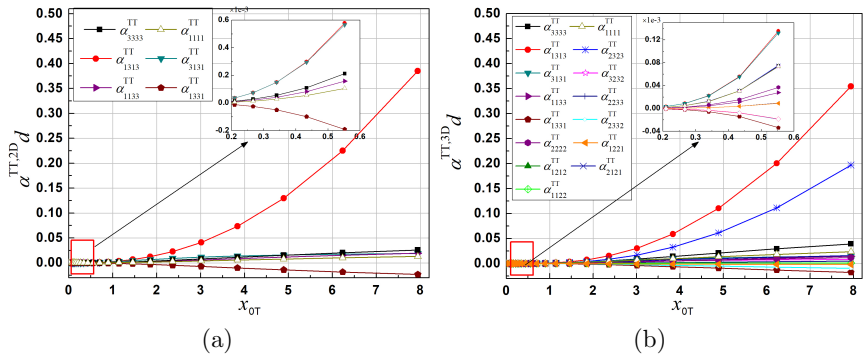


Figure 7: Evolution of the transverse-to-transverse wave scattering-induced attenuation,  $\alpha_{klmn}^{TT}$ , w.r.t. the normalized frequency in (a) 2D and (b) 3D case, with furthermore an enlarged view at low frequencies in the Rayleigh region  $x_{OT} \in [0.2, 0.6]$ .

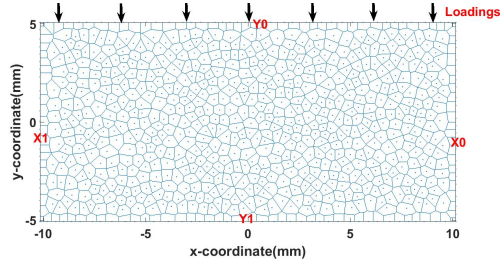


Figure 8: Illustration of the 2D FE model with a Voronoi-type polycrystalline microstructure.

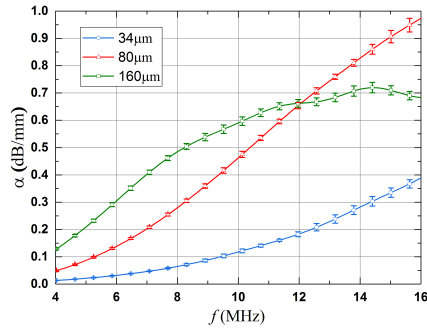


Figure 9: Standard deviation (bars) and mean (solid circles) estimations of the attenuation coefficient versus frequency for a longitudinal wave in a  $\beta$ -titanium polycrystal with three different grain sizes.

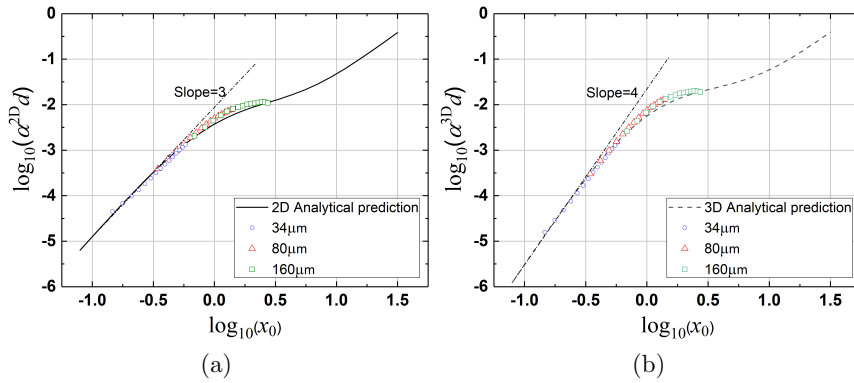


Figure 10: Numerical estimations for normalized attenuation coefficient versus normalized frequency using logarithmic scales,  $\log_{10}(\alpha d)$  vs.  $\log_{10}(x_0)$ , for a longitudinal wave in a  $\beta$ -titanium polycrystal with three different grain sizes: (a) the 2D results and (b) the deduced 3D results based on the ratio of analytical attenuation between 2D and 3D models  $\alpha^{3D}/\alpha^{2D}$ , compared to the analytical predictions.

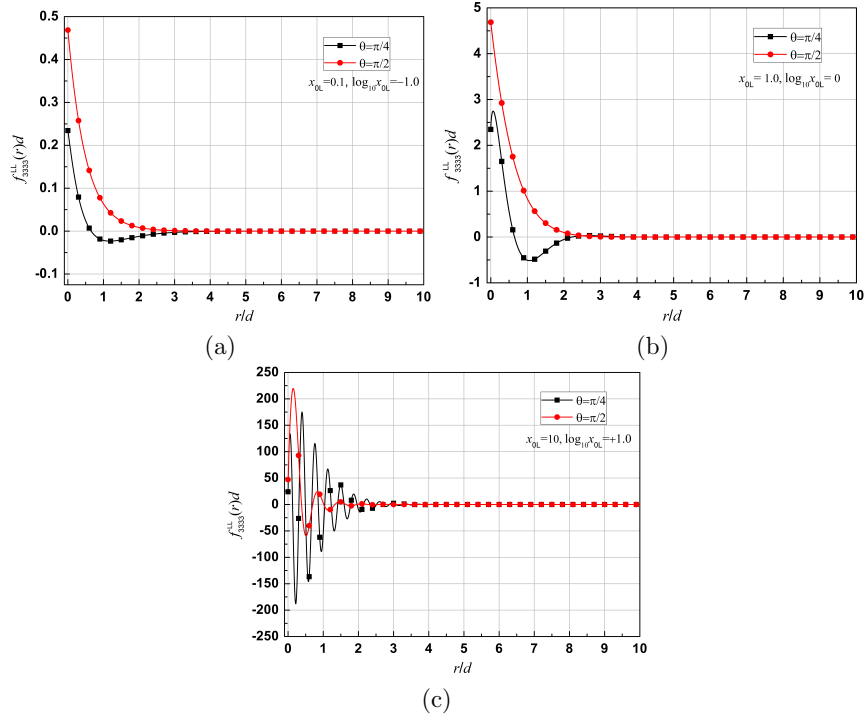


Figure 11: In the 2D case, normalized integrand function  $f_{3333}^{LL}d$  as a function of the normalized integrand variable  $r/d$  in Eq.(25) at three different normalized frequencies (a)  $x_{0L} = 0.1$ , (b)  $x_{0L} = 1.0$ , and (c)  $x_{0L} = 10$  for the grain size of  $d = 80\mu\text{m}$ , with  $f_{3333}^{LL} \equiv \text{Im} \left( \frac{k_{0\beta} \langle \delta C_{3333} \delta C_{3333} \rangle}{2C_{3333}^0} r G_{33}^L(r, \theta) D_{33}^L(r, \theta) \right)$  and for  $\theta = \pi/4, \pi/2$ .

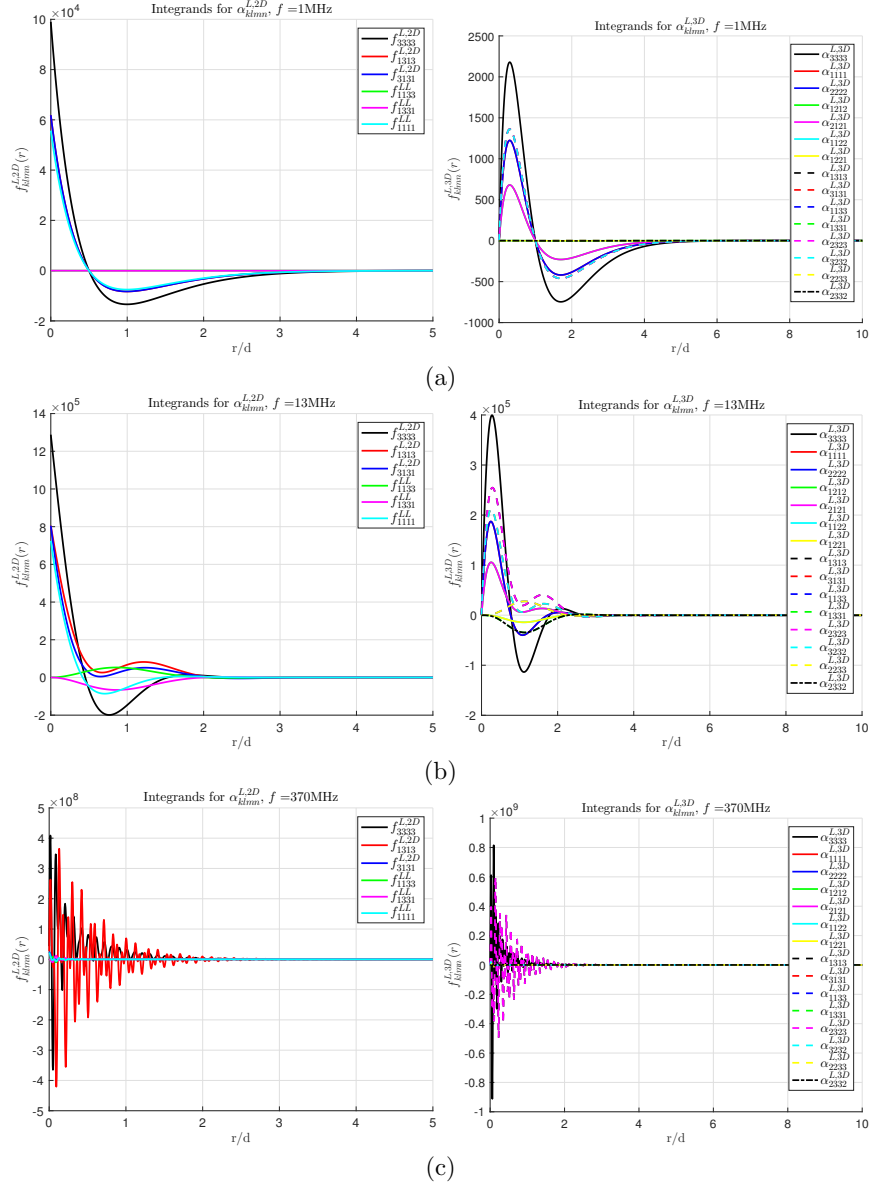


Figure 12: Integrands  $f_{klmn}^L(r) = f_{klmn}^{LL}(r) + f_{klmn}^{LT}(r)$ , defined in (25) and after analytical integration with respect to  $\theta$  in 2D and to  $(\theta, \varphi)$  in 3D, plotted at three different frequencies  $f =$  (a) 1MHz ( $x_0 = 0.08$ ), (b) 13MHz ( $x_0 = 1.0$ ), and (c) 370MHz ( $x_0 = 32.2$ ) for the grain size of  $d = 80\mu\text{m}$ , with  $f_{klmn}^L \equiv \text{Im} \left( \frac{k_{0\beta} \delta C_{33kl} \delta C_{mn33}}{2C_{3333}^0} \frac{1}{4\pi\rho\omega^2} (\eta_{kmln}^{LL} + \eta_{kmln}^{LT}) \right)$

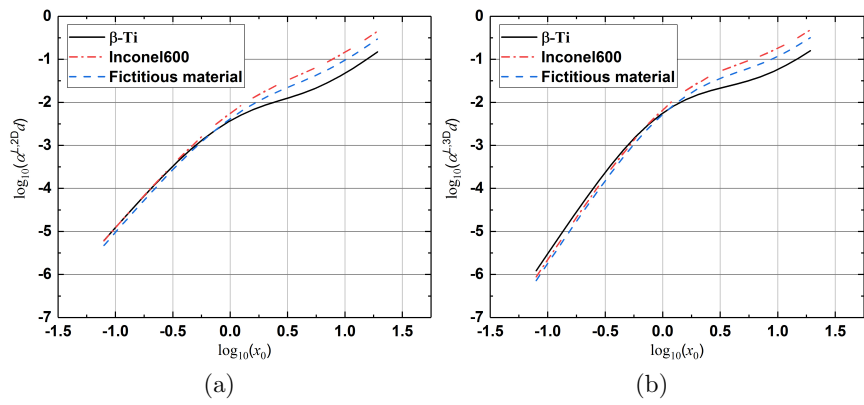


Figure 13: Comparison of the longitudinal wave attenuation coefficient between three materials for both (a) 2D and (b) 3D cases