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# INFLUENCE OF GRAIN MORPHOLOGY AND SIZE ON ULTRASONIC ATTENUATION IN POLYCRISTALLINE ISOTROPIC MATERIALS

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### ABSTRACT

EDF R&D carries out studies for many years in order to improve and quantify the performances of the ultrasonic NDT process implemented on nuclear power plants. The detection and sizing of defects in coarse grained materials is a very challenging issue related to the inspection of critical components of nuclear power plants. Indeed in coarse grained material, the scattering of the ultrasonic wave at grain boundaries is responsible for the high attenuation which highly degrades the detection performances. This unfavorable phenomenon is predominant where the mean grain size is comparable to the wavelength of the control. In this framework, EDF R&D has carried out studies on the simulation of the ultrasonic propagation in complex materials with the finite elements code ATHENA.

2D and 3D finite element modeling approaches of ultrasonic propagation have been implemented, combined with a description of the microstructure of coarse grain materials [1]. The aim of this study is to demonstrate that the integration of a relevant description of the microstructure of macroscopically isotropic grain materials in a numerical simulation is an efficient tool to predict the ultrasonic attenuation in those materials. In addition, the influence of grain morphology, size and orientation on the ultrasonic attenuation coefficient is studied. The simulation results are compared with theoretical models and experimental measurement performed on an isotropic polycrystalline material (coarse grain Ni-based alloy).

Keywords: scattering, ultrasonic attenuation, finite element modeling, grain morphology, coarse grain Ni-based alloy

### NOMENCLATURE

α	attenuation coefficient
f	probability density function
k	wavenumber
d	mean grain size

### 1. INTRODUCTION

The ultrasonic inspection of some polycrystalline materials that can be found in components of the primary circuit of nuclear reactors is very challenging for the detection and sizing defects. Indeed, when ultrasonic waves propagate through coarse grain materials, the incident energy is scattered by grain boundaries due to highly anisotropic and inhomogeneities. This is mainly determined by the elastic properties of the crystals, the density between adjacent grains, the grains sizes and shapes, the crystallographic texture. The scattering of ultrasonic waves can decrease the detection and sizing of defects capabilities in ultrasonic inspection by two phenomena: ultrasonic attenuation and structural noise. These unfavorable phenomena are predominant in materials where the mean grain size is comparable to the wavelength used for the control. The ultrasonic attenuation measures the amplitude decay of elastic waves propagating in a polycrystalline material and is usually quantified by a scalar named the scattering attenuation coefficient  $\alpha$ .

Aiming at better understanding of these phenomena and the wave propagation within these heterogeneous structures, EDF R&D has extensively used numerical simulation to improve the performance of the ultrasonic technique and to evaluate its sensitiveness to the material parameters. In this framework, EDF R&D has developed a finite elements code ATHENA dedicated to the simulation of the ultrasonic propagation in heterogeneous media. So a numerical approach has been developed to model the ultrasonic attenuation caused by the scattering in coarse grained polycrystalline materials. The present study presents recent developments of realistically large and detailed the Grain-Scale modeling (GSM) of ultrasonic attenuation in polycrystalline isotropic materials, demonstrating new simulation possibilities in 2D and 3D [1]. It investigates the capability of GSM approach to model the different scattering behaviours of ultrasonic longitudinal waves within coarse grained isotropic materials with equiaxed microstructure.

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In this context, the objective of this article is to quantify the influence of several parameters on the attenuation like the grain morphology and size, the grain shape, the crystallographic orientation and the probe frequency in the isotropic material Nickel-based alloy – Inconel 600<sup>®</sup>. The numerical results of 2D and 3D simulations are compared to theoretical predictions obtained from the unified theory of Stanke and Kino [2] and the 2D adaptation of Stanke and Kino model by Xue Bai [3] and experimental measurements of scattering attenuation coefficient.

### 2. MATERIALS AND METHODS

### 2.1. Grain-scale modeling approach

The GSM approach aims to combine the finite elements code ATHENA which enables to simulate the ultrasonic wave propagation in heterogeneous and anisotropic media with a realistic description of the microstructure of polycrystalline materials.

### 2.1.1. Finite elements code modeling ATHENA

The modeling of the ultrasonic propagation is performed with the finite elements code ATHENA which is implemented in both 2D and 3D versions. This code simulates the propagation of ultrasonic waves in all kinds of elastic media and in particular, heterogeneous and anisotropic media. ATHENA solves the elastodynamic equations expressed with the stresses and the velocities by a finite element method. The finite elements method used in ATHENA is implemented with a square and regular mesh for the calculation zone. Furthermore, absorbing conditions can be set on the boundary of the computation zone with the use of Perfectly Matched Layers [4]. It enables to avoid edge reflection and thus to simulate a virtually infinite area.

# 2.1.2. Grain-scale description of polycrystalline microstructure

The grain-scale description consists of creating an artificial microstructure which accounts for the geometric, elastic and crystallographic properties of the studied material. The 2D modeling of an isotropic microstructure is usually carried out using the Voronoï diagrams [5]. The 2D Voronoï diagrams are mathematical decompositions of a metric space determined by distances to a specified set of discrete points- the seeds. Poisson-Voronoï diagrams are a variety of Voronoï diagrams where the metric is the Euclidian distance and the seeds are randomly distributed with a Poisson algorithm. State of the art function to generate a 2D Poisson-Voronoï tessellation are included in MATLAB, which is used in the presented work (Figure 1.a). The same material properties are assigned to each cell (each grain). The elastic properties of the material are defined by the stiffness tensor of the single crystal. Moreover, the crystallographic properties of a modeled microstructure are specified by the crystallographic orientation of every grain (assimilated to single crystal). For the isotropic material (Ni-based alloy with coarse grains), each grain is assigned with a random orientation, defined in order to ensure an isotropic space distribution of the orientations defined by the Euler angles in the Roe convention.

To improve and generalize the simulation of the ultrasonic scattering, the isotropic microstructure with equiaxed grains is also modeled in 3D using the open source Dream3D software. A 3D representation of the random equiaxed microstructure is successfully reached (Figure 1.b). The geometric description is focused on a log-normal grain size distribution which is controlled by the probability density function f. Similarly to the 2D model, the elastic and crystallographic properties are defined in the same way. Figure 1.a and Figure 1.b show the ability of 2D and 3D modeling to mimic the realistic equiaxed microstructure of isotropic material characterized by the EBSD analysis (Electron Backscattered Diffraction) (Figure 1.c).



FIGURE 1: POLYCRISTALLINE ISOTROPIC MICORSTRUCTURE : (a) 2D MODEL, (b) 3D MODEL, (c) EXPERIMENTAL ANALYSIS - EBSD

#### 2.2. Attenuation computation

The attenuation is computed with the multiple backwall echoes method. It is based on the progressive decay of the amplitude of successive backwall echoes. A 10 mm-thin metal slab with parallel faces is inspected with an immersion ultrasonic probe of diameter 12.7 mm in normal incidence in order to generate only the longitudinal waves. The water height is chosen so that the sample is located in the far field of the probe to overcome inhomogeneities of the ultrasonic beam. Aiming to consider only the contribution of scattering and to eliminate the contribution of beam divergence, the attenuation is computed by the comparison between a grain-scale simulation in an heterogeneous media and a simulation in an equivalent homogenized media which is characterized by the Voigt average homogenized elastic coefficients. The two first backwall echoes are taken into account for the computation of the attenuation coefficient [1].

## 3. RESULTS AND DISCUSSION

### 3.1. Comparison of grain distribution

The microstructure of isotropic material is examined by an EBSD analysis as shows Figure 1.c. Moreover, Figure 2 compares the experimental grain size distribution with the 2D and 3D numerical grain size distributions obtained respectively with Poisson-Voronoï tessellations and the Dream3D code. The average of five different grain size distributions in 2D and in 3D are plotted in this figure. The 2D and 3D numerical grain size distributions are calculated respectively with about 559 and 6086 grains whereas the experimental grain size distribution is computed with about 540 grains.



**FIGURE 2:** COMPARISON OF THE EXPERIMENTAL GRAIN SIZE DISTRIBUTION WITH THE 2D AND 3D NUMERICAL GRAIN SIZE DISTRIBUTIONS

The mean grain size and the distribution width (standard deviation) are determined by log-normal fitting distributions. Figure 2, highlights the very good agreement between the experimental distribution and the 3D numerical distribution, though an important gap is shown with the 2D numerical distribution. Indeed, the first two ones are relatively wide. The mean grain size of the experimental characterization and the 3D model are respectively 775  $\mu$ m, 800  $\mu$ m and with a same standard deviation 650  $\mu$ m and a peak of 350  $\mu$ m (mode of distribution). However, the 2D numerical distribution is very narrow and centered around a mean grain size of 800  $\mu$ m and a standard deviation of 250  $\mu$ m.

### 3.2. Ultrasonic attenuation

The attenuation values obtained with the GSM method are compared with experimental measurements and theoretical predictions which are provided by the unified theory of Stanke and Kino in 3D [2] and the adaptation of this model in 2D made by Xue Bai [3]. The scattering attenuation coefficient  $\alpha$ , normalized through multiplication with the mean grain size *d*, is plotted against the normalized frequency (product of wavenumber k and d) on a *log-log* scale in Figure 3. This latter indicates that the scattering phenomenon is established according to three regimes: Rayleigh for the ratio between wavenumber and grain size  $kd \ll 1$  (low frequency), stochastic  $kd \approx 1$  (high frequency) and a transitional regime exists between the Rayleigh and stochastic regime. Regarding the comparison between different curves, the 3D simulation show a good agreement with the 3D analytical predictions and experimental data in the transitional regime. Otherwise, we note the underestimation of the attenuation by the 2D simulation compared with experimental data and the 3D simulation.



**FIGURE 3:** COMPARISON OF THEORITICAL, EXPERIMENTAL AND SIMULATION DDATA (2D, 3D) OF ATTENUATION COEFFICIENT FOR NI-BASED ALLOY

### 4. CONCLUSION

The objective of this study is to give an overview of the recent progress achieved by EDF R&D in capabilities of finite elements modeling to simulate the wave propagation in polycrystalline isotropic materials with an accurate integration of the microstructure. The present 2D and 3D numerical results show promising ability of the GSM approach to predict the behaviour of the ultrasonic attenuation in coarse-grained material.

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