Numerical computation of ultrasonic attenuation in polycrystalline materials with finite element modelling and grain-scale material description

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Abstract

A 3D finite element modeling approach of ultrasonic propagation combined with a description of the microstructure at the scale of the grains has been implemented. The simulations seek to determine the contribution of scattering to the ultrasonic attenuation in polycrystalline materials. The approach is applied into isotropic microstructures. The ultrasonic propagation is computed with the finite element code ATHENA 3D that developed by EDF. The description of the propagation media accounts for the geometric, elastic and crystallographic properties of coarse-grained material. The attenuation was computed from the decay of simulated multiple backwall echoes. The contribution of the microstructure scattering was isolated by a correction of the attenuation data with the attenuation obtained in an equivalent homogenized material. The simulation investigates the variation of attenuation as a function of several key parameters: grain size, grain orientation, probe frequency.

1. Introduction and context

Non-Destructive Evaluation (NDE) is extensively used to ensure the structural integrity of important and safety-related components in the nuclear industry. In this context, the inspection of some polycrystalline materials that can be found in components of the primary circuit is an important scientific challenge. However, the solidification phenomenon occurring during the fabrication process leads to a highly anisotropic and heterogeneous microstructure. Indeed, these materials (nickel-based alloys, austenitic stainless steel welds, etc.) remain difficult to inspect with common ultrasonic control because the interaction of the incident wave with the microstructure is complex and leads to uncontrolled degradation of the incident beam during its propagation. In the case where the mean grain size is of the order of the typical wavelength, the scattering of elastic waves at grain boundaries attenuates, distorts the wave and generates a noise which is called «structural noise». These unfavorable phenomena decrease the detection and sizing of defects capabilities in ultrasonic inspection. The attenuation measures the amplitude decay of elastic waves propagating in a polycrystalline material and is usually quantified by a scalar named the attenuation coefficient $\alpha$. This phenomenon is caused by three contributions, the divergence of the beam, absorption, and scattering, where the two latter are related to properties of the material. The first contribution to attenuation is due to the divergence of the ultrasonic beam. It is purely geometric and related to the diffraction pattern of the probe used for the inspection. Attenuation by absorption is due to energy transformation into heat due to dislocations. In general, in the application of ultrasonic
NDE, the contribution of the absorption phenomenon is negligible in polycrystalline materials. Then the third contribution is the attenuation by scattering and is attributed to interactions between waves and grain boundaries due to inhomogeneities in elastic properties and in density between adjacent grains. It is mainly determined by the elastic properties of the crystals, the grains sizes and shapes, the crystallographic texture. So 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. Therefore, an approach has been developed to model the ultrasonic attenuation caused by the scattering in coarse grained polycrystalline materials. Grain-scale modelling (GSM) of polycrystalline materials has been successfully undertaken in various fields of research including ultrasonic NDE (Chassignole [1,2], Lhuillier [3,4]) but were limited to 2D. Although several approaches have been adopted, all of those mentioned here that consider geometrically varying grains, rely on Voronoï tessellations to numerically generate a morphology which is geometrically similar to a naturally occurring polycrystalline microstructure. Recently we have succeeded to implement the 3D model of the coarse grained isotropic microstructure with equiaxed grains. In this context, the objective of our study is to generalize the modelling of scattering attenuation in coarse grained polycrystalline materials like in the case of Ni-based Alloy. The present study aims to identify the influence of several parameters on the attenuation like the grain size, the grain shape, the crystallographic orientation and the probe frequency in the isotropic material Nickel-based Alloy – Inconel 600®. The GSM approach is described in section 2.

2. Modelling Approach: Grain-Scale Modelling

The aim of the Grain-Scale Modelling approach is 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. The approach aims to reproduce the beam perturbations, the ultrasonic attenuation and the appearance of structural noise due to scattering of the wave at grain boundaries.

2.1. Finite elements code modelling ATHENA

The modeling of the ultrasonic propagation was performed with the finite elements code ATHENA which exists in a 2D and a 3D version. The implementation of this code is based on the solving of the elastodynamic equations expressed with the stresses and the particle velocities by a finite elements method [1,2]. The code is dedicated to model the propagation of ultrasonic waves in all kinds of elastic media and in particular, heterogeneous and anisotropic media. The finite elements method used in ATHENA is implemented with a square and regular mesh for the calculation zone. Furthermore, the code enables to set reflecting or absorbing boundary conditions of the calculation zone which are denoted as Perfectly Matched Layers (PML) [5]. The use of PML removes edge reflection and thus enables to simulate a virtually infinite area.
2.2. Grain scale description of polycrystalline microstructure

In order to simulate the contribution of the polycrystalline microstructure to the ultrasonic scattering, the propagation media was modelled at the scale of the microstructure. The GSM approach consists of creating an artificial microstructure which accounts for the geometric, elastic and crystallographic properties of the studied material. The modelling of the isotropic microstructure was implemented in 2D with the use of Voronoi diagrams. Moreover, to improve and generalize the simulation of the ultrasonic scattering, the isotropic microstructure with equiaxed grains was also modelled in 3D using the open source Dream3D code.

2.2.1. Geometric description

The geometric description of the microstructure consists to define a geometric subdivision which mimics the grains of the polycrystalline material. A 3D representation of the random equiaxed microstructure of an isotropic coarse grain material (Ni-based alloy) has been successfully reached in this study. The geometric description is focused on a log-normal grain size distribution. The grain sizes are expressed with the equivalent sphere diameter (ESD) of grains. The ESD represents the diameter of a sphere that has the equivalent volume of grains. The control of grain sizes is done by the input statistic parameters: mean ($\mu$) and standard deviation ($\sigma$) which are mentioned in the probability density function $f(x)$ of the log-normal distribution:

$$f(x) = \frac{1}{x \sigma \sqrt{2\pi}} \exp \left( -\frac{(\ln x - \mu)^2}{2\sigma^2} \right)$$  \hspace{1cm} (1)

Where $x$ denotes the grain size (the equivalent sphere diameter (ESD)).

2.2.2. Crystallographic properties

The crystallographic properties of a modelled structure is defined 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. The orientations of each grain are defined by the Euler angles in the Roe convention. To ensure the definition of isotropic behaviour of microstructure the 3 angles ($\varphi$, $\theta$, $\psi$) are randomly picked with respect to the following rotations respectively with $z$, $y'$ and $z''$ axes in the crystal frame.
2.2.3. Elastic properties

The elastic properties of the studied material are defined by the stiffness tensor of the single crystal with a cubic symmetry. The stiffness tensor is characterized by the three independent coefficients $C_{11}$, $C_{12}$ and $C_{44}$ which are the same for each grain of the microstructure. The constants specify the properties of the heterogeneous media at the scale of grain. These coefficients are illustrated in Table1. Moreover, in a homogeneous medium (without grains) the homogenized elastic constants are computed with the single crystal elastic coefficients and the knowledge of the Orientation Distribution Function (ODF). The detailed computation of the homogenized elastic coefficients is described in [4].

Table 1: Single-crystal coefficients and homogenized elastic coefficients of Ni-based Alloy 600 and 316L Stainless Steel (in GPa)

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<tr>
<th>Materiel</th>
<th>Single Crystal Elastic Coefficients</th>
<th>Homogenized Elastic Constants</th>
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<tr>
<td></td>
<td>$C_{11}$, $C_{12}$, $C_{44}$</td>
<td>$C_{11}$, $C_{33}$, $C_{44}$, $C_{66}$, $C_{12}$, $C_{13}$</td>
</tr>
<tr>
<td>Ni-based Alloy 600</td>
<td>235, 145, 126</td>
<td>283, 283, 79, 126, 126</td>
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3. Attenuation computation

The attenuation was computed with the multiple backwall echoes method developed by Haldipur [6]. This method is a simple technique to evaluate the ultrasonic attenuation due to grain scattering. It is based on the progressive decay of the amplitude of successive backwall echoes. In order to apply this method, a thin slab for both studied materials is inspected with an immersion ultrasonic probe of diameter 12.7 mm in normal incidence to generate only the longitudinal waves. The thickness of the inspected sample is 10 mm and 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. Moreover, we have mentioned in the section 1 that the signal decay in polycrystalline materials is generated by the multiple scattering phenomenon and the divergence of the beam. So aiming to eliminate the contribution of beam divergence and to consider only the contribution of scattering, the attenuation is computed by the comparison between a grain-scale simulation in an heterogeneous media (see Fig.2.a) and a simulation in an equivalent homogenized media (see Fig.2.b) which is characterized by the homogenized elastic coefficients (see Table1). The two first backwall echoes were taken into account for the computation of the attenuation coefficient. The first step consists to extract the two first backwall echoes and to apply a Hanning windowing on each echo. A Fourier transform is then applied to the windowed echoes. The scattering attenuation is obtained by the following relation:

$$
\alpha_{diff}(w) = \alpha_{het}(w) - \alpha_{hom}(w) = \frac{20}{2d} \log \left[ \frac{r1_{het}(w) r2_{hom}(w)}{r1_{het}(w) r2_{hom}(w)} \right]
$$

Where $\alpha_{diff}$ denotes the diffusion attenuation coefficient, $\alpha_{het}$ is the attenuation coefficient obtained from the grain-scale simulation, $\alpha_{hom}$ is the attenuation coefficient computed from homogenized simulation, $r1$ and $r2$ are the frequency spectra of the first and second backwall echoes and $d$ is the thickness of the sample.
Figure 2: Principle of the method of multiple backwall echoes to compute the ultrasonic attenuation. (a) Grain-scale simulation. (b) Homogenized simulation.

4. Results and discussion

In this section, the recent results of the ultrasonic attenuation obtained by the GSM approach are presented as well as the experimental and theoretical validation of the numerical results.

4.1. Evaluation of ultrasonic attenuation for the isotropic material: Ni-based Alloy

In order to study the attenuation for the isotropic material Ni-based Alloy, 3D simulations at the grain scale level for three different grain sizes: 500 µm, 800 µm, 1000 µm have been performed. These results were compared with recent ones obtained by 2D simulations which are based on the coupling between the finite elements code ATHENA2D and the description of the microstructure using Voronoï diagrams. Figure 3 represents the variation of the attenuation coefficient in the different cases for a probe central frequency of 2.25 MHz. The different curves of attenuation were plotted in frequency range of [1.25 MHz, 3.25 MHz].

Figure 3: Comparison of 3D and 2D simulation data of the attenuation as function of the frequency for a probe central frequency of 2.25 MHZ, for the three different grain sizes 500 µm, 800 µm, 1000 µm.
Figure 3 shows that the attenuation increases monotonically with both frequency and grain size, which initially suggests a good coherence with the expected behavior. Indeed, we observe for 2D simulations as well as for 3D ones that in this frequency range, the attenuation increases with the grain size. The agreement of 2D and 3D results is very good for 500 µm and 800 µm up to 2 MHz. Moreover, we note that at high frequency a concave hump is observed especially in the case of grain size of 1000 µm. This hump might correspond to the transition from the Rayleigh scattering regime to the stochastic scattering regime. It is observed that the larger the grain size the earlier transition to the hump. By comparing the 2D and 3D numerical results for different grain sizes, we note that the 2D simulation underestimates the attenuation compared to the 3D simulation for a frequency above 2 MHz. This can be explained by the simplification of the 2D configuration. In this context, it will be necessary in our study to compare the numerical results obtained by 2D and 3D simulations with theoretical predictions and experimental measurements in order to evaluate these results.

4.2. Theoretical and experimental validation

To evaluate the numerical results and identify the different regimes of the scattering mechanism, we compared the numerical values with theoretical predictions which are obtained by the Unified Theory of Stanke and Kino [7]. This theory 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), geometric $kd \gg 1$ where the attenuation evolves in the first and second regime as a function of the frequency and the grain size respectively as $f^4$, $d^3$ (in Rayleigh regime) and $f^2$, $d$ (in stochastic regime). However, in the geometric regime, the attenuation coefficient is independent of the frequency and dependent the grain size to $1/d$. Thus, a transitional regime exists between the Rayleigh and stochastic regime where the frequency dependence can vary before converging to the stochastic asymptote.

![Figure 4](image_url): Comparison of theoretical, experimental and simulation data (3D and 2D) of attenuation for Ni-based Alloy for $d = 500$ µm and $F = 2.25$ MHz: (a) Comparison of numerical values of attenuation with normalized predictions of attenuation coefficient deduced from the Stanke and Kino model [7]. (b) Comparison of the numerical values of attenuation with experimental data.
Indeed, this transitional regime is characterized by two successive humps: a concave and a convex hump. According to the Unified Theory, the theoretical and numerical curves of attenuation coefficient $\alpha$ were normalised through multiplication with the grain size $d$ (equivalent sphere diameter) and plotted in Figure 4.a against the normalized frequency (product of wavenumber $k$ and $d$) on a log-log scale. These results correspond to the microstructure whose the equivalent grain size is in the order of 500 $\mu$m.

Regarding the comparison between the theoretical and the numerical curves, these latter show a good agreement with the analytical predictions (See Figure 4.a). This suggests that the grain-scale modelling is able to model the changing in scattering behaviours. However, we note that the numerical results overestimate the attenuation at low frequency ($\log (kd) < 0$), Rayleigh regime) in both cases. Otherwise, the transition from the Rayleigh scattering region to stochastic scattering region is confirmed by the numerical results. In this context, Figure 4.a shows the good coherence between the 3D model and the theoretical curve in this transitional regime and the underestimation of the 2D simulation observed in Figure 3. This was confirmed by Van Pamela [8,9] and Xue Bai [10] in their studies. The authors show the pertinence of 3D simulation to model the attenuation phenomenon and explain the origin of the underestimation of the 2D simulation. Indeed, they demonstrate the dimensional dependence of the scattering induced attenuation on frequency or wavenumber for various scattering regimes in 2D and in 3D. The authors show that in the Rayleigh regime, the attenuation is proportional to $f^{D+1}$, where $D$ denotes the dimension. However, in the stochastic regime, the attenuation is proportional to $f^2$ regardless of the dimension. So the underestimation of the attenuation by the 2D simulation is explained by the frequency dependence of the attenuation coefficient to $f^3$ and not $f^4$ as in the case of 3D simulation. In this context, to have a more representative theoretical confrontation for the 2D simulation data, Xue Bai [10] should adapt the Stanke and Kino model by giving 2D analytical formulas for ultrasonic attenuation coefficient. The numerical values obtained with simulations are performed for the grain size of 500 $\mu$m and the probe frequency 2.25 MHz were then compared with experimental data which are measured on a block of Inconel 600® whose average grain size is in the order of 500 $\mu$m. The different results are displayed in Figure 4.b. The GSM simulation, especially the 3D simulation shows a very good agreement with the experimental data. Furthermore, we pick that the evolution of curves is very similar and the values of attenuation are very close. For example, at a frequency of 2.25 MHz, the numerical values of attenuation for the 2D and 3D simulation are respectively 0.26 dB and 0.3 dB while the experimental measurement is 0.29 dB. This corresponds to a gap in the order of 10% and 3.5%, respectively. The exposed results demonstrate the efficiency of the GSM especially the 3D modelling approach to estimate the scattering attenuation in the isotropic media: coarse grain Ni-based alloy.

5. Conclusion

The objective of this article was to give an overview of the recent progress achieved by EDF R&D in capabilities of finite elements modelling to simulate the wave propagation in complex polycrystalline materials with an accurate integration of the microstructure. A numerical modelling approach which combines the finite elements code ATHENA with a description of the isotropic coarse grain microstructure at the grain-scale has been implemented in 3D. The Grain-Scale Modeling approach aims at determining the contribution of the attenuation due to the ultrasonic wave scattering by the microstructure.
This approach has been applied on the coarse-grained Ni-based Alloy material (Inconel600). The computation of the ultrasonic attenuation was based on a comparison of a simulation with a grain-scale description of the microstructure and a simulation with a homogenized media. The simulation enabled to investigate the variation of attenuation as a function of two parameters: the grain size and the probe frequency. Preliminary results of the 3D simulations have been presented and compared with recent results of the 2D simulation [4]. These numerical results have shown promising ability of the GSM method to predict the behaviour of the ultrasonic attenuation in the coarse-grained material in 2D and 3D. Moreover, the simulated attenuation data has been confronted to experimental data and to theoretical predictions obtained by the Unified Theory of Stanke and Kino [7]. The comparison shows very good agreement of the numerical results especially the 3D simulation data with experimental and theoretical results. This demonstrates the pertinence of the 3D approach to simulate the complex phenomena related to wave scattering by the microstructure, namely the attenuation. However, modelling limitations were also highlighted. It was shown that the 2D model underestimates the attenuation in the transitional regime. Overall, it is proposed that the progress and understanding presented in this article will favor the ongoing improvement of FE simulations of ultrasonic NDE of polycrystalline anisotropic materials like the austenitic welds.

References

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