Image-Based Finite Element Simulation of Ultrasonic Wave in Polycrystalline Metal using Phase-Field Modeling

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Abstract. When modeling ultrasonic wave testing in metals with coarse grains, it is important to introduce crystalline structures because the anisotropy of the crystal structure and the heterogeneity of grains disturb ultrasonic waves. To improve inspection capabilities for the polycrystalline metal in ultrasonic testing, an image-based simulation which can model the mesoscopic metal structure becomes an effective tool. In this research, a three-dimensional (3D) polycrystalline structure generated by multiphase-field modelling was introduced to ultrasonic wave simulation. 3D finite element simulations of ultrasonic waves were validated and compared with visualization results obtained from laser Doppler vibrometer measurements. The simulation results and measurements showed good agreement with respect to the wave velocity, as well as multiple scattering from grains.

1. Introduction

In the ultrasonic testing (UT) for metals with coarse grains, such as austenitic steel, ultrasonic wave is disturbed by the anisotropy of the crystal structure and by the heterogeneity of metal grains with different orientations. These two factors result in the skewing of the ultrasonic beam and energy diffusion. Local scattering from the grains reduces the signal-to-noise ratio of ultrasonic echoes, and beam skewing leads to incorrect positioning and sizing of flaws. Several studies for austenitic steel in the past several decades have described mathematical weld models and methods for evaluating flaws in welds. The ray-tracing method proposed by Ogilvy [1,2] is a model-based approach used to predict wave propagation in a weld. Recently, image based approaches using convex cells of the Voronoi partition have been proposed to imitate the texture of the weld [3,4]. Although it can accurately describe grains with equiaxed structures, the Voronoi model is not easy to use for creating arbitrarily shaped grains such as columnar crystals.

In this study, a 3D grain model generated through a phase-field method [5] is introduced to the UT simulation. The phase-field method is a mathematical model that solves moving interfacial problems that has been used in solidification dynamics, solid-state phase transformations, martensitic transformations, and grain growth, among others. To treat multigrain structures of the metal, we adopt the multiphase-field (MPF) model proposed by Steinbach [6]. The 3D numerical model of the polycrystalline metal is fed into the simulation tool of the finite-element method (FEM). In FEM, the voxel element is used because the digital volume image from the MPF model can be used directly as a simulation data set.
ultrasonic wave simulations for the investigation are performed by using MPF models with different grain sizes and orientations. The simulation is validated by comparison with the visualization results obtained from laser Doppler vibrometer (LDV) measurements [7].

2. Image-based FEM

2.1 Explicit FEM with Voxel Element

In transient-wave analyses, the FEM can be classified as either implicit or explicit in general. Finite-element equations in the explicit approach can be solved directly by using previously known solutions. Although the explicit scheme has to fulfill the Courant-Friedrichs-Lewy condition to avoid numerical divergence, it is easy to incorporate the parallel computation technique for a large scale simulation. Here, we adopt an explicit procedure, and show a brief outline of the explicit FEM in the following paragraph.

The position vector \( \mathbf{x} = (x_1, x_2, x_3) \) is defined in the Cartesian coordinates with the base unit vectors \( \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3 \). We start with the virtual-work-principle form of the Cauchy equation of motion:

\[
\int_V \left( \partial_t \mathbf{w} \right)^T \mathbf{F} \, dV(x) + \int_V \rho \mathbf{w}^T \ddot{\mathbf{u}} \, dV(x) = \int_S \mathbf{w}^T \tau \, dS(x)
\]

vector \( \mathbf{u} = (u, v, w) \) is the displacement vector, \( \rho \) is the density, \( \mathbf{t} = (t_x, t_y, t_z) \) is the traction vector, \( \mathbf{w} = (w_x, w_y, w_z) \) is the virtual displacement, \( \partial \) is the differential operator matrix, \( (\partial^T \partial) \) is transposed matrices, and \( \ddot{\mathbf{u}} = \partial^2 \mathbf{u} / \partial t^2 \). \( \tau \) is the stress tensor of the second rank, which satisfies the following constitutive law:

\[
\tau_{ij} = c_{ijkl} \varepsilon_{kl}, \quad (i, j = 1, 2, 3)
\]

where \( c_{ijkl} \) is the fourth-rank tensor which shows the elastic stiffness. The summation convention rule for \( k \) and \( l \) applies. A stiffness tensor, \( c_{ijkl} \), which is measured in a crystal coordinate system \( (x^i_1, x^i_2, x^i_3) \) with coordinate unit vectors of \( (e^i_1, e^i_2, e^i_3) \) is expressed as \( c^i_{ijkl} \). To treat various crystal orientations, the transformation of \( c^i_{ijkl} \) in the crystal coordinate system into the coordinate system \( (x_1, x_2, x_3) \) is performed through the transformation law [8].

\[
c_{ijkl} = c_{ijkl}^{C} \sum_{ln} l_{im} l_{jn} l_{kp} l_{pq}, \quad (i, j, k, l = 1, 2, 3)
\]

where \( l_{im} \) is the direction cosine between two coordinate systems, which can be written as \( \cos(\mathbf{e}_i, \mathbf{e}_m^C) \).

By using an eight-node isoparametric hexahedral element with side length of \( \Delta x \), the finite-element matrix equations can be derived from Eq. (1):

\[
M \ddot{\mathbf{u}} + K \mathbf{u} = \mathbf{f}
\]

where \( \mathbf{f} \) is the nodal forces, \( \mathbf{u} \) is the nodal displacement, \( M \) and \( K \) are the global-mass and stiffness matrices, respectively. Here, the voxel element is used in the FEM because the digital volume image can be used directly as the simulation data set. In this case, material parameters are assumed to be constant in an element.

Next we consider the discretization of Eq. (4) in the time domain. The current time step and step interval are denoted by the integer \( k \) and \( \Delta t \), respectively. By using the central-difference formula, Eq. (4) gives

\[
\mathbf{u}^{k+1} = (2I - \Delta t^2 M^{-1}K)\mathbf{u}^k + \Delta t^2 M^{-1}\mathbf{f}^k - \mathbf{u}^{k-1}
\]
where $E$ is the unit matrix, and $M^{-1}$ is the lumped mass matrix, which has values only at the diagonal components. The above equation shows that the displacement of the step $k+1$ can be obtained directly by using the known solutions at steps $k$ and $k-1$. In the explicit FEM, we only allocate the computational memory for the displacement node, but prepare two step previous displacement data.

2.2 Property of Austenitic Steel

In this study, we consider a modeling of austenitic stainless steel. Since the austenitic stainless steel has a cubic structure, we use the following elastic parameter:

$$
\begin{bmatrix}
   c_{111}^C & c_{122}^C & c_{112}^C & 0 & 0 & 0 \\
   c_{122}^C & c_{111}^C & c_{122}^C & 0 & 0 & 0 \\
   c_{112}^C & c_{112}^C & c_{111}^C & 0 & 0 & 0 \\
   0 & 0 & 0 & c_{323}^C & 0 \\
   0 & 0 & 0 & 0 & c_{323}^C \\
   0 & 0 & 0 & 0 & 0 & c_{323}^C
\end{bmatrix} \begin{bmatrix}
   212.0 & 133.2 & 133.2 & 0 & 0 & 0 \\
   133.2 & 212.0 & 133.2 & 0 & 0 & 0 \\
   133.2 & 133.2 & 212.0 & 0 & 0 & 0 \\
   0 & 0 & 0 & 0 & 119.6 & 0 \\
   0 & 0 & 0 & 0 & 0 & 119.6 \\
   0 & 0 & 0 & 0 & 0 & 119.6
\end{bmatrix} = [\text{GPa}] \ (6)
$$

The density of the steel is 7.8 g/cm$^3$. Figure 1 shows the group velocity curves of Pressure wave (P wave) and Shear waves (S1 and S2 waves) calculated with the stiffness component in Eq. (6).

![Fig. 1. Distributions of group velocities of austenitic stainless steel with cubic structure $c_{\mu\nu}^C$ in Eq. (6).](image)

3. Multiphase-field Model

The phase-field method has become a powerful tool for simulating microstructural evolution in a wide variety of material processes, such as solidification, solid-state phase transformations, martensitic transformations, and grain growth. The shape and mutual distribution of the grains are represented by phase-field variables that are continuous in space and time. To treat multigrain multiphase structures in metal, we adopt the MPF model proposed by Steinbach [6]. The microstructure is expressed in terms of a set of order parameters, each of which is related to a specific crystalline orientation. The phase field variable $\phi_\alpha(x,t)$ indicates the $\alpha$-th grain. In the MPF modeling, $n$ is the local number of grains. The following sum constraint applies:

$$
\sum_{\alpha=1}^{n} \phi_\alpha(x,t) = 1. \tag{7}
$$
The MPF equations are derived as follows:

\[
\frac{\partial \phi}{\partial t} = -\frac{2}{n} \sum_{j=1}^{n} M_{ij}^{\phi} \left[ \sum_{k=1}^{n} \left( W_{ik} - W_{jk} \right) \phi_k + \frac{1}{2} (a_{ik}^2 - a_{jk}^2) \nabla^2 \phi_k \right] - \frac{8}{\pi} \sqrt{\phi \phi_{ij}} \Delta f_{ij}
\]

where \( \nabla^2 \) is the Laplacian operator; \( \gamma_{ij} \) is the energy of the interface between grain \( i \) and \( j \); \( M_{ij}^{\phi} \) is the mobility; \( \delta \) is the interface width, which is treated as a single value for all interfaces in this model; and \( \Delta f_{ij} \) is the chemical free energy. The evolution of the phase-field variables is expressed by partial differential equations, which can be solved numerically. Equation (8) can be solved through the finite-difference scheme with grid size \( \Delta x \) and time interval \( \Delta t \). We use the forward difference with respect to time and the central difference for space as follows:

\[
\begin{align*}
\frac{\partial \phi}{\partial t} & \rightarrow \frac{\Phi_{i}^{k+1}(l,m,n) - \Phi_{i}^{k}(l,m,n)}{\Delta t} \\
\frac{\partial^2 \phi}{\partial x_1^2} & \rightarrow \frac{\Phi_{i}^{k}(l-1,m,n) - 2\Phi_{i}^{k}(l,m,n) + \Phi_{i}^{k}(l+1,m,n)}{\Delta x_1^2} \\
\frac{\partial^2 \phi}{\partial x_2^2} & \rightarrow \frac{\Phi_{i}^{k}(l,m-1,n) - 2\Phi_{i}^{k}(l,m,n) + \Phi_{i}^{k}(l,m+1,n)}{\Delta x_2^2} \\
\frac{\partial^2 \phi}{\partial x_3^2} & \rightarrow \frac{\Phi_{i}^{k}(l,m,n-1) - 2\Phi_{i}^{k}(l,m,n) + \Phi_{i}^{k}(l,m,n+1)}{\Delta x_3^2}
\end{align*}
\]

where \( \Phi_{i}^{k}(l,m,n) \) are computational arrays to store the value \( \phi_i(x,t) \), and the superscript \( k \) is the time step. Our primary objective is to be able to generate the final form of a 3D metal texture, which has a realistic appearance, while disregarding the progress of grain growth at each time step. Therefore, we use the normalized parameters of the interface energy \( \gamma \), the mobility \( M \), and chemical free energy \( \Delta f \). Here, \( \delta \) is set such that \( \delta = 7\Delta x \) in the MPF simulation. However, the time increment should fulfill the following relation \( \Delta t \leq (\Delta x)^2 / (6 M^\phi \alpha^2) \) for the stable calculation.

4. Simulation of Wave Propagation in Polycrystalline Metal using MPF Model

We performed 3D MPF simulations for the growth of polycrystalline crystals in a region with dimensions of 30 x 10 x 30 [mm]. In this simulation, we make two models with different size and orientation. Figures 2(a-1) and (b-1) show the grain model A and B, respectively. In Model A and B, spatially distributed nuclei of the number 104 and 12498 were present at the first step in the MPF simulation, respectively. The color of the grain in Figs. 2(a-1) and (b-1) indicates the grain ID assigned at the first step. After the MPF simulation, the average diameter of the columnar grain became approximately 1.5 mm and 0.7 mm in Model A and B, respectively.

In the ultrasonic-wave simulation with the FEM, we had to tie up the grain to the crystalline orientation, that is, the Euler angle. Here, we classified 26 dominant groups of Euler angles. All the surfaces on the numerical model show the stress free condition. We assume that an incident wave with a center frequency 1.0 MHz is emitted from a contact transducer region with diameter 12.7 mm on the top surface of the specimen. The incident pressure is distributed uniformly across the transducer surface. In the FEM, we choose \( \Delta x = 0.02 \) mm and \( \Delta t = 1.75 \) ns to keep the convergence of the simulation. Therefore, the total voxel number becomes 1500 x 500 x 1500.
Fig. 2. FEM simulation results (snapshot of displacement field) of the wave propagation in the interior of the Model A and B generated from MPF simulations.

Figures 2(a-2) and (a-3) show the snapshot of wave propagation (absolute value of the displacement vector, \( |\mathbf{u}| = \sqrt{u_1^2 + u_2^2 + u_3^2} \)) in Model A. Figures 2(b-2) and (b-3) show the absolute value of the displacement vector in Model B. In Fig. 2, the wave front of the P wave is visible, however, the S waves are scarcely observable because of strong grain scattering and attenuation. The displacement in Model B is slightly larger than the one in Model A. The Fourier spectra of displacement \( u_3 \) obtained at the depth 10 mm and 25 mm from the top surface are plotted in Fig.3. The frequency is shifted to the lower side in spite of the incident wave with the center frequency of 1 MHz. Furthermore, the ultrasonic wave is strongly attenuated at the deep position. Although, in general, the disturbance due to grain scattering becomes significant as the diameter of the grain increases, the simulation results in Model A and B show slight difference. The reason is that the grain size in Model A and B is sufficiently small compared with the wave length of incident wave.

Fig. 3. Fourier spectra of displacement \( u_3 \) in Model A and B at 10mm and 25mm depth from the top surface.
5. Validation of Image-based FEM Simulation

In order to check the validation of the image-based FEM, we compare the numerical result with the measured data. Here, we used an austenitic stainless steel specimen that was unidirectionally solidified. The material is ER316L, which is used for welding low-carbon molybdenum-bearing austenitic alloys. Figure 4 shows the picture of ER316L specimen. From the EBSD pattern, it was found that the grains with around 1 mm diameter were mainly solidified, and the columnar grain extended along the $x_3$ direction. Here, we performed simulations for the growth of polycrystalline crystals in a region with dimensions of 30 x 30 x 10 [mm]. Figure 4(a) shows the grain growth from spatially distributed nuclei. In the MPF simulation, 744 nuclei were present at the first step. The color of the grain in Fig. 4(a) indicates the grain ID of nucleus assigned at the first step. Here, we used the stiffness matrix expressed in Eq. (6), and classified 25 dominant groups using the rotation equation in Eq. (3). The information was applied into the generated grain. On the other hand, the motion due to wave propagation is experimentally visualized by LDV measurements, as shown in Fig. 4(b). An incident wave with a center frequency 2.0 MHz is emitted from a contact transducer region with diameter 12.7 mm on the top surface of the specimen.

Fig. 4. (a) 3D model of austenitic stainless steel that was unidirectionally solidified. (b) Experimental setup with LDV device for visualization of wave propagation.

Figures 5(a) and (b) show the visualizations of $|u|$ on the surface of the austenitic steel by the image-based FEM and the anti-plane displacement $|\sigma_2|$ measured by the LDV, respectively. In the image-based FEM, we choose $\Delta x = 0.02$ mm and $\Delta t = 1.75$ ns to keep the convergence of the simulation. The total voxel number and time incremental number become 1500 x 500 x 1500 and 3500, respectively. The simulated and measured snapshots are in good agreement with the front shape of the P wave. Furthermore, the average of the velocity in the simulation is a good approximation of the one in the measurement. Grain scattering in the simulation continues for a slightly longer time than in that in the measurement. We need to introduce an attenuation factor due to intrinsic absorption and non-reflective boundary condition into the FEM.

6. Conclusions

In this study, a 3D multigrain structure generated by MPF modeling was introduced into ultrasonic UT simulation. The 3D numerical model was imported into the simulation tool of
the image-based FEM. Using the MPF model, we can describe the propagation direction of the ultrasonic wave as well as the multiple scattering by the grains. We showed that the disturbance by grain scattering became significant as the diameter of the grain increased. The accuracy of the image-based FEM simulation was validated with visualizations of wave propagation by LDV measurement. The specimen with unidirectionally solidified austenitic steel was used. The simulation and measurement results were in good agreement with respect to the wave velocity and front shape of the P wave.

We will apply the image-based FEM to more realistic simulations for wave propagation in metals such as dissimilar metal welding and rolled steel bar.

![Image of wave visualization](image1.png)

**Fig. 5.** Visualization of the wave motion on the surface of austenitic steel specimen (ER316L) by image-based FEM (a) and LDV measurement (b).

**References**


