OVERVIEW OF THE RECENT DEVELOPMENTS ON GRAIN-SCALE MODELING TO
SIMULATE ULTRASONIC SCATTERING WITH A 2D FINITE ELEMENT CODE

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Abstract

Numerous studies were undertaken by EDF R&D for a few years to improve the NDT process on
these applications and to help to their qualification. In many cases, the inspected components may
exhibit a coarse grain microstructure which induces severe beam disturbances and reduces the
reliability of the control. Moreover, modeling is more and more used to evaluate the beam to structure
or to defect interaction and to perform parametric studies. However, the modeling of the scattering
phenomena - attenuation and structural noise – must be based on accurate input data for the material
description.

The methodology proposed by EDF R&D to simulate the inspection of coarse grain structures
is to combine the finite element code ATHENA 2D with a grain scale description of the materials. The
method reproduces the beam perturbations, the attenuation and the appearance of structural noise due
to scattering of the wave at grain boundaries. It enables to compute macroscopic attenuation
coefficient. In the case of anisotropic structure like austenitic welds, the anisotropic evolution of the
attenuation in the inspection plane can be simulated.

The performances and the limits of the grain-scale modeling approach are illustrated on several
configurations. Firstly the influence of the microstructure model on the accuracy of simulation results
have been investigated on isotropic coarse grain INCONEL 600 components. Two specific
illustrations are presented and compared to experimental results, which are the modeling of a multi-
layer isotropic structure (centrifugally cast stainless steel) and a complex anisotropic structure
(austenitic weld).

Introduction

For several years, EDF has extensively used numerical models to improve the design, qualification
and implementation of NDT processes. Several studies and experimental validations have already
been carried out with the ATHENA code to simulate ultrasonic inspections in simple and complex
cases. In particular, the ability of the code to accurately reproduce complex phenomena occurring
during the propagation in heterogeneous media like welds (beam deviation, division or attenuation…) has already been the subject of several publications [1-4]. In these studies, the heterogeneous medium
is described as a set of homogeneous anisotropic domains characterized by their elastic and attenuation
properties.

In addition to the development of the finite elements (FE) code ATHENA, EDF has recently
carried out studies on the grain-scale modeling of the ultrasonic scattering in coarse grain structure.
The method relies on the coupling of the FE simulation and a modeling of the microstructure at the
description level of the grain.

The objective of this paper is to give an overview of the recent developments achieved by EDF
R&D in the field of the grain-scale simulation of ultrasonic inspections with the 2D version of the
ATHENA code.
Firstly, a brief description of the features implemented in ATHENA 2D is given. Then the models used to describe the microstructure of polycrystalline materials are detailed. Eventually, the results of grain scale modeling are presented. It gives an evaluation of the main parameters of the microstructure models impacting the reliability and the performances of the simulations.

1. **Numerical modeling**

The main features of the 2D version of the ATHENA code are presented here, more details can be found in [5].

ATHENA2D is a finite element code for elastodynamic developed by EDF R&D. The code solves the equation of elastodynamic expressed in a mixed formulation combining stress and velocity terms. The code is dedicated to the simulation of wave propagation in all kinds of elastic media and in particular, heterogeneous and anisotropic materials. One important feature of the code is the use of the fictitious domain method [6]. It relies on the combined use of a regular discretization of the calculation zone with a non-regular meshing of the defects. It allows taking advantage of the rapidity of regular mesh calculation with the possibility to model arbitrary shaped defects. Furthermore, ATHENA 2D gives the possibility to use Perfectly Matched Layers (PML) to define the boundaries of the calculation domain [7]. The use of PML removes spurious reflections on artificial edges of the calculation zone and thus enables to model virtually infinite components. Finally, ATHENA 2D integrates the possibility to simulate various inspection configurations (pulse-echo, tandem, TOFD) with a wide range of transducers (single element and phased array), inspection mode (contact or immersion), materials and defects. The code has been widely used by EDF to simulate the inspection of complex structures such as austenitic welds [3, 8, 9].

2. **Polycrystalline material modeling**

The aim of the grain-scale modeling is to combine the accuracy of the FE simulation of the ultrasonic propagation in heterogeneous and anisotropic media with a fine description of the microstructure of polycrystalline materials. The approach enables to simultaneously simulate the structural noise and attenuation due to ultrasonic scattering in coarse grain structures.

2.1. **Microstructure modeling**

In 2D grain scale modeling, the inspected component is modeled by a 2D tessellation of the plane which mimics the morphology of polycrystalline microstructure. In this paper the polycrystalline microstructure was modeled by several variety of plane tessellation based on Voronoi diagrams.

Voronoi tessellations are a mathematical tool which enables to subdivide the plane with convex cells. Each variety of Voronoi diagram relies on a basic construction procedure. A set of points, called seeds, is withdrawn on the portion of plane to be subdivided. The plane is subdivided in cells which contains the points closer from a given seed than any other. The way to withdrawn the seed in the first step and the metric used to compute the distances in the second step define the variety of Voronoi tessellations. Three kinds of Voronoi tessellations have been used to model the polycrystalline microstructure: the Poisson-Voronoi, Laguerre-Voronoi and heterogeneous Voronoi diagram.

a) The Poisson-Voronoi diagrams use an uniform distribution of seed and the Euclidian metric [10] (Figure 1.a).

b) The Laguerre-Voronoi diagrams also use a uniform distribution of seeds but the distance to the seeds is computed via the Laguerre distance [11] (Figure 1.b).

c) The variety of tessellation called heterogeneous diagrams in this study is generated by a recursive procedure based on Poisson-Voronoi diagram. A macroscopic Poisson-Voronoi tessellation with an average cell size greater than the final expected grain is constructed. A set of seeds is withdrawn on each cell of the macro-diagram with a local uniform distribution and a given density which varies from one macro-cell to another. The set of all the seeds belonging to the macro-cells is used to compute the final tessellation (Figure 1.c).
The Poisson-Voronoi model has been used because of its ease of implementation whereas the Laguerre-Voronoi and heterogeneous Voronoi models have been chosen in order to control the shape of the grain size distribution. In terms of basic morphology, Poisson-Voronoi diagrams model grains exhibiting a sharp grain size distribution. On the contrary, the heterogeneous Voronoi diagrams provide highly inhomogeneous grain size repartition with local concentration of small and large grains.

2.2. Material properties

Once the inspection plane is partitioned into cells representing the grains, each domain is assigned with a random orientation — defined by three Euler angles - accounting for its crystallographic orientation. The elastic properties of each grain are derived from the single crystal’s stiffness tensor and the three Euler angles. To accurately reproduce equiaxed materials, the 3 Euler angles are drawn following a random statistical law chosen to ensure the creation of a macroscopically isotropic medium. One set of random grain orientations plus one tessellation of the computation area give in one ‘‘realization’’ of the random microstructure.

3. Results and discussion

Thereafter, the recent results obtained by EDF R&D in the field of the grain-scale modeling are presented.

3.1. Influential parameters in grain-scale modeling

The aim of this section was to investigate the impact of the main parameters characterizing the description of the microstructure on the simulation performances. In particular, the objective was to evaluate the influence of the grain size distribution on the simulations.

We focused on the inspection of a homogeneous and isotropic block. The configuration implemented in both experimental set-up and simulations is shown in Figure 2. The mock-up is made of INCONEL 600 alloy which was thermally treated and exhibits a mean grain size of ~750 µm. The mock-up was inspected with a single element probe at 2.25 MHz generating longitudinal waves at 45°.

The elastic coefficients of the INCONEL 600 single crystal are given in Table 1. In this study, we analyze the beam-to-defect interaction for a side-drilled hole (SDH) located at a 30 mm depth.

<table>
<thead>
<tr>
<th>INCONEL 600</th>
<th>Elastic coefficients (GPa)</th>
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<tbody>
<tr>
<td>Mean grain size (µm)</td>
<td>C₁₁</td>
</tr>
<tr>
<td>750</td>
<td>235</td>
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</tbody>
</table>

Table 1: Elastic coefficients of INCONEL 600 single crystal.
The three different Voronoi models detailed in section 2.1 were chosen to study the impact of the grain size distribution on the simulation results. Figure 3 shows the grain size distributions obtained with the three models. The distributions have been computed so that they exhibit the same average grain size, ~750 µm. They are compared to the experimental grain size distribution obtained after micrographic observations on the mock-up.

One can see that the Poisson-Voronoi model exhibits a sharp grain size distribution. The “heterogeneous Voronoi” and Laguerre-Voronoi enable to compute simulated microstructure with grain size distributions which are much more similar to the measured grain size distribution. In particular, the models allow reproducing the high amount of small grains and also allow to account for the tail of the experimental distribution corresponding to the large grain sizes. Nevertheless the implementation of the Laguerre-Voronoi and heterogeneous Voronoi algorithms is much more complex and time consuming. As a consequence, the question of the level of refinement of the microstructure model required as regard to the expected simulation accuracy is an important issue.

As a preliminary study the Poisson-Voronoi model has been used to investigate the stability and convergence of the simulated results. It has thus been shown that about 10 simulations are required to constraints the average SDH echo amplitude within a confidence interval of 5%. Moreover 30 simulations are hardly enough to constraint the average value in a 1% confidence interval. Nevertheless the estimation of the required number of simulations is only valid for the considered configuration and need to be evaluated for each study.

As a consequence in the following study, the amplitude of the SDH located at 30 mm was simulated with 30 realizations of each microstructure model. In order to compare the simulated and experimental data, the echo of a SDH located at 10 mm in depth in a homogeneous block was used as reference for amplitude and time scales. The results are shown in Figure 4. One can see that the mean value of the three models are very close from each other. It thus shows that the differences in the grain size distribution due to the microstructure description seem to induce a very shallow impact of the simulated results. In addition, the differences between the mean simulated amplitudes of the 3 models and the experimental data are lower than 3 dB. The grain scale model is thus in this configuration rather efficient to reproduce the amplitude of SDH echoes in a highly scattering material. One can also note that the simulated results exhibit a slight time divergence (~1 µs) as regard to the experimental echo. The difference is more likely to be due to the uncertainties of the homogenized elastic coefficients used to simulate the time reference.

The trend of the noise profiles averaged over 30 simulations for the three simulation models and over 25 transducer positions for the experimental data are displayed in Figure 4. The three microstructure models show very similar trends for the noise. Indeed, each of the averaged profile is contained in the standard deviation of the two others. This observation confirms the previous conclusion on the slight influence of the grain size distribution on the results. Moreover, Figure 4 shows that the simulation does not well reproduce the experimental noise profile.
Figure 4: a) Noise profile (trend computed over 30 simulations) and b) amplitude of the SDH located at z = 30 mm obtained experimentally and simulated with 3 different microstructure models.

This preliminary study has shown that the grain-scale modeling exhibits great efficiency to reproduce the decay of the SDH echo and thus the attenuation due to the scattering of the wave at the grain boundaries. In addition, the grain-scale modeling generates a high level of structural noise. Nevertheless, the average trend of the noise profile is highly overestimated by the grain-scale modeling. Finally, the 3 microstructure models implemented show highly similar results both in terms of attenuation and noise level.

3.2. Multi-layer isotropic structure: Centrifugally Cast Stainless Steel

This section deals with the inspection of Centrifugally Cast Stainless Steel. The microstructure of CCSS components may be highly complex and depends on the solidification conditions.

In the present case, the studied component is made of biphasic austeno-ferritic stainless steel. The metallographic observations (Figure 5.a) revealed that the microstructure varies along the depth in the block. The component was thus modeled as a multi-layer microstructure (4 layers) with a mean grain size varying along the depth (Figure 5.b). A second level of microstructure description was also introduced in order to take into account the subdivision of the initial ferritic grains into austenite colonies during the solidification process (usually called A type solidification). The corresponding simulated microstructure is obtained by subdivising each grain with a second poisson-Voronoi based procedure (Figure 5.c).

Figure 5: a) Metallographic observation of Centrifugally Cast Stainless Steel, b) Multi-layer grain scale model of CCSS, c) Multi-layer grain scale model of CCSS including a second refinement level of the microstructure.

In addition, the studied CCSS is a biphasic material containing 88% of austenite and 12% of residual ferrite. As a consequence 2 different set of elastic coefficients were used and assigned to the grains. The first set of elastic constant corresponds the austenite single crystal. Those input properties neglect the residual ferrite. They have been used in models #1 & #3 (see Table 2). The second set includes the residual ferrite by using a homogenized elastic tensor computed with the frame of the Voigt model (see model #2, Table 2). Eventually, 3 different models have been used and are described in Table 2. One aim of this study was thus to investigate the influence of the material modeling on the UT simulation results.
The 3 models have been used to compute the amplitude of the 4 SDH presented in Figure 6 and the amplitude of the backwall echo. The results are displayed in Figure 7. The echo amplitudes obtained with the three microstructure models are compared to the measurements performed for three probe position along the direction of the SDH axis. The SDH at 34 mm has been chosen as reference for the amplitude comparison. The general trend of the experimental data is well reproduced by the three simulation models. Especially the high amplitude difference between the SDH echoes and the backwall echo is well estimated. Nevertheless all three models globally overestimate the amplitude of the SDH echoes. It means that the attenuation due to the ultrasonic scattering generated by the microstructure is underestimated by the numerical model. In addition, as in the previous section, the 3 different models exhibit very similar results. It is thus highly difficult to discriminate the models.

![Figure 7: SDH echo amplitudes simulated with the 3 microstructure models and experimentally acquired on 3 different positions on the mock-up.](image)

### 3.3. Complex anisotropic structure: Austenitic weld

In this application, the grain-scale modeling approach has been implemented in order to compute the anisotropic attenuation coefficient in an austenitic weld. The structure of austenitic weld is characterized by columnar grains generated by epitaxic growth during the solidification. The microstructure exhibits a crystallographic fiber axis and is thus highly anisotropic. In those conditions, the ultrasonic propagation through the structure highly depends on the angle $\alpha$ between the ultrasonic beam propagation direction and the fiber axis. Nevertheless, the determination of the variations of the attenuation coefficient as a function of the $\alpha$ angle is very hard to achieve experimentally[12].

In order to obtain this data for longitudinal waves, a simulation approach based on grain-scale modeling has been proposed. The simulated configuration is displayed on Figure 8 and consists on a single element immersion transducer at normal incidence on the inspected block. The mock-up is made of anisotropic austenitic INCONEL weld modeled at the grain scale.
The morphologic columnar structure was modeled by a Poisson-Voronoi tessellation which was elongated in the direction of the crystallographic fiber axis. The grain size is characterized by the mean length in the fiber direction and the width in the transverse direction. The grain size has been characterized by metallographic observations and was set to $5 \times 0.25 \text{ mm}$.

The assumption of a transverse isotropic symmetry is made for the elastic properties assigned to the grains. The grains exhibit a common $<100>$ crystallographic axis corresponding to the fiber axis. The elastic coefficients used are displayed in Table 3 and correspond to the values for INCONEL 600.

<table>
<thead>
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<th>Elastic coefficients (GPa)</th>
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<tbody>
<tr>
<td></td>
<td>length width</td>
<td>C11</td>
</tr>
<tr>
<td>5000</td>
<td>250</td>
<td>234</td>
</tr>
</tbody>
</table>

Figure 8: Simulation configuration for the determination of the anisotropic attenuation coefficient of P-waves vs the $\alpha$ angle between the beam propagation and the fiber axis.

The objective of the study was to determine the contribution of the attenuation due to the wave scattering at the grain boundaries. In order to avoid the contribution of the beam divergence, a second computation was done with a homogeneous medium and was subtracted to the initial computation. The $\alpha$ value was incremented from 0 (vertical fiber axis) to 90° (perpendicular fiber axis) in order to investigate the attenuation variations versus the fiber axis orientation. For each set of input parameters the attenuation coefficient was averaged over 30 realizations of the microstructure. The computation of the attenuation coefficient uses the amplitudes of two successive backwall echoes.

The variations of the attenuation coefficient have been computed for 2 different frequencies – 2 MHz and 8 MHz- and are displayed in Figure 9. The simulated values at 2 MHz are compared to the experimental data available. They were estimated from attenuation measurements with a specific set-up on 316L weld samples, slightly adjusted from experimental data on SDH [13].

Unlike an isotropic medium, the results show strong variations of the attenuation depending on the direction of propagation. The maximum attenuation is obtained for propagation perpendicular to the fiber axis ($\alpha = 90^\circ$). This evolution of the attenuation as a function of the angle is in good agreement with the results of previous experimental and theoretical studies [3, 14, 15].

Moreover, the simulation results show a very good agreement with the experimental data at 2 MHz. The modeling approach seems to be highly reliable to estimate the scattering attenuation in an anisotropic weld.

Figure 9: Evolution of the attenuation coefficient as a function of the $\alpha$ angle between the propagation direction of the ultrasonic beam and the crystallographic fiber axis of the austenitic weld.
Conclusion
The objective of this paper was to give an overview of the recent developments achieved by EDF R&D in the field of the grain-scale simulation of ultrasonic inspections with the 2D version of the ATHENA code developed by EDF R&D. The method relies on the coupling of the FE simulation and a modeling of the microstructure at the description level of the grain. The main functionalities of the finite element code ATHENA 2D has been given. Three different mathematical models based on Voronoi diagram have been used to describe the microstructure of polycrystalline materials and to control the grain size distribution.

The grain-scale approach has been implemented on three different cases.

The first case deals with the simulation of the inspection isotropic coarse grain structure made of INCONEL 600 and was dedicated to the investigation of impact of the description of the microstructure on the reliability of the simulations. Three different models of microstructure based on Voronoi diagrams have been implemented in order to control the grain size distribution. Then the grain-scale approach has been applied on two others applications which are the inspection of multi-layer isotropic structure made of centrifugally cast stainless steel and the determination of the attenuation in an anisotropic structure of an austenitic weld.

Globally, the grain-scale modeling has proven a great efficiency to reproduce the decay of the SDH echo and thus the attenuation due to the scattering. The modeling enables to generate a high level of structural noise. Nevertheless, the average trend of the noise profile is highly overestimated by the grain-scale modeling. In the first application, the different microstructure models implemented show highly similar results both in terms of attenuation and noise level. It suggests that the grains size distribution is not a major influential parameter of the computation. In addition, the grain-scale modeling appears to be an efficient way to estimate the attenuation properties of complex structures when the data is experimentally hard to achieve.

Eventually, the discrepancy between experiment and modeling as regard to the noise level can be due to the 2D approximation of the finite elements code or the mathematical tool used to describe the microstructure of coarse grain material. The consequence of the 2D hypothesis would be to virtually concentrate the ultrasonic backscattered energy in the inspection plane and may raise the backscattering phenomena. The future perspective of the grain-scale modeling at EDF R&D will implement the 3D version of the ATHENA finite element code. Nevertheless the creation of 3D microstructure usually requires more than 100,000 grains and become a challenging issue of the grain-scale approach.

References