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Finite element modeling of grain size effects on the ultrasonic microstructural noise backscattering in polycrystalline materials

X. Bai [1], B. Tie *, J.-H. Schmitt, D. Aubry

MSSMat, CNRS, CentraleSupélec, Université Paris-Saclay, Bât. Eiffel, 8-10 Rue Joliot Curie, 91190 Gif-sur-Yvette, France

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ABSTRACT

The correlation between ultrasonic wave propagation and polycrystalline microstructures has significant implications in nondestructive evaluation. An original numerical approach using the finite element method to quantify in both time and frequency domains the ultrasonic noise scattering due to the elastic heterogeneity of polycrystalline microstructures is presented. Based on the reciprocity theorem, it allows the scattering evaluation using mechanical data recorded only on the boundary of polycrystal instead of within its volume and is applicable to any polycrystalline aggregate regardless of its crystallographic or morphological characteristics. Consequently it gives a more realistic and accurate access of polycrystalline microstructures than the classical analytical models developed under the assumption of single scattering and the Born approximation.

The numerical approach is proposed within the same unified theoretical framework as the classical analytical models, so it is possible to validate it in the cases of idealized microstructures for which the considered analytical models remain relevant. As an original result, assuming single phase, untextured and equiaxed microstructures, two-dimensional (2D) theoretical formulas are developed and a frequency-dependent coefficient is found compared to the classical three-dimensional (3D) formulas. 2D numerical simulations are then performed for idealized microstructures composed of hexagonal grains with a uniform grain-size. Three grain sizes are considered herein and involve different scattering regions. Good comparisons are obtained between theoretical and numerical estimates of the backscattering coefficient, which validate the numerical approach. Effects of the grain boundary orientations are analyzed by modeling an irregular hexagonal grain morphology and a random grain morphology generated by an established Voronoi approach. The origin of the significant oscillation level of backscattering is then investigated and discussed.

1. Introduction

The motivation for the research on the ultrasonic wave propagation in polycrystalline materials is found in nondestructive evaluation (NDE). When ultrasonic waves propagate through polycrystalline materials, the incident energy is scattered by grain boundaries due to heterogeneities of mechanical properties, such as the elastic stiffness tensor and the density. Two phenomena therefore occur: amplitude attenuations and microstructural noise signals. Important theoretical investigations have been done for the scattering induced attenuation (e.g. [1–5]). In some circumstances the NDE measurement can be restricted by uncontrolled high noise-to-signal ratio, for it is difficult or even impossible to identify echo signals of interest when their amplitudes are of the same order of magnitude as noise level. Thus efforts have been dedicated to the study of scattered noise signals in order to improve nondestructive inspection and evaluation of microstructures and of their evolution.

Theoretical developments to evaluate the scattering effectiveness are based on two seminal works:

The first one initiated by Gubernatis et al. [1] is based on a single-scattering assumption and provides the solutions of scattering amplitudes of ultrasonic waves caused by a bounded isolated scatter embedded in an infinite isotropic and homogeneous elastic medium. To obtain explicit formulas for the scattering coefficient, the Born approximation was applied and the author concluded that the theoretical formulas were valid only for frequencies below the very high frequency range, often called the geometric region [6]. Based on the same approach, further theoretical investigations were proposed by

* Corresponding author.
E-mail address: bing.tie@centralesupelec.fr (B. Tie).
[1] Present address: Laser Institute, Qilu University of Technology (Shandong Academy Of Sciences), 250103, Shandong, China.

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Han, predicting the ultrasonic backscattering in duplex microstructures composed of randomly-oriented macrograins composed of colonies with crystallographically related orientations [7].

The second method is based on the reciprocity theorem, initially used to prove the interchangeability between a source and a receiver in the electromagnetic wave and elastic wave transmission problems [8]. Kino adapted the scattering matrix defined for electromagnetic waves to elastic waves to derive scattering formulas and made a fundamental contribution to the application of the reciprocity principle to the scattering of elastic waves by flaws [9]. Finally, explicit formulas of backscattering coefficient were proposed by Rose for single-phase and macroscopically isotropic and homogeneous polycrystalline materials with the use of the Born approximation in three-dimensional cases [10].

The equivalence of both methods was proven by Rose [10] and Margetan et al. [11] with the assumption that the elastic properties of the macroscopic effective medium are defined by the unweighted Voigt average of the elastic properties of the polycrystalline microstructure and in the weak scattering case for which the use of the Born approximation is pertinent. Analytical formulas for backscattering in equiaxed polycrystals under the single-scattering assumption were developed [10] and extended to general pitch-catch configurations [11]. More recently, Ghoshal et al. developed a multiple-scattering framework using the Wigner distribution [12]. Based on this multiple-scattering framework, a model for double scattering is recently developed by Hu et al. [13], which showed a strong potential to analyze strongly scattering materials.

However, despite the theoretical results, significant difficulties still remain to develop analytical formulas of ultrasonic scattering coefficients in polycrystalline materials with a more complex microstructure. Therefore it is believed that numerical modeling should be a powerful alternative to access more real and complex polycrystalline microstructures and to improve the understanding of their interactions with ultrasonic waves. Among possible numerical methods, full-field numerical modeling using the finite element method (FEM) allows taking into account polycrystalline microstructures without any simplifying assumptions and therefore grasping of complex phenomena of wave propagation in polycrystals, especially effects of the multiple scattering [14–16]. FE modeling is applicable to quantify the scattering effectiveness due to grain boundaries of numerically generated polycrystalline microstructures. Furthermore, progress in the electron backscatter diffraction (EBSD) technique makes possible to obtain input maps of real microstructures to take into account by FE meshes [17]. Its accuracy and versatility in modeling numerical or real polycrystalline microstructures make the FEM a promising tool for further developments of nondestructive inspection.

Former works on FE simulations focused on the evaluation of ultrasonic attenuation in polycrystalline materials, e.g. [14,15,18,19]. However there is relatively little work on the development of methods based on FE full-field modeling, which allows precise evaluation of microstructural noise levels [20]. The purpose of the present work is to propose a versatile FE approach that leads to an evaluation of scattering effectiveness in an arbitrary spatial direction in any polycrystalline medium. The FE approach is developed within the unified framework based on the reciprocity theorem. Before being applied for analyzing experimental results, it must be checked the proposed modeling avoids any numerical artifacts. Therefore it is validated by comparison with the classical theoretical models in the case of analyzing grain size effects on the ultrasonic backscattering in single phase, untextured and equiaxed polycrystals with idealized but representative theoretical microstructures.

Only 2D FE simulations are conducted. To exclude the grain size distribution effects [21], especially at the transition between the different regimes, for instance, Rayleigh-to-stochastic transition, microstructures with numerically generated single-size regular hexagonal grains are mainly considered. This is obviously far from the actual grain structure in a polycrystal, but it gives a kind of asymptotic result. Such a hypothesis leads obviously to the periodicity of the grain morphology, possibly causing numerical artifacts. Two other cases of microstructures with geometrically varying grains are therefore discussed: an irregular hexagonal grain morphology and a Voronoi tessellation, both of which have a narrow dispersion of grain size and are geometrically close to a naturally occurring polycrystalline microstructure [15]. An external pressure loading is used to produce an incident signal, which simulates, for instance, the broadband laser-generated ultrasound pulse [22]. Frequency content of the incident signal is large enough to account for different scattering regions with respect to three studied grains sizes. This example of laser-generated ultrasonic waves also justifies a first 2D numerical approach, since it is of significance to the cases where transducers with a cylindrical focus are used for the inspection of heterogeneous materials [20]. This is, for instance, the case for ultrasonic characterization of the microstructure using a laser pulse following the work by Monchalin [23]. The backscattering coefficient is calculated in both time and frequency domains using numerically recorded data at several receivers placed at the boundary of the polycrystals. Dependence of the backscattering coefficient on the frequency and the grain size are therefore analyzed and compared with theoretical predictions.

The paper is organized as follows: A unified framework for theoretical and numerical evaluations of noise scattering is presented in Section 2. Classical analytical models are recalled, 2D analytical formulas of the backscattering coefficient are developed, especially the constant of proportionality between the grain-noise scattering coefficient and the received power due to the grain scattering, which was proposed and already identified by Margetan et al. [11] in the 3D case, is derived. The ratio of this constant between the 2D and 3D cases is proved to be frequency dependent. Numerical measure procedure is then proposed. In Section 3, FE ultrasonic propagation models for backscattering measurement are defined, quality analysis of numerical simulations is presented with a mesh convergence analysis and a study of phase velocities in polycrystalline materials. Section 4 presents numerical results concerning the grain size effects on the ultrasonic backscattering coefficient, followed by some main conclusions given in Section 5.

2. A unified framework for theoretical and numerical evaluations

A unified theoretical framework based on the reciprocity theorem for the evaluation of the ultrasonic noise scattering in both 2D and 3D cases is presented. Analytical formulas for the scattering coefficient are obtained by considering the equivalence between the amplitudes of scattered noise signals obtained using two different methods: the one based on the well-known Auld's electromechanical reciprocity relation, which adapts the reciprocity theorem to the evaluation of scattering coefficients using transducer output signals [8,9], and the other one based on far-field analysis of an isolated scatterer, which also refers to the reciprocity theorem for obtaining full elastodynamic wave fields [24]. The key assumption is the weak scattering so the Born approximation can be applied.

As a principal result of this work, a numerical evaluation approach is defined within the unified framework of Auld's reciprocity theorem and the corresponding expressions of the ultrasonic noise backscattering coefficient using FE modeling in both 2D and 3D cases are proposed.

2.1. Reciprocity gap due to the microstructural scattering

Consider a polycrystalline material occupying a region Ω of space dimension $N_{dim}(=2,3)$ and bounded by a surface $\partial\Omega$ and