Finite Element Modelling of Elastic Wave Propagation in Polycrystalline Media

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Abstract

Ultrasonic Non-destructive evaluation has shown great potential in microstructural characterization and determination of structural integrity for a wide range of materials. Components being polycrystalline in nature are composed of grains having explicit size distribution and random crystallographic orientations. When a beam of ultrasound propagates in a polycrystalline medium, acoustic energy gets scattered at grain interfaces. This scattering results in loss of acoustic energy from the beam, resulting in variation of phase velocity, beam skewing and energy attenuation. Attenuation can significantly affect the ability to detect defects during inspection. Finite element (FE) modeling has shown the ability of handling complex multiple scattering occurring during these interactions. In this paper, an autogenic FE code is developed to study wave propagation phenomena in a two dimensional (2D) polycrystalline microstructure. Controlled Voronoi tessellations are generated to represent the grain structure in the polycrystalline medium. The physical domain is discretized into triangular elements and the governing equations are solved by direct time integration (explicit) scheme to approximate the solution at the nodes.

A preliminary study on an isotropic model has been performed using the in-house solver, compared with commercial FE package and also validated experimentally. This work has been further extended to study wave propagation phenomena in polycrystalline materials. The computational efficiency of the solver is examined in various case studies against that of commercial FE package.

Keywords: Polycrystalline materials, Voronoi tessellation, Finite Element Method

1. Introduction

Ultrasonic Non-Destructive Testing (NDT) techniques are extensively employed in almost all areas of Engineering for the characterization of materials and detection of defects in structures. Most metallic materials to be evaluated by NDE are heterogeneous and Polycrystalline at the mesoscale, exhibiting anisotropic behaviour. When an ultrasonic wave propagates in a Polycrystalline material, it scatters at the grain boundaries on account of crystallographic mis-orientations among the grains [1]. Each grain boundary induces an acoustic impedance step and triggers scattering of the ultrasonic signal. Local scattering leads to loss of energy of the propagating wave, resulting in wave attenuation, which depends on the wave frequency, grain size and shape, and elastic properties of the crystallites. These phenomena reduce signal- to- noise ratio (SNR) and cause beam skewing, leading to loss in detection performance [2, 3]. Hence, it is important to gain insight about the microstructure in order to improve ultrasonic NDE techniques.

In order to interpret the experimental results and obtain knowledge of the microstructural parameters from ultrasound measurements, quantitative models are necessary [4].
Hence, the development of an accurate model is significant in describing the transient propagation of ultrasonic waves through a variety of materials. Analytical modelling approaches to elastic wave propagation in solids are difficult to apply in ultrasonic testing systems, where one is interested in predicting displacement fields from ultrasound interactions. Hence, numerical modelling of ultrasound serves as a flexible tool for examining elastic wave propagation in solids [4, 5]. Finite Element Method (FEM) is a well-established numerical method which can predict the displacement field but requires high computational cost to model polycrystalline materials [6].

The objective of this paper is to build a robust FE solver in order to describe elastic wave propagation in a Polycrystalline medium based on the Finite Element Method (FEM). For this purpose, an autogenic FE code has been developed, validated and utilized to perform simulations on a 2-dimensional (2D) domain with the view of tackling the computational cost involved. The numerical code solves for transient displacement fields by integrating the system directly in time using plane strain formulation. The results obtained using the code are presented and discussed. They are validated with simulation results obtained from a commercially available FE package and experimental procedures.

The reminder of the paper is organized as follows; the mathematical formulation employed to develop the code is introduced in section 2. Section 3 describes the grain scale microstructural modelling and its discretisation. The numerical results are presented and discussed in section 4; along with validation. The computational efficiency of the in-house solver is presented in section 5. Finally, the work is summarized along with the concluding remarks in section 6.

2. Finite Element Formulation

The physical basis governing ultrasonic wave propagation and interaction in polycrystalline media is the wave equation, which in the absence of body forces is given by [7]

\[
T_{ij,j} - \frac{\partial^2 u_i}{\partial t^2} = 0
\]  

(1)

where \( T_{ij}, u_i \) and \( \rho \) denote the stress tensor, displacement vector, and material density respectively.

The stress tensor can be expressed by the modified Hooke’s law [8]

\[
T_{ij} = C_{ijkl}\varepsilon_{kl}
\]  

(2)

where \( C_{ijkl} \) and \( \varepsilon_{kl} \) are fourth order elastic constants and second order strain tensor respectively.

The strain tensor can be expressed in terms of displacements as

\[
\varepsilon_{kl} = \frac{1}{2}(u_{k,j} + u_{l,j})
\]  

(3)
The numerical implementation of eqn. (1) involves converting the governing wave equation to a discrete spatial and temporal numerical representation. The Finite Element Method (FEM) discretises the region (2D domain) into a series of finite elements where the field quantity \( u \) in the element is related to its nodal values through a set of approximation or shape functions [9]

\[
u_i = [N(i,j)]u_j
\]  

(4)

Substitution of eqn. (4) into eqn. (3) and utilizing the constitutive relation in eqn. (2) yields the elemental matrix equation by means of the weighted residual method [9]

\[
[M] \{\ddot{u}_j\} + [K] \{u_j\} = \{R\} 
\]  

(5)

\([M]\) and \([K]\) are called elemental lumped mass and stiffness matrices respectively while \([R]\) is the force vector. Equation (5) is subsequently assembled into a global matrix form encompassing all individual elemental contributions.

\[
[M] \{\dddot{u}\} + [K] \{u\} = \{R\} 
\]  

(6)

The FE solver is developed for the computer implementation of (6). The transient solution of (6) for the nodal displacements (as a function of time) is determined by an explicit, central difference, numerical integration scheme [10] which approximates \( \ddot{u} \) as

\[
\ddot{u}(t) \equiv \frac{1}{\Delta t^2} (u_{t+\Delta t} - 2u_t + u_{t-\Delta t}) 
\]  

(7)

where \( \Delta t \) is the time step.

Inserting (7) into (6) yields

\[
\frac{1}{\Delta t^2} [M] u_{t+\Delta t} = \{R\} - \left( [K] - \frac{2}{\Delta t^2} [M] \right) u_t - \frac{1}{\Delta t^2} [M] u_{t-\Delta t} 
\]  

(8)

If the reference coordinate system of a grain in the polycrystalline structure does not coincide with the natural coordinate system of the domain, the element stiffness matrix undergoes transformation given by

\[
[K]^{\ast} = [C] [K] [C]^T 
\]  

(9)

where \([K]^{\ast}\) represents the rotated elastic stiffness matrix and \([C]\) represents the Bond Transformation matrix [11] and is a function of an operator containing the direction cosines for the desired rotation.
3. **Modelling Approach**

The modelling of the ultrasonic propagation is performed with the Finite Element code developed using MATLAB R2014a [12]. In this work, we consider Copper as the Polycrystalline material for modelling.

3.1 **Microstructural Modelling**

The domain of the Polycrystalline material is modelled by Voronoi tessellation [13], which is accepted as a good approach by researchers in the field of crystallography. A Voronoi tessellation is used to subdivide a given domain into polygons to numerically generate a morphology that is geometrically similar to the grain structure of naturally occurring polycrystalline material. The tessellation is built from a stochastic distribution of seed points in the domain. Every point lying on the grain boundary is equidistant from the seed points of grains, sharing that boundary. These grain boundaries are a consequence of change in crystallographic orientation between each grain. In our simulations, studies are performed with varying grain densities. The tessellation is generated by an open-source, Unix based package Neper [14].

The elastic properties of each grain are transformed as per equn. (9) in the formulation according to its crystallographic orientation. Therefore, a grain boundary between 2 cells of different crystallographic orientations represents a step of acoustic impedance and induces the scattering of the ultrasonic beam.

3.2 **Mesh Generation**

Spatial and temporal discretisation of the Voronoi tessellation, in conjunction with a suitable choice of element type, is critical for the convergence of the numerical results. This research utilizes 2D, 3 noded, 2 degrees-of-freedom triangular elements in order to discretise the entire domain into an unstructured mesh in order to ensure mesh conformity with the geometry.

The spatial ($dh$) and temporal ($dt$) resolution are selected based on stability criteria. This is obtained using the courant condition [15].

\[
\frac{dt}{dh} C_{\text{max}} \leq \frac{1}{\sqrt{n}}
\]  

(11)
where \( C_{\text{max}} \) is the L-wave velocity, and \( n = 2 \), for a 2-dimensional grid.

For the optimization and accuracy of results, the value of \( dh \) must be of the order of \( \lambda/8 \) to \( \lambda/20 \) [16].

Figure 1 shows the FE mesh for the 2D Voronoi tessellation, generated using Neper. The data from Nepe is imported into the solver, developed in MATLAB to carry out the numerical simulations.

![Figure 1. Polycrystalline microstructure generated using Neper by (a) Voronoi tessellation (b) discretised domain.](image)

3.3 Boundary and loading conditions

The transient excitation pulse is specified by a displacement vector applied normal to the top edge of the domain, which produces the initial displacement field that simulates transducer action. A Hanning windowed, tone burst pulse is used as the input load which is given by:

\[
u(t) = a \left( 1 - \cos \left( \frac{2 \pi ft}{N} \right) \right) \cos(2 \pi ft)
(0 \leq t \leq t_0)
\]

where \( f \) is the excitation frequency and \( N \) is the number of cycles, \( a \) is the maximum amplitude of the pulse and \( t_0 \) is the overall duration of the signal; outside of this time interval the waveform is assumed to be identically zero.

All the surfaces on the numerical model are set to stress-free conditions (free boundary, \( T_y n_j = 0 \)). Table 1 gives a summary of the loading conditions. The time domain input pulse and its corresponding FFT are shown in figure 3.
### Table 1. Loading conditions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frequency (f)</td>
<td>1 MHz</td>
</tr>
<tr>
<td>Excitation Pulse</td>
<td>3-cycles, Hanning, tone burst</td>
</tr>
<tr>
<td>Max. Amplitude</td>
<td>20 nm</td>
</tr>
<tr>
<td>Pulse Width</td>
<td>3 µs</td>
</tr>
</tbody>
</table>

Figure 2. Loading conditions (a) the input pulse (b) FFT of the pulse.

4. **Numerical Results and Discussion**

The models generated using the methodology described in the previous section are simulated in the in-house FE solver. The simulation results obtained from isotropic case studies are compared with ones generated using commercial FE package COMSOL Multiphysics [17] and experimental measurements in order to validate our solver. The validated solver is implemented for the study of ultrasonic wave propagation in polycrystalline models.

4.1 Validation of in-house model

Table 2 enlists the modelling parameters for comparison with COMSOL (case I) and experimental procedures (case II).

Table 2. Isotropic Model Parameters for case I: Simulation using COMSOL and; case II: Experimental measurement

<table>
<thead>
<tr>
<th>Material Properties</th>
<th>I</th>
<th>II</th>
</tr>
</thead>
<tbody>
<tr>
<td>Domain (×10⁻³m)</td>
<td>12.5x60</td>
<td>100x25</td>
</tr>
<tr>
<td>Density (kg/m³)</td>
<td>8930</td>
<td>8950</td>
</tr>
<tr>
<td>Young’s Modulus (GPa)</td>
<td>120</td>
<td>139</td>
</tr>
<tr>
<td>Poisson’s Ratio</td>
<td>0.285</td>
<td>0.269</td>
</tr>
<tr>
<td>Longitudinal velocity (m/s)</td>
<td>4170</td>
<td>4400</td>
</tr>
<tr>
<td>Shear velocity (m/s)</td>
<td>2860</td>
<td>2473</td>
</tr>
</tbody>
</table>

6
Discretisation parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>FE solver</th>
<th>COMSOL</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean mesh size (x10^-5 m)</td>
<td>6.5</td>
<td>2.3</td>
</tr>
<tr>
<td>Time step (x10^-8 s)</td>
<td>1.1</td>
<td>2.3</td>
</tr>
</tbody>
</table>

The model, mesh and boundary conditions are identical for both FE solver and COMSOL. The ultrasonic experiments are performed in conventional through transmission mode with a pair of 1 MHz L-wave transducer (V103, Panametrics) of 0.5” aperture kept at the opposite faces of a copper specimen of thickness 25 mm available at our research facility. The 3-cycle Hanning tone burst is triggered by a Ritec Pulser/receiver and the output is digitized and displayed in a Digital Storage Oscilloscope of sampling rate 2 GHz (Keysight Technologies).

The simulation results from the in-house solver in comparison with both cases I and II are shown in figures 3 and 4 respectively.

Figure 3. FE code vs COMSOL; (a) A-scan comparison (b) Comparison of their corresponding FFT plots.

Figure 4. FE solver vs experimental results.
The match between the A-scan plots in figure 3 in terms of time of arrival, signal shape and phase demonstrate the accuracy of our solver for modelling isotropic media. Also, the numerical and experimental results are in good agreement with each other with an error of approximately 0.5 %. This suggests the capability of the FE solver as an effective tool to model ultrasonic wave propagation.

4.2 Wave propagation in Polycrystalline microstructure

Elastic wave propagation in polycrystalline medium is studied under various cases, which are detailed in table 3. The case studies are conducted by varying the number of grains in the domain, keeping the other parameters constant. The nodal displacements are monitored across the 60mm thickness at the back wall of the domain.

Table 3. Polycrystalline model parameters

<table>
<thead>
<tr>
<th>Material Parameters</th>
<th>8930</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (kg/m³)</td>
<td></td>
</tr>
<tr>
<td>Elastic constants (GPa)</td>
<td>C₃₁=168</td>
</tr>
<tr>
<td></td>
<td>C₃₂=121</td>
</tr>
<tr>
<td></td>
<td>C₄₄=75</td>
</tr>
<tr>
<td>Longitudinal velocity (m/s)</td>
<td>4337</td>
</tr>
<tr>
<td>Transverse velocity (m/s)</td>
<td>2898</td>
</tr>
<tr>
<td>Domain(x10⁻³m)</td>
<td>12.5x60</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Case studies</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of grains</td>
</tr>
<tr>
<td>Average grain size (×10⁻⁶m)</td>
</tr>
<tr>
<td>Regularity Parameter</td>
</tr>
</tbody>
</table>

The displacement plots and the corresponding frequency spectra for the different case studies are shown in figure 5.
Figure 5. Case studies on ultrasonic wave propagation in polycrystalline material with 750, 6000 and 15000 grains showing (a) Time domain signals (b) FFT plots.

The FFT plots indicate an apparent shift in the frequency of the received signal, which approaches that of the isotropic case with increase in grain density. The high frequency components encounter scattering at the grain interfaces, which is a function of the grain size in the domain. Furthermore, a decrease in signal amplitude with increasing grain size can be observed from the time domain plots, which gives a quantitative representation of the attenuation due to the scattering phenomena. The degree of scattering on account of grain density affects the ultrasonic material characterization of the polycrystalline structure. An illustration of wave propagation through the polycrystalline structure in contrast to that of the isotropic model is shown in figure 6.
5. Solver Efficiency

The main focus of this work is to develop an efficient FE solver that can handle complex geometries, fine discretisation and boundary conditions by utilizing minimal computational resources. The computational efficiency of the current FE solver has been examined in terms of solving time; as opposed to that of the commercial FE package. Case studies are done on a set of models with varying number of elements and time step as shown in table 4.

<table>
<thead>
<tr>
<th>Case</th>
<th>Domain (mm)</th>
<th>Time step (ns)</th>
<th>Number of time steps</th>
<th>Number of elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>30x12.5</td>
<td>14.2</td>
<td>1759</td>
<td>23898</td>
</tr>
<tr>
<td>2</td>
<td>60x15</td>
<td>9.9</td>
<td>2508</td>
<td>107862</td>
</tr>
<tr>
<td>3</td>
<td>12.5x60</td>
<td>11</td>
<td>2253</td>
<td>173152</td>
</tr>
<tr>
<td>4</td>
<td>90x25</td>
<td>10.1</td>
<td>2464</td>
<td>266946</td>
</tr>
<tr>
<td>5</td>
<td>120x40</td>
<td>9.5</td>
<td>3664</td>
<td>567208</td>
</tr>
<tr>
<td>6</td>
<td>200x50</td>
<td>11</td>
<td>2500</td>
<td>1918526</td>
</tr>
</tbody>
</table>

The computation time depends on the discretisation of the model. In reference to the computations performed by the MATLAB code and COMSOL, figure 7a shows a plot of solution time vs number of elements for both the cases. Overall, for the case studies conducted, the in-house FE solver reduces the computational effort by 98% as compared to COMSOL.
In case of Polycrystalline models, the computation time is dependent on the model discretisation as well as complexity of grains in the domain, which affects the average mesh size. Studies on polycrystalline models are done as listed in table 5. The solution time for these models are compared with similar ones simulated using COMSOL and is plotted in figure 7b.

<table>
<thead>
<tr>
<th>Case</th>
<th>Number of grains</th>
<th>Number of Elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>750</td>
<td>201349</td>
</tr>
<tr>
<td>2</td>
<td>1500</td>
<td>212812</td>
</tr>
<tr>
<td>3</td>
<td>3000</td>
<td>246382</td>
</tr>
<tr>
<td>4</td>
<td>6000</td>
<td>252130</td>
</tr>
</tbody>
</table>

Figure 7. Comparison of solution time between in-house FE solver and COMSOL for (a) Isotropic models (b) Polycrystalline models.

6. Conclusions and Prospects

This paper describes the creation of an efficient FE solver that is capable of simulating ultrasonic wave propagation in polycrystalline materials in 2D with reduced computational cost. The formulation used to develop the solver has been introduced. The well-established method of voronoi tessellations has been employed to generate the grain morphology, which is then discretised and solved for transient displacement fields. The solver is validated across commercial FE package and experimental procedures in order to reaffirm the accuracy and feasibility of the solver to simulate ultrasonic wave propagation. The scattering phenomenon in polycrystalline media has been examined in different case studies with varying grain densities. The studies show the decay of higher frequency components with increasing grain size. The computational efficiency of the solver has been demonstrated as it outperforms the commercial FE package in terms of solver time.

Work is currently underway to extend the modelling capabilities of this solver to 3D polycrystalline media, along with the implementation of GPU to further enhance the computational efficiency. A user-friendly Graphical User Interface (GUI) needs to be developed.
References


