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**National Seminar of ISNT**
**Chennai, 5. – 7. 12. 2002**
**www.nde2002.org**

# Ultrasonic attenuation and backscattering in polycrystalline materials with nonspherical grains

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**Abstract:** An ultrasonic wave propagating through a microscopically inhomogeneous medium, such as polycrystalline materials, is subject to scattering at the grain boundaries as well as other inhomogenities. The fraction of energy removed from the incident wave is responsible for important phenomenon like attenuation, dispersion, and background “noise" associated with a given ultrasonic inspection system. Quantitative knowledge of attenuation, phase velocity, and scattered wave field are extremely important for a reliable nondestructive evaluation of such materials. Expected propagation characteristics of ultrasonic waves in randomly oriented equiaxed grains are fairly well understood. But when the grains are elongated and/or preferentially oriented, the wave propagation constants exhibit anisotropic behavior. The present paper sheds more light on the effect of grain shape on the attenuation and dispersion of ultrasonic waves in polycrystals. Specifically, theoretical results are presented showing the effects of different grain aspect ratios. It is observed that for the same effective grain volume, grain elongation has smaller effect on attenuation. Although considerable attention has been given to the understanding of mean propagation characteristics of an ultrasonic beam, until recently, there have been relatively little efforts devoted towards rigorous treatments of backscattered signals from the material microstructure. In this paper, we also attempt to include some degree of multiple scattering in the calculation of the backscattered signals by developing a formalism that relates mean wave propagation characteristics to the noise.

## INTRODUCTION

A polycrystalline material is composed of numerous discrete grains, each having a regular, crystalline atomic structure. The elastic properties of the grains are anisotropic and their crystallographic axes are oriented differently. When an acoustic wave propagates through such a polycrystalline aggregate, it is attenuated by scattering at the grain boundaries, with the value of this attenuation and the related shift in the propagation velocity depending on the size, shape, orientation distributions, and crystalline anisotropy of the grains. If the grains are equiaxed and randomly oriented, these propagation properties are independent of direction, but such is not the case when the grains are elongated and/or have preferred crystallographic orientation. Therefore, reliable ultrasonic testing of engineering alloy components require the knowledge of the anisotropies in the attenuation and velocities of ultrasonic waves due to preferred grain orientations and elongated shapes.

The propagation of elastic waves in randomly oriented, equiaxed polycrystals has received considerable attention, with most recent contributions for the cubic materials being made by Hirsekorn [1,2] Stanke and Kino [3,4], Beltzer and Brauner [5], and Turner [6]. Stanke and Kino present their ``unified theory" based on the second order Keller approximation [7] and the use of a geometric autocorrelation function to describe the grain size distribution. Stanke and Kino argue that their approach is to be preferred because i) the unified theory more fully treats multiple scattering, ii) the unified theory avoids the high frequency oscillations which are coherent artifacts of the single-sized, spherical grains assumed by Hirsekorn, and iii) the unified theory correctly captures the high frequency “geometric regime” in which the Born approximation breaks down. The theoretical treatment of ultrasonic wave propagation in preferentially oriented grains is more limited. Hirsekorn has extended her theory to the case of preferred crystallographic orientation while retaining the assumption of spherical grain shape [8], and has performed numerical calculations for the case of stainless steel with fully aligned [001] axes [9]. Turner, on the other hand, derives the Dyson equation using anisotropic Green's functions to predict the mean ultrasonic field in macroscopically anisotropic medium [6]. He then proceeds to obtain the solution of the Dyson equation for the case of equiaxed grains with aligned [001] axes.

Previously we have employed the formalism of Stanke and Kino [3,4] in [001] aligned stainless steel polycrystal to compute the mean attenuation and phase velocity of plane ultrasonic waves [10,11]. In this paper we revisit our earlier calculations for the case of elongated grains and focus our attention on the effect of grain shape on the mean propagation characteristics. Specifically, we consider two cases: 1) the [001] crystallographic axes are aligned with the *z*-axis of the laboratory coordinate system while remaining two axes are randomly oriented and 2) all the crystallographic axes are randomly oriented. In both cases, the crystallites have cubic symmetry and the grains are considered to be ellipsoidal with either their major or minor axis parallel to the *z*-direction of the laboratory coordinate system. Numerical results for the attenuation and phase velocity of longitudinal wave in these two polycrystals are presented here. The material properties of the two media are listed in Table 1.

Until recently, there have been fewer attempts to develop rigorous expressions for backscattered signals. Margetan et. al. [21] formulated backscattered power using independent scatterer approximation. More recently, Rose [22] has developed a general formalism, based on Auld's [23] electro-mechanical reciprocity relations. Since this formalism is basically intractable, he then proceeded with the relevant calculations using Born and the single scattering approximations. We have, in the past [24], employed Rose's formalism to calculate the backscattered power due to preferentially oriented spherical and nonspherical grains. In this paper, we describe a formalism that accounts for some degree of multiple scattering in the calculation of the backscattered signals. Computed results for the cases of randomly oriented equiaxed and elongated grains are also presented in this paper.

Table 1. Material Properties

| Material | $c_{11}$ $(N/m^2)$ | $c_{12}$ $(N/m^2)$ | $c_{44}$ $(N/m^2)$ | $\rho$ $(kg/m^3)$ |
|---|---|---|---|---|
| Iron | $21.6 \times 10^{10}$ | $14.5 \times 10^{10}$ | $12.9 \times 10^{10}$ | $7.86 \times 10^3$ |

## THEORY

### Mean wave propagation

The displacement field due to an ultrasonic wave propagating in a polycrystalline material can be described by the stochastic wave equation

$$[C^{\xi}{}_{ijkl}(\vec{r})u^{\xi}{}_{kl}(\vec{r})]_{,j} + \rho^{\xi}(\vec{r})\omega^2 u^{\xi}{}_i(\vec{r}) = 0\,, \tag{1}$$

where $C^{\xi}{}_{ijkl}(\vec{r})$ is the actual local elastic tensor, $\rho^{\xi}(\vec{r})$ is the actual local density, and $u^{\xi}{}_i(\vec{r})$ is the actual displacement field in the medium ξ. The set of elastic tensors and the probability density function $p(\xi)$, which is the probability of choosing any particular medium, form a stochastic process. In a medium with no density variation, the application of the unified theory of Stanke and Kino [3] to the wave equation yields the generalized following Christoffel's equation for the expected propagation constant *k*.

$$[\Gamma_{ik} - \rho\omega^2 / k^2 \delta_{ik}] = \vec{0} \tag{2a}$$

where

$$\begin{aligned}\Gamma_{ik} = \hat{k}_j \hat{k}_l \{C^{o}{}_{ijkl} + \varepsilon < \Delta_{ijkl} > + \varepsilon^2 [< \Delta_{ij\alpha\beta}\Delta_{\gamma\delta kl} > - < \Delta_{ij\alpha\beta} >< \Delta_{\gamma\delta kl} >] \\ \int G_{\alpha\gamma}(\vec{s})[W(\vec{s})e^{ik\vec{s}.\hat{k}}]_{,\beta\delta} d^3\vec{s}\},\end{aligned} \tag{2b}$$

$\varepsilon\Delta_{ijkl} = C_{ijkl}(\vec{r}) - C^{o}{}_{ijkl,}$ $G_{\alpha\gamma}(\vec{s})$ is a Green's function taken from the work of Lifshits and Parkhamovski [14], $C^{o}{}_{ijkl}$ are the Voigt [15] averaged elastic constants, and $W(\vec{s})$ represents the geometric autocorrelation function (the probability that two points, placed randomly in the material and separated by a displacement $\vec{s}$, fall in the same crystallite). Equation (2) describes the expected propagation constant $k$ of plane waves of the form $< u_i >= a\hat{u}e^{-ik\hat{k}.\vec{r}-i\omega t}$, where ω is the angular frequency and $\vec{k} = k\hat{k}$ is the propagation vector in the direction of propagation $\hat{k}$. *k* is related to phase velocity $v_p$ and attenuation coefficient α through the relationship $k = \omega / v_p - i\alpha$.

Equation (2) admits solutions for $\hat{u}$ only if the determinant of the matrix in brackets on the left-hand side vanishes. In the absence of scattering, these occur for three distinct real values of $\omega^2 / k^2$; one for each of the two quasi-shear waves and one for the quasi-longitudinal wave. In the presence of scattering, requiring the determinant to vanish defines a transcendental equation which may support many roots. The correct root was selected by seeking the real part of the root closest to the root in the absence of scattering and requiring that the imaginary part $\alpha \geq 0$. The wave polarizations are given by the corresponding eigenvectors.

## Particular Case for Calculations

We have extended our previous calculations [10] for polycrystals of cubic symmetry to accommodate grain elongation in the *z*-direction. Generalizing on Stanke and Kino [3], the geometric autocorrelation function $W(\vec{s})$ is assumed to have the form [14]

$$W(\vec{s}) = e^{-2/d\sqrt{1+(d^2/h^2-1)\cos^2\theta}} \tag{3}$$

where *d* is the mean grain diameter in the plane perpendicular to the *z*-axis, *h* is the grain height along the *z*-direction, and θ is the angle measured with respect to the *z*-axis. Stanke and Kino pointed out the suitability of this choice when $d = h$ for real materials [4] and have used it in a previous publication [6,15]. It is to be noted that small values of *d/h* correspond to elongated (cigar shaped) grains, while large values correspond to flattened (pancake shaped) grains. As mentioned before, we shall present our calculations for expected propagation constants in polycrystalline materials with or without macroscopic texture. The particular texture considered in this work has the [001] crystallographic axes of all grains parallel to the *z*-axis of the laboratory coordinate system while the [100] and the [010] axes are randomly oriented about this direction. This simplifies the averaging procedure. Thus, if φ is the rotation of the [100] axis from the *x*-axis in the laboratory system,

$$< f > = \frac{1}{2\pi}\int_0^{2\pi} f(\phi)d\phi \tag{4}$$

Following the general procedure to obtain the complex propagations constants and polarizations as described before, we were able to develop an integral equation for the expected propagation constant for elastic waves propagating along arbitrary directions in the *yz*-plane. In order to do this, it was found convenient to rotate the laboratory coordinate system (*x, y, z*) by an angle θ about the *x*-axis resulting in a primed (*x'*=*x, y', z'*) coordinate system and choose the $z'$-axis (direction 3) as the propagation direction. Waves with arbitrary propagation direction are, in general, not purely longitudinal or shear in a medium with macroscopic texture. However, for cubic crystals with small single crystal anisotropy $A = c_{11} - c_{12} - 2c_{44}$ compared to $C^o{}_{ijkl}$, the deviations of the polarizations from those of pure modes are not expected to be large. Therefore, we have neglected the deviation of the polarizations from the pure mode values in the polycrystalline aggregate under consideration. With this assumption, we only need the averages $\varepsilon < \Delta_{3333} >$ and $\varepsilon^2[< \Delta_{33kl}\Delta_{mn33} > - < \Delta_{33kl} >< \Delta_{mn33} >]$.

## **Backscattered Ultrasonic Power**

The displacement field $u_i$ associated with time-harmonic elastic wave with angular frequency ω in a particular medium is given by

$$[C_{ijkl}(\vec{r})u_{kl}(\vec{r})]_{,j} + \rho(\vec{r})\omega^2 u_i(\vec{r}) = 0\,, \tag{5}$$

where $C_{ijkl}(\vec{r})$ is the actual local elastic tensor, $\rho(\vec{r})$ is the actual local density, and $u_i(\vec{r})$ is the actual displacement field. We decompose the elastic constants and the displacement field in the following way

$$C_{ijkl}(\vec{r}) = C^o{}_{ijkl}(\omega) + \delta C_{ijkl}(\vec{r}) \tag{6}$$

$$u_i(\vec{r}) = < u_i > + \delta u_i(\vec{r}) \tag{7}$$

where $C^o{}_{ijkl}(\omega)$ are frequency dependent "expected" elastic constants prescribed by some "suitable" theory and $\delta u_i(\vec{r})$ is the fluctuation of the particle displacement relative to the mean value $< u_i >$ in a statistically independent homogeneous medium. Obviously, the expected field $< u_i >$ satisfies the following wave equation in a constant density medium.

$$C^o{}_{ijkl} < u_{kl} >_{,jl} + \rho\omega^2 < u_i > = 0 \tag{8}$$

Application of the decomposition specified in Equations (6) and (7) to equation (5) yields the following equation for the fluctuation field $\delta u_i(\vec{r})$.

$$C^o{}_{ijkl}\delta u_{k,jl}(\vec{r}) + \rho\omega^2 \delta u_i(\vec{r}) = -[\delta C_{ijkl}(\vec{r})\{\frac{\partial < u_k >}{\partial x_l} + \frac{\partial(\delta u_k)}{\partial x_l}\}]_{,j} \tag{9}$$

Equation (9) is intractable since the source term on the right hand side also contains the unknown $\delta u_i(\vec{r})$. One can, however, seek an iterative solution. This is the approach we follow here. In an unbounded region, the first order iterative solution can then be written as

$$\delta u_i(\vec{r}) = -\int_v G_{im}(\vec{r} - \vec{r}\,')[\delta C_{mjkl}(\vec{r}\,') < u_k >_{,l'}]_{,j'} d^3\vec{r}\,' \tag{10}$$

where $G_{im}(\vec{r} - \vec{r}\,')$ is the Green's function for the average medium and the primed subscripts indicating differentiation with respect to the primed coordinate system. For mean plane waves of the form $< u_i > = a\hat{u}e^{-ik\hat{k}.\vec{r} - i\omega t}$, application of Green's divergence theorem to the foregoing equation yields

$$\delta u_i(\vec{r}) = -ik\hat{u}_k\hat{k}_l \int_v G_{im,j'}(\vec{r} - \vec{r}\,')\delta C_{mjkl}(\vec{r}\,')e^{-i\vec{k}.\vec{r}\,'} d^3\vec{r}\,' \tag{11}$$

The expected scattered power in a statistically homogeneous medium is then given by

$$< \delta u_i \delta u_p{}^* >= \hat{u}_k \hat{u}_\gamma \hat{k}_l \hat{k}_\delta k k^* < \delta C_{mjkl} \delta C_{q\alpha\gamma\delta} > \\ \int_v G_{im,j'}(\vec{r}-\vec{r}\,')[\int_v G^*{}_{pq,\alpha''} W(\vec{r}-\vec{r}\,'') e^{i\vec{k}^*.\vec{r}\,''} d^3\vec{r}\,''] e^{-i\vec{k}.\vec{r}\,'} d^3\vec{r}\,' \tag{12}$$

Here $W(\vec{r}\,'-\vec{r}\,'')$ represents the probability that two points, placed randomly in the material and separated by a displacement $\vec{r}\,'-\vec{r}\,''$ fall in the same crystallite and the superscript * represent complex conjugate.

Simplified Calculation

We have simplified the evaluation of backscattered signals indicated by Equation (12) by considering a polycrystal with randomly oriented and weakly scattering equiaxed grains. This allows us, at low frequencies, to employ the independent scatterer approximation. Following the approach of Gubernatis et. al. [25], the scattered field at $\vec{r}$ when $|\vec{r}-\vec{r}\,'|$ is large, is written as

$$\delta u_i(\vec{r}) = \frac{e^{i\alpha r}}{r} A_i + \frac{e^{i\beta r}}{r} B_i\,, \tag{13}$$

where the vectors $A_i$ and $B_i$ are called the scattering amplitudes and α and β are the longitudinal and the transverse wave numbers, respectively, in the average attenuative medium. We choose this average medium to be described by the unified theory of Stanke and Kino. That is the complex $C^o{}_{ijkl}(\omega)$ is given by

$$C^o{}_{ijkl}(\omega) = \overline{C}_{ijkl} + \varepsilon < \Delta_{ijkl} > + \varepsilon^2 [< \Delta_{ij\alpha\beta} \Delta_{\gamma\delta kl} > - < \Delta_{ij\alpha\beta} >< \Delta_{\gamma\delta kl} >] \times \\ \int G_{\alpha\gamma}(\vec{r}) \{W(\vec{r}) e^{i\vec{k}.\vec{r}}\}_{,\beta\delta} d^3\vec{r}, \tag{14}$$

where $\overline{C}_{ijkl}$ represent the Voigt averaged elastic constants. After some required manipulation, the expected backscattered power for a longitudinal wave propagating in the 3-direction can be written as

$$< A_3 A_3{}^* >= \frac{\alpha^4 (\alpha^4)^*}{(4\pi\rho\omega^2)^2} < \delta C_{3333} \delta C^*{}_{3333} > S(2\alpha) S^*(2\alpha)\,. \tag{15}$$

In the above equation, $S(2\alpha) = \int_v e^{i2\vec{\alpha}.\vec{r}} d^3\vec{r}$ is the shape factor of an individual grain. We define the backscatter coefficient as

$$\eta = N < A_3 A_3{}^* >^{1/2}, \tag{16}$$

where *N* is the number of grains per unit volume insonified by the incident ultrasonic wave.

## RESULTS

## Mean Propagation Constants for L-waves

To obtain the attenuation per wavelength $\alpha / k_{ol}$ and the normalized shift in phase velocity $(v_l - v_{ol})/v_{ol}$ for plane waves in the considered textured medium, the integral equation for the expected propagation constants, Equation (2), was solved numerically. Here and in what follows, $v_o$ and $k_o$ refer to phase velocity and wave number, respectively, based on Voigt averaged elastic constants in the absence of preferred grain orientation. The subscript 'l' associated with the Voigt averaged quantity refer to *L*-waves and $v_{mean}$ refers to mean grain volume. In the process, the single crystal elastic constants used for stainless steel [13] are listed in Table 1.

Directional dependence of the normalized attenuation coefficient of *L*-waves propagating at an angle φ relative to the axis of rotational symmetry (*z*-axis) for $k_{ol}(v_{mean})^{1/3} = 1$ is shown in Fig. 1. It is seen that when ultrasonic wave propagates along the preferred direction, there is no attenuation at all. This is to be expected since the wave propagating in this direction does not see any acoustic mismatch from grain to grain. As φ increases from 0 degree to 90 degrees, the attenuation monotonously increases. However, it is to be noted that the grain elongation affects the attenuation in a more complex way. Figure 2 shows the directional dependence of the normalized variation of phase velocity for $k_{ol}(v_{mean})^{1/3} = 1$ and for five different grain aspect ratios. Grain shape is seen to have no effect on phase velocity when $\varphi \le 45^\circ$. For $\varphi > 45^\circ$, grain shape again affects the phase velocity in a complex way.

Fig. 3 shows the dependence of the normalized attenuation coefficient $\alpha / k_{ol}$ for *L*-waves in untextured iron on the normalized frequency $k_{ol}(v_{mean})^{1/3}$ for different grain aspect ratios *d/h*. At very low frequencies ( Rayleigh frequency regime), for the same mean grain volume, attenuation per wavelength is hardly affected by grain elongation. Careful observation of Fig. 4 however reveals that elongation in the direction perpendicular to the wave propagation direction causes slightly greater attenuation. It is also seen that in the stochastic region where $k_{ol}(v_{mean})^{1/3} = O(1)$, deviation from the non-spherical shape of the grains decreases the attenuation. Looking back at Fig. 3, we observe that grain elongation delays the transition to the "geometric" frequency regime where attenuation varies inversely as $(v_{mean})^{1/3}$. It is clear that in the "stochastic-geometric" transition regime, slender grains cause more attenuation than the more flattened grains. This is consistent with the intuitive notion that when ultrasonic waves behave as rays, slender grains having more projected area, remove more energy from the beam through reflection at the grain boundaries.

In Fig. 5, we have plotted the normalized shift in phase velocity $(v_l - v_{ol})/v_{ol}$ in texture free iron against the normalized frequency $k_{ol}(v_{mean})^{1/3}$ for *L*-waves with *d/h* as a parameter. In this case we observe that, at low frequencies, the acoustic wave becomes increasingly dispersive with grain elongation. In the entire frequency regime considered here, it is observed that grains flattened in the direction of mean propagating wave are less dispersive. The complicated behavior of the phase velocities for different grain shapes when $k_{ol}(v_{mean})^{1/3} \geq 10$ is believed to be associated with differing "Rayleigh-stochastic-geometric" transition regimes.

## <u>Backscatter Coefficient for L-waves</u>

Using Equation (16), we have calculated the backscattered coefficient for ultrasonic wave propagation in texture free iron with elongated grains. The material properties of the chosen medium are listed in Table 1. Figure 6 shows the frequency dependence of the computed backscatter coefficients using the averaged elastic constants extracted from the unified theory of Stanke and Kino [3]. It is seen that at low frequencies, the slender grains scatter more energy backwards than the flatter grains. For slightly higher frequencies, in the "stochastic" frequency regime, the shape dependence becomes more complicated and not completely understood by the author. Figure 7 compares the predictions based on Voigt averaged medium and the lossy expected medium. At low frequencies both the representations of the average medium yield the same result.
This is to be expected since the incident beam is not significantly scattered in the medium at these frequencies. As the normalized frequency $k_{ol}(v_{mean})^{1/3}$ increases, effects of some degree of multiple scattering begin to appear. Some of the early-time scattered signals due to the grains are further scattered back to the observation point, thereby increasing the backscatter coefficient.

## CONCLUDING REMARKS

We have applied the unified theory of Stanke and Kino [3] to determine the propagation constants in a textured polycrystalline material with elongated grains where the crystallites have cubic symmetry. We have presented computed ultrasonic wave propagation characteristics in two different mediums: 1) [001] aligned stainless steel and 2) iron with randomly oriented grains. Our numerical results show that the attenuation is largely controlled by grain volume. The predominant effect of grain shape is to alter the onsets of the "Rayleigh-stochastic" and the "stochastic-geometric" transition regimes and the extent of each of these frequency regimes. The effect of grain shape on phase velocity is also quite small.

The simple scheme to account for some degree of multiple scattering in the computation of backscatter coefficient shows promise. It must be reiterated that the formalism referred to in this paper does not restrict the calculation to be performed using independent scatterer approximation. We are currently in the process of performing more detailed evaluation of the formalism.

## ACKNOWLEDGEMENT

This work was supported by Department of Energy under Contract DE-AC 06-76RLO 1830.

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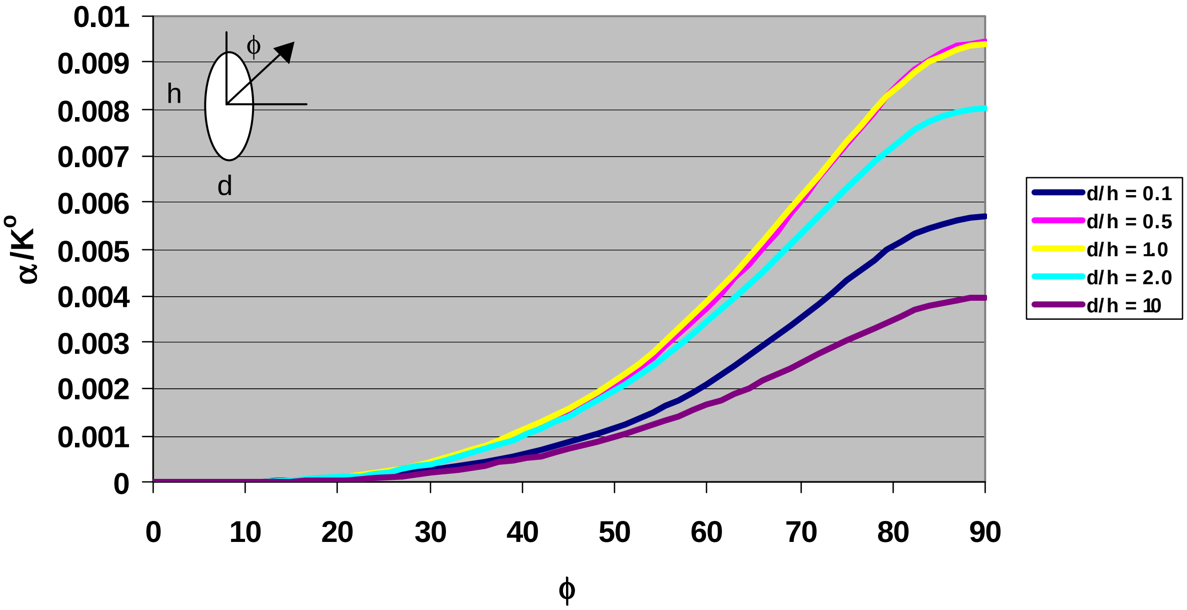


Figure1: Directional dependence of normalized attenuation in [001] aligned stainless steel; $k_{ol}(v_{mean})^{1/3} = 1$.

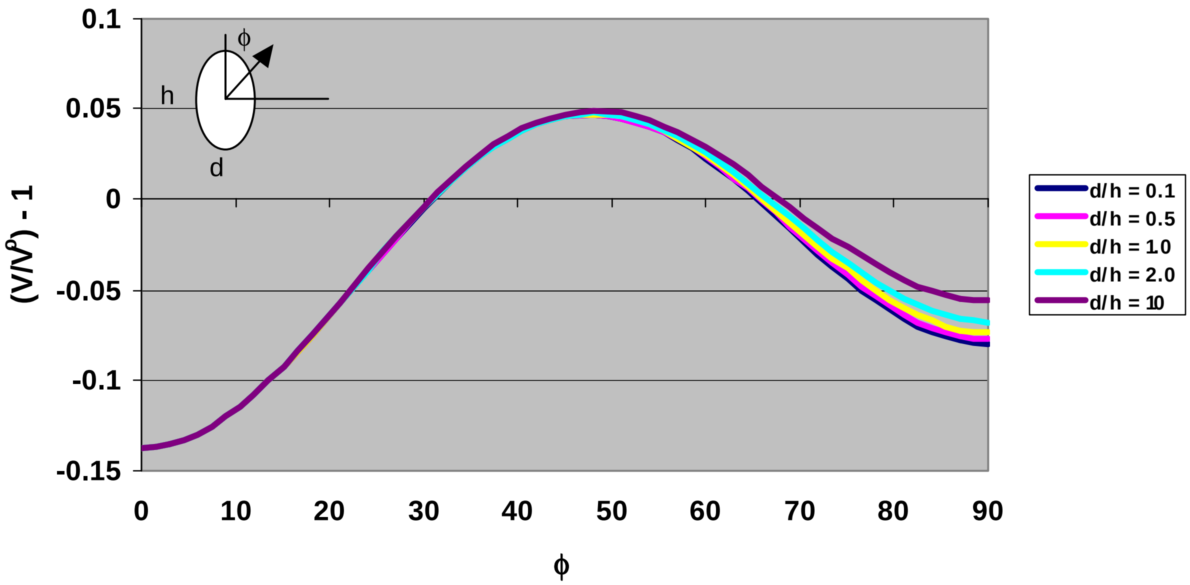


Figure 2: Directional dependence of normalized phase velocity in [001] aligned stainless steel; $k_{ol}(v_{mean})^{1/3} = 1$.

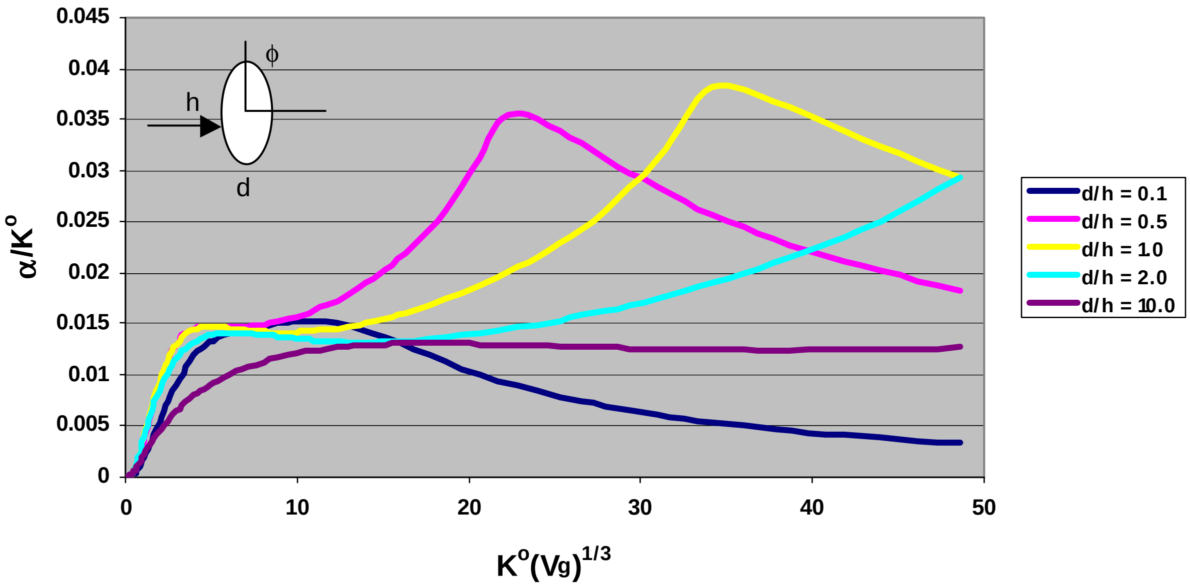


Figure 3: Frequency dependence of attenuation in untexured iron.

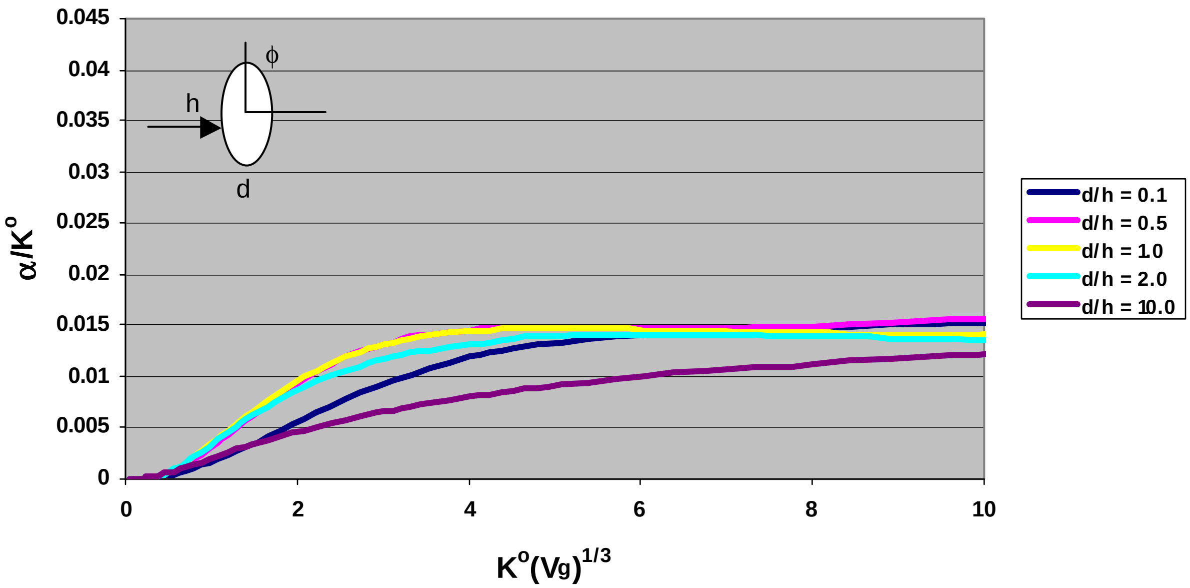


Figure 4: Frequency dependence of attenuation in untextured iron.

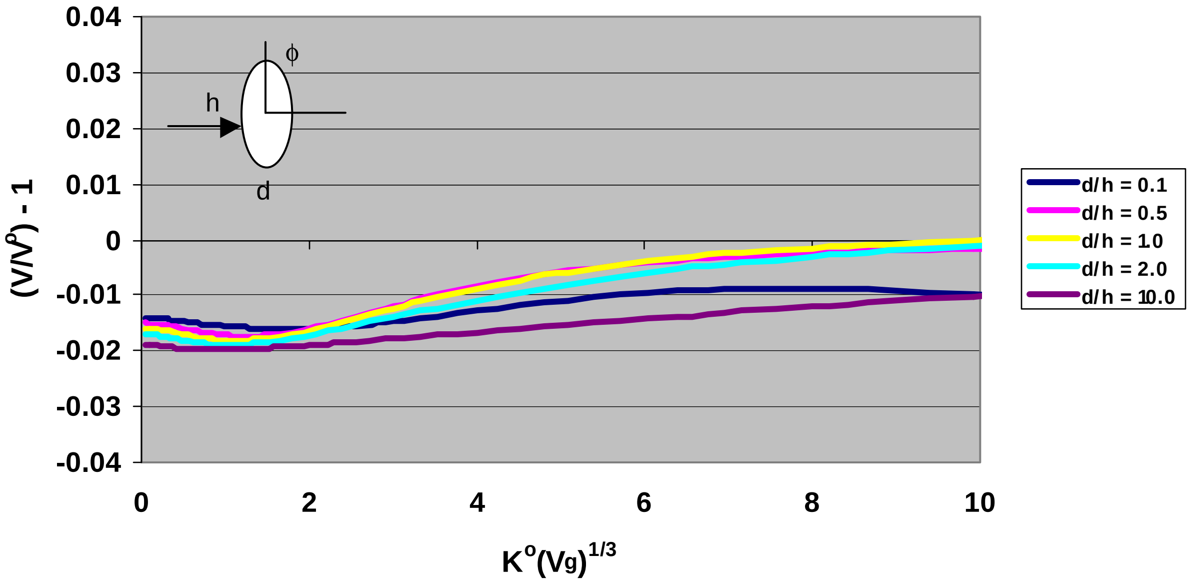


Figure 5: Frequency dependence of phase velocity in untexured iron.

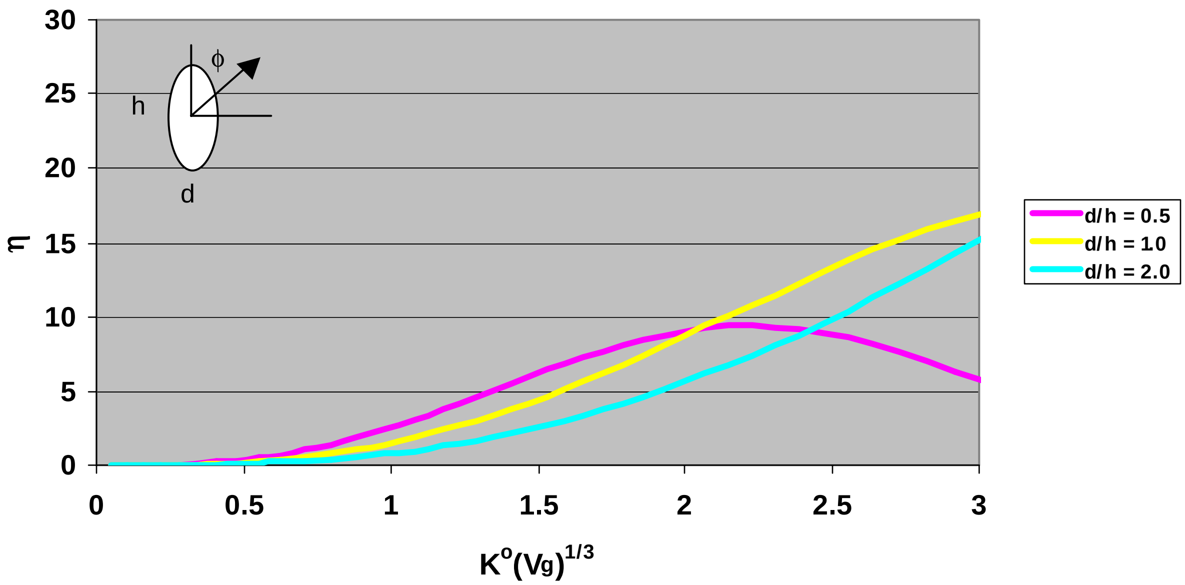


Figure 6: Frequency dependence of backscatter coefficient in untexured iron.

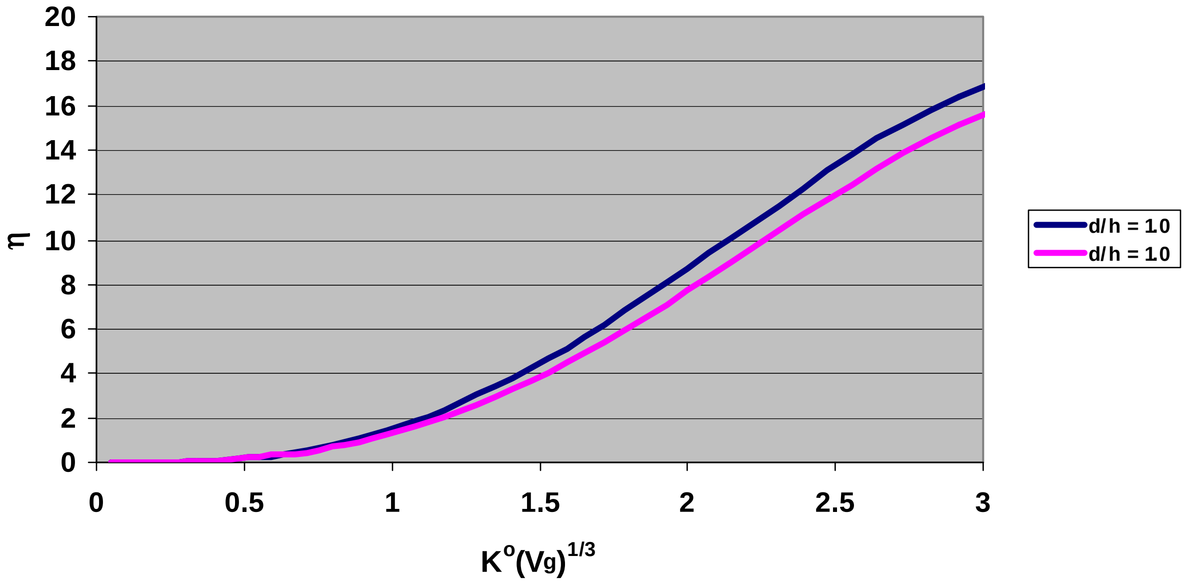


Figure 7: Comparison of backscatter predictions based on Voight averaged and "Stanke-Kino" media.