Relation between ultrasonic scattering and microstructure of polycrystalline materials

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Abstract: Ultrasonic testing is a very common volumetric technique used in industry in order to detect and characterized defects. Within the framework of the maintenance of its nuclear power stations, Electricité de France (EDF) uses this technique on various components. In the case of polycrystalline materials, the scattering of the ultrasonic wave can result in an important attenuation of the signal and the appearance of structural noise. In the present study, we propose to analyze scattering noise in relation to the microstructure of the material. Both experimental and 2D finite elements modelling results are presented for different controlled structure of an homogeneous and isotropic Ni-based alloy.

1 – Introduction

Maintenance represents, for Electricité de France (EDF), a major issue to guaranty the safety of its nuclear power plants. In order to detect and characterize a potential defect, the use of ultrasonic inspection is widely spread. In this technique, the detection is mostly based on an amplitude criterion of the signal reflected from the defect. But while the ultrasonic wave is propagating inside the component, it interacts with the structure resulting in a random scattering of the wave. This phenomenon induces two main effects on the recorded echo: the attenuation of signal and a disturbing backscattered noise. In specific configurations, these effects are so important that the performances of ultrasonic techniques are not guaranteed. These conditions have been studied in previous works [1-4] and analytical expressions of the attenuation as a function of wavelength to grain size ratio ($\lambda/D$) have been proposed [2, 5].

For onsite nuclear inspection, the use of one non destructive testing (NDT) method is conditioned by a pre-qualification which has to demonstrate the performances of the chosen technique. In this context, modelling codes can be very helpful in the performance demonstration by parametric studies. Nonetheless, in order to get quantitative modelling results, all physical phenomena and particularly beam-to-structure interactions have to be taken into account.

In the literature, several modelling codes have been used to describe ultrasound wave propagation in solid media including analytical and semi-analytical approaches and Finite Element methods [1-4], [6-8]. EDF concentrates its efforts on one finite elements code called ATHENA 2D developed in collaboration with the French national Institute for research in Computer Science and Control (INRIA) [9]. In order to implement the wave scattering in the model, recent developments have been performed [10, 11]. The reproduction of the attenuation by the model can be implemented using two different approaches. The first one consists in modifications of the mathematical formulation of the equations,
with the introduction of a tensor determined on the basis of experimental values of ultrasonic attenuation coefficients [11]. This development of the code has proven its efficiency in reproducing the attenuation of the acoustic wave during its propagation but can inherently not reproduce structural noise.

The second solution consists in coupling the conventional elastic model with a description of the material sophisticated enough to correctly reproduce the scattering phenomenon. The objective of the present study is to evaluate the relevance of a grain scale description of the material for the simulation of the ultrasonic beam scattering for a wide range of $\lambda/D$ ratio. This paper is dedicated to the validation of this modelling approach on backscattered noise criteria. The first part introduces the experimental mock-ups, defects and measurements. In the second part, the ATHENA code and the modelling of the microstructure are introduced. Finally, experimental and modelling results are discussed with a view to validate this approach.

2. Experimental set-up

2.1. Material characterization

The scattering of ultrasound in polycrystalline materials is complex as it involves interaction with microstructural features of the material (grain boundaries, precipitates, twins…). For simplification considerations, the study is conducted on forged bars of 135 mm diameter in Inconel 600®, a nickel based alloy used in the nuclear sector. Indeed, this material is purely austenitic and exhibits a homogeneous structure in terms of chemical composition and grain size.

Moreover, the metallographic examinations performed on this material (Figure 1) reveal an equiaxed structure characteristic of isotropic elastic properties. The mean grain size diameter ($D$), estimated according to American Society for Testing and Materials (ASTM) standards, is equal to 220 microns. The presence of twins has furthermore been observed.

In order to study the scattering phenomenon on different microstructures in term of grain size, we have chosen to apply heat treatments at different temperatures on several samples. The consequence of those treatments is the increase of the mean grain size [12]. From 1150°C and a holding time of 90 minutes, the mean grain size increases and reaches a value of 450 microns (Figure 1b). After a treatment at 1200°C, the grain size is estimated at 1 mm (Figure 1c). Table 1 summarizes the characteristics of the various microstructures studied in this work.

![Figure 1](image)

*Figure 1*: (a) Initial state; (b) 1050°C; (c) 1200°C.

**Table 1.** Characteristics of microstructures studied.

| Sample | Heat treatment temperature (°C) | Heat treatment duration (mins) | Grain size (µm) |
|--------|---------------------------------|--------------------------------|-----------------|
| 1      | Initial state                   |                                | 220             |
| 2      | 1150                            | 90                             | 450             |
| 3      | 1200                            | 360                            | 1000            |
2.2 Inspection configuration

The objective of the experimental set-up is to produce some reference data to be compared to modelling results. Figure 2 presents the mock-up geometry. It consists of a section of the forged bar with a 100 mm thickness and a 135 mm diameter.

The reference defects used in this study are flat bottom holes of 30 mm height and respectively 3 mm, 5 mm and 8 mm diameter.

![Figure 2. Schematic representation of the experimental set-up.](image)

The ultrasonic inspection consists in an immersion inspection with longitudinal waves at 0° incidence. Three probes with different central frequencies (1 MHz, 2.25 MHz and 5 MHz) are selected in order to analyze the ultrasonic scattering for a large range of \( \lambda/D \) ratio.

The position of the probe from the upper surface of the mock-up is selected to perform a far field inspection. Once the distance from the upper surface is adjusted, the orientation of the probe is controlled by obtaining the maximum amplitude of the echo reflected by the upper surface in order to assure the orthogonality between the ultrasonic beam and the sample surface. The machining respects the parallelity of the upper, backwall and the flat-bottom hole (FBH) surfaces.

2.3. Estimation of the SNR

The comparison between experiment and modelling is based on the signal to noise ratio estimation. The signal corresponds to the specular echo reflected by the flat bottom hole. The highest echo amplitude on the whole scan is kept in. The backscattered noise is defined as the maximum of echo amplitude out of defect localization and in a time gate of 1 µs located around the top of the FBH.

3. Modelling approach : ATHENA 2D Code

3.1. ATHENA 2D Code

ATHENA 2D is a finite elements code for elastodynamics developed by EDF Research and Development Division in collaboration with INRIA [9]. The model uses a regular mesh for the calculation zone. Contact and immersed transducers are implemented. Calculations can be performed for all type of structures, especially anisotropic and heterogeneous structures [13] and take into account wave attenuation due to grain scattering [10, 11]. The beam propagation and beam to defect interactions are calculated with all conversion modes. Furthermore, defects are represented with the fictitious domain method which gives the opportunity to separate the defect and the component meshes [14].

3.2. Grain scale modelling compatible with ATHENA 2D

A study of the attenuation parameter has estimated the judicious scale necessary to describe the structure [15, 16]. Indeed, it has been demonstrated that, if the first order parameter was grain boundaries, twins have also to be taken into account to correctly reproduce the scattering phenomenon. Indeed, twins are 2D crystallographic defects corresponding to a stacking fault of the dense planes, leading to a mirror symmetry of 60° relatively to the \{111\} plane. In first
approximation, twins can be considered as grain boundaries. Consequently twin modelling can be achieved by reducing the mean grain size of the microstructure evaluated by a metallographic examination.

Microstructure modelling of polycrystalline materials can be computed using Voronoï diagrams. Voronoï polycrystals have already been used to study elastic wave scattering and provided a reliable description of a polycrystalline structure [8]. Figure 3 shows an example of a Voronoï microstructure. An example of the comparison between the simulated and the experimental grain size distribution is shown in Figure 4.

As the forged bar in Inconel 600® exhibits an isotropic structure, the determination of the orientation of one individual grain, represented by a Voronoï cell, is made through a random drawing on a thousand possible orientations. The matrix of elastic constants of each grain, expressed in the reference sample is then determined based on the single crystal elastic constants (\(C_{11} = 234.6\) GPa, \(C_{12} = 145.4\) GPa, \(C_{44} = 126.2\) GPa in the single crystal reference) [17] and the crystallographic orientation of each grain. Finally, since the 2D version of ATHENA software is used, only the four elastic constants whose indices correspond to the propagation plan are considered.

4. Results

Typical Bscan images are presented in the Figure 5 for both experimental and modelling results for the inspection at 5 MHz frequency of the sample with a mean grain size equal to 850 \(\mu\)m. These results demonstrate the relevance of finite elements and grain-scale modelling to reproduce the following scattering phenomena:

1. The presence of a backscattered noise in the form of random echoes whose amplitude decreases as the time of flight increases. This result is attributed to the attenuation of the backscattered signal and to its spatial diffusivity.
2. The poor signal to noise ratios for the FBH echoes due to both the attenuation of the defect echo and the high level of structural noise.
Figure 5: Experimental and modelling results for the 850 µm grain size mock-up with a 100 mm thickness.

To complete this validation study, quantitative values of signal to noise ratios were evaluated for every inspection configurations. The comparison between experimental and modelling SNR are presented in table 2 and table 3 for microstructures with a mean grain diameter respectively equal to 370 µm and 850 µm.

As the local microstructure around the defect is unknown, the amplitude of the FBH signal in modelling corresponds to the mean of echo amplitudes obtained from 10 different Voronoï descriptions. On the other hand, the backscattered noise in modelling corresponds to the maximum amplitude estimated for each 2D Voronoï description in order to be in agreement with the experimental procedure.

A limitation of the present approach is that 2D modelling overestimates the amplitude of the FBH echo for certain configurations (especially for 3 mm diameter FBH and low frequencies) because the fact that the beam width is higher than the defect diameter in the third dimension is not taken into account. To overcome this difficulty, the 2D effect is compensated using correction coefficients calculated for each defect and each probe. They are defined as the difference between experimental and modelling FBH to backwall echo amplitude ratio estimated in a structure with small grains corresponding to a very low attenuation.

Table 2: Experimental and modelling results in term of signal to noise ratio (dB) for a mean grain size equal to 370 µm.

| Frequency (MHz) | FBH 3 mm | | FBH 5 mm | | FBH 8 mm |
|----------------|----------|----------|----------|----------|----------|
|                | Experiment | ATHENA 2D | Experiment | ATHENA 2D | Experiment | ATHENA 2D |
| 1              | 6.0       | 5.9      | 10.9      | 11.0      | 16.2      | 15.4      |
| 2.25           | 3.4       | 5.3      | 8.8       | 10.0      | 15.9      | 15.4      |
| 5              | Not detected | Not detected | 0.2       | 0.2       | 4.8       | 4.0       |

Table 3: Experimental and modelling results in term of signal to noise ratio (dB) for a mean grain size equal to 850 µm.

| Frequency (MHz) | FBH 3 mm | | FBH 5 mm | | FBH 8 mm |
|----------------|----------|----------|----------|----------|----------|
|                | Experiment | ATHENA 2D | Experiment | ATHENA 2D | Experiment | ATHENA 2D |
| 1              | 3.7       | 2.2      | 8.0       | 6.1       | 11.5      | 11.2      |
| 2.25           | 0.2       | Not detected | 3.9      | 3.4       | 10.7      | 10.6      |
| 5              | Not detected | Not detected | Not detected | Not detected | 0.7      | 0.7       |

From table 2 and table 3, we can make the following comments:

- for one FBH : the signal-to-noise ratio (SNR) decreases as the frequency increases ;
- the SNR decreases as the grain diameter increases;
Those two results indicate that the scattering phenomenon is increasing with the mean grain diameter and with the frequency. These results are consistent with those obtained on the attenuation coefficient in the Rayleigh and stochastic scattering domains [15]. It is important to note that a mean grain size of 850 µm and a 5 MHz frequency conduct to a $\lambda/D$ ratio equal to 1.4. This value is characteristic of the stochastic domain and is associated to a maximal value of attenuation. Higher grain sizes or higher frequencies should be studied to analyze the variation of SNR in the geometric domain in which the attenuation is only dependent on the grain size and decreases when D increases. Finally, modelling results fit well the experimental data, with differences inferior to 2 dB over all the configurations tested.

This demonstrates the relevance of the modelling approach consisting in describing the microstructure at the twin and grain scale and confirms that the Voronoï diagrams are well adapted to represent a polycrystalline material. Consequently this study presents a validation of the finite elements code ATHENA 2D to simulate the scattering of a longitudinal wave propagating in a polycrystalline material.

5. Conclusion

In conclusion, the present study gives an experimental validation of ATHENA 2D code to model the scattering phenomenon of an ultrasonic compression wave propagating at 0° incidence in a polycrystalline material. The description of the microstructure at the grain scale is necessary to simulate the scattering phenomena and the level of refinement must integrate the crystallographic defects that are the grain boundaries and twins. It has furthermore been demonstrated that the Voronoï diagrams are appropriate to describe the structure. With this approach, it has been demonstrated that the FE model gives quantitative accurate results. Furthermore, it is important to notice that the multi-scattering is intrinsically integrated in the model. This is a very important difference and advantage of FE code compared to analytical models or semi-analytical models which systematically make the assumption of single scattering.

In perspectives, this study will be carried on in different directions. The first one will be dedicated to the validation of the code for shear waves and angular incidences. Finite elements modelling could also be an useful tool to develop methods of material characterization (grain size) from information given by the backscattered signals. For example, preliminary experimental works highlight differences between microstructures from the observation of a retro-scattering pick [18]. The last effort would be to develop the 3D code and associated 3D grain scale modelling. Indeed, thanks to the high computer performances and the joined parallelization of the code, this target is ambitious but realistic.

6. References

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