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Numerical modeling of grain size effect on the ultrasonic propagation in polycrystalline materials

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Abstract — Grain size effect on the ultrasonic propagation in single phase, untextured and equiaxed polycrystalline materials by numerical modeling is studied. Attenuation levels and backscattered noise signals are calculated in both time and frequency domains according to the response of several receivers. Coherent comparisons are obtained between our numerical results and some well-known classical theories.

Key words — Ultrasonic wave propagation, Attenuation, Backscattering, Polycrystals, Grain size

1. Introduction

The motivation for the research on the ultrasonic wave propagation in polycrystalline materials is found in nondestructive evaluation (NDE)^[1]. When ultrasonic wave propagates through polycrystalline materials, the incident energy of input signals can be scattered by the inhomogeneity of the elastic properties and the density of individual crystallites. Consequently scattered waves are generated and the wave propagation suffers from the amplitude attenuation and a phase velocity variation^[2]. The scattered signals in a given direction and the amplitude attenuation for a given wave mode can be used to obtain information on the microstructure such as the grain size or the flaws. A good understanding of how elastic waves are attenuated and backscattered by the polycrystalline microstructures is meaningful to improve the flaw inspection and the evaluation of microstructural evolution^[3]. However, the correlation between the ultrasonic propagation properties with the microstructural characteristics still remains today poorly understood and research efforts are therefore required.

The present work focuses on the analysis of grain size effect on the ultrasonic attenuation and backscattering in single phase, untextured and equiaxed polycrystalline materials by numerical modeling. Finite element models are defined for theoretical polycrystalline microstructures with randomly oriented, single sized grains. Attenuation levels and backscattered noise signals are calculated in both time and frequency domains according to the simulated response of several receivers. Numerical results for the dependence of attenuation coefficient and backscattered noise signals on the frequency and the grain size are presented, and then compared with predictions of the classical theories.

2. Classical theories of ultrasonic attenuation and backscattering

Here is presented a brief summary of some classical theories of the ultrasonic attenuation and backscattering to which the numerical results are compared.

2.1. Attenuation

The general formulation for attenuation coefficient of longitudinal wave α_l is given by the unified theory of Stanke and Kino^[4]. It is accurate to the second order of the inhomogeneity degree and applicable for single-phase, untextured, equiaxed polycrystalline materials with cubic symmetrical

crystallites and valid for time-harmonic wave in all frequency regions. According to this theory, the analytical form for attenuation in Rayleigh region for longitudinal wave reads as^[4]:

$$\alpha_l^R = \frac{1}{375} \frac{\nu^2}{(C_{11}^0)^2} \left(1 + \frac{3}{2} \frac{(v_{0l})^5}{(v_{0s})^5} \right) (k_{0l})^4 \bar{d}^3 \quad (1)$$

And in the stochastic region reads as^[4]:

$$\alpha_l^S = \frac{2}{525} \frac{\nu^2}{(C_{11}^0)^2} (k_{0l})^2 \bar{d} \quad (2)$$

Here, \bar{d} is the effective average diameter of grains, v_{0l}, v_{0s} represent the phase velocity of longitudinal and transverse wave respectively, and k_{0l} indicates the propagation constant in the equivalent homogeneous material, ν represents the invariant anisotropy factor, dependent on the elastic properties of materials.

2.2. Backscattering

Following a series of articles by J.E.Gubernatis^[1,5,6] and J.H.Rose^[2], the backscattering coefficient η is defined as the differential scattering cross section per unit volume in the backscattered direction^[7]:

$$\eta = \frac{\langle \delta C_{ijkl} \delta C_{pqrs} \rangle}{(4\pi\rho(v_{0l})^2)^2} \frac{\pi \bar{d}^3 (k_{0l})^4}{(1 + (k_{0l})^2 \bar{d}^2)^2} \quad (3)$$

Equation (3) gives the general expression for the backscattering coefficient of longitudinal wave derived from the reciprocity theorem based on the single scattering approximation and Born approximation. It is applicable for the randomly oriented, single-phase, equiaxed polycrystals without density variation. Here, δC is the variation in elastic stiffness tensor within the crystallites, ρ is the density.

3. Numerical modeling of ultrasonic wave propagation

3.1. Setting of Numerical Model

The elastodynamic equations describing the ultrasonic wave propagation in polycrystalline materials are solved by finite element methods. The geometry of the finite element model is defined as Fig.1. The blue part is a homogeneous and isotropic surrounding material; the red part is an untextured, single-phase polycrystalline microstructure with single-size regular hexagonal cubic symmetric crystallites without density variation. A random distribution of crystallographic orientations is set up, so the studied polycrystalline material can be considered as macroscopically uniform and isotropic and its equivalent homogenized isotropic material served as the reference material. Several grain sizes and different random distributions of crystallographic orientation for each size are considered to analyze the propagation characteristics of a longitudinal wave in terms of attenuation and backscattered noise levels in both time and frequency domains.

There are 11 transmitters on the top side and 11 receivers inside which are located 2.0 mm away from the top side, with horizontal distance between two adjacent transmitters or receivers equal to 0.28 mm. Two different Ricker signals^[8] with the same peak amplitude are applied on the emitter line, whose central peak frequencies are 5 MHz and 10 MHz respectively. To reduce the effect of transverse wave, the peak amplitude of Ricker signals on the emitter line is multiplied by a Gaussian

type apodization function, which decreases the peak amplitudes of input signals smoothly down to zero at the edges of emitters lines.

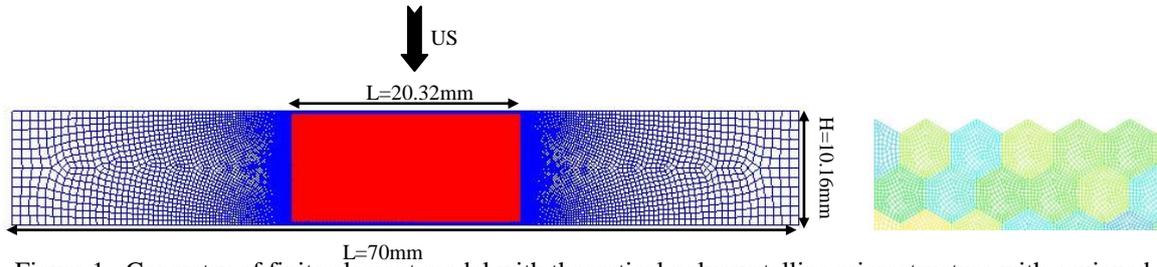


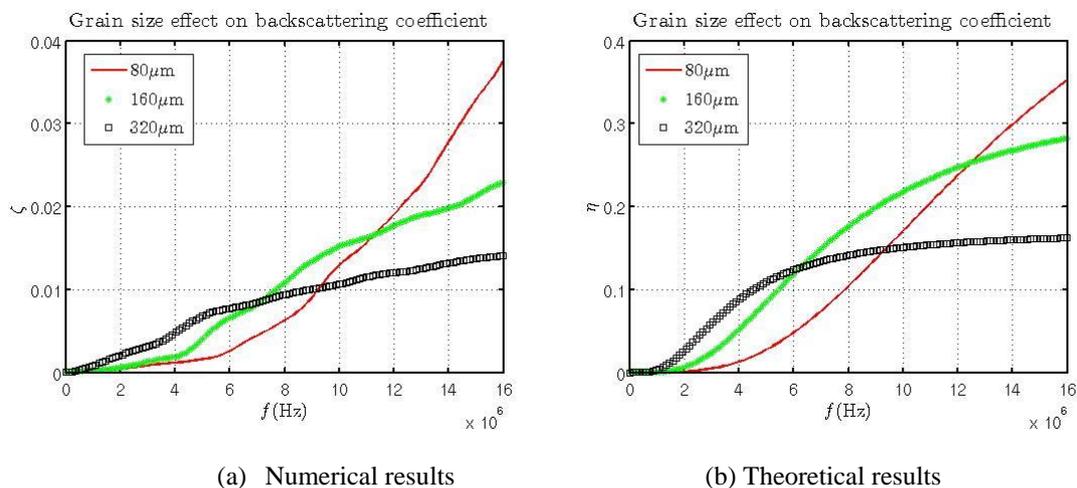
Figure 1 –Geometry of finite element model with theoretical polycrystalline microstructure with equiaxed hexagonal grains

3.2. Numerical measurement of attenuation and backscattering

Vertical displacements in the ultrasound inspection direction are recorded numerically in time domain at the transmitters and receivers. The longitudinal attenuation is evaluated as the ratio of reflected signal power to incident signal power in time domain or in frequency domain using Fourier transform. As for the level of backscattered noise $\zeta(f)$, it is calculated as the ratio between the spectral powers of the backscattered noises to the incident signals, accumulated for the frequency domain $[0, f]$.

4. Numerical investigation of grain size effects

Due to space of the article, only the numerical result about the grain size effect on the backscattering noise levels is presented here. As shown in Fig.2 (a), the backscattering level $\zeta(f)$ is influenced greatly by the ratio between the grain size and the wavelength. Indeed, larger grain size backscatters more energy in low frequency region and smaller grain size shows larger backscattering in high frequency region. For a given grain size, the backscattering increases rapidly in Rayleigh region and then gradually increases to a plateau in stochastic region, which can be observed for the large grain size in the studied frequency region (shown as the curve corresponding to the grain size equal to $320 \mu\text{m}$ in Fig. 2). Compared with the analytical results^[7] (Fig.2 (b)), coherent variation tendencies for the grain size effect and frequency influence on the backscattering are obtained. However, the amplitudes are not in agreement between the theoretical and numerical results, since the present calculation uses the ultrasonic wave characteristics recorded only at several receivers inside the materials, rather than in the whole sample.



(a) Numerical results (b) Theoretical results
Figure 2 –Grain size effect on the backscattering coefficient

Besides, the effect of grain size and frequency on the longitudinal attenuation is analyzed in detail: the attenuation coefficient for longitudinal waves due to scattering increases with the increase of grain size in Rayleigh region and the characteristic hump during the transition region from Rayleigh to stochastic is observed. Compared with the existing classical theory, a good agreement is found in terms of the variation tendency of the curves. Moreover, the simulations with microstructures with irregular hexagonal equiaxed grains, obtained by slightly and randomly perturbing the shape of regular hexagonal equiaxed grains while keeping the same grain area, are conducted, in order to eliminate the suspicion of possible artefacts due to regularly oriented grain boundaries. Our numerical results show that, in this case, the influence of grain boundary orientation is small on the attenuation and backscattered noise levels.

5. Conclusions

This work presents a numerical way to simulate the influence of the grain size on ultrasonic wave attenuation and backscattering as a function of the frequency. The calculation based on finite element method indicates that, for single phase, untextured and equiaxed polycrystalline materials without density variation, the attenuation coefficient for longitudinal waves due to scattering increases as the grain size increases and the backscattered noise level is controlled greatly by the ratio between the grain size and the wavelength. These numerical results are in good agreement with the previous classical theories, which indicates the validity and effectiveness of the present method for the analysis of ultrasonic attenuation and backscattered noise level of longitudinal wave. The advantage of the numerical approach is the ability to study the ultrasonic attenuation and backscattering in more complex polycrystalline materials. This is the ongoing work.

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