Effect of columnar grain shape modeling on the microscopic stress distribution at the clad weld metal surface of Ni base alloy

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Abstract. Recently, crystal plasticity simulations have been widely used to evaluate microscopic stress. However, the appropriate simulation model has not yet been determined. In this study, the microscopic stresses in the clad weld metal of Ni base alloy were simulated. A series of simulations using columnar grain shape models with different thicknesses indicated that a sufficient thickness is required for the evaluation of microscopic stress at the surface and that the adequate model thickness could be determined by the proposed approach. Additionally, a series of simulations using models with different column axes indicated that the column axis has little effect on the microscopic stresses at the surface of the metal.

1. Introduction
The increase in atmospheric carbon dioxide is a global problem. A large part of human carbon dioxide emissions comes from fossil-fuelled thermal power plants. Nuclear power generation can replace thermal power generation; however, the risk associated with nuclear power plants is a major concern. Recently, intergranular stress corrosion cracking (IGSCC) has been observed in Ni base alloy weld metal in nuclear power plants. The microscopic stress at the surface is an important factor. The stress concentrations near grain boundaries and triple junctions are caused by the different crystal orientations of neighboring grains. Therefore, a numerical simulation that considers the crystal orientations is needed to calculate the microscopic stress. The crystal plasticity finite element method (CP-FEM) is a numerical method that considers crystal orientation and has recently been widely used.

Although it is known that the simulation results are affected by the geometrical model used, the appropriate model for CP-FEM simulations has not yet been determined. To calculate the microscopic stress distribution at the surface of Ni base alloy weld metal, the appropriate model needs to be established. In particular, the grain cross sections and the crystal orientation distribution of a section can easily be measured using the electron backscatter diffraction (EBSD) technique. However, it is difficult to obtain accurate three-dimensional grain shapes. So, the effect of grain shape modeling on the simulation result should be investigated.

Generally, the crystalline structure of weld metal consists of columnar grains, which are slender in shape. In particular, columnar grains constituting clad weld metal are aligned as shown in Figure 1. So, the crystalline structure of clad weld metal can be characterized by the column axis, which is the longitudinal direction of the columnar grain. The column axis corresponds to the grain growth direction, and the grain growth direction depends on the welding conditions and the welding direction.
The purpose of this study is to investigate the effects of the model thickness and the column axis on the microscopic stress distribution at the surface of the clad weld metal of Ni base alloy. In this study, columnar grain shape models with different thicknesses and different column axes were generated based on the crystal orientation distribution measured using the EBSD technique. Then, the microscopic stresses at the surface of the clad weld metal of Ni base alloy were calculated using CP-FEM.

![Column axis](image)

**Figure 1.** Illustration of the crystalline structure of clad weld metal.

2. **Crystal orientation distribution at the surface of the clad weld metal of Ni base alloy**

First, a clad weld specimen was fabricated. Two layers of Ni base alloy were deposited on low alloy steel by submerged arc welding using a band electrode. The welding conditions are shown in Table 1. The low alloy steel (SQV2A) was 226 mm in width, 410 mm in length, and 167 mm in thickness. The Alloy 82 electrode was 75 mm in width and 0.4 mm in thickness. The chemical composition of the low alloy steel is shown in Table 2, and the chemical composition of Alloy 82 is shown in Table 3. An overview of the clad weld joint is shown in Figure 2. The $X$ direction was the welding direction, the $Y$ direction was perpendicular to the welding direction, and the $Z = 0$ plane was the surface of the weld metal. A specimen for measuring the crystal orientations was cut from the center of the last pass as shown in Figure 2. Then, the crystal orientation distribution at the surface of the weld metal was measured using the EBSD technique. The inverse pole figure (IPF) map is shown in Figure 3. As seen in the figure, the $<100>$ direction is mainly observed along the direction perpendicular to the surface of the weld metal. Additionally, the average grain diameter (equivalent to the average width of the columnar grains on the surface) was $2.5 \times 10^2 \mu m$.

**Table 1.** Welding conditions.

| Power source | Welding current (A) | Arc voltage (V) | Welding speed (cm/min) | Wire extension (mm) | Preheating and interpass temperature (ºC) |
|--------------|---------------------|-----------------|------------------------|---------------------|------------------------------------------|
| DC           | 1100–1300           | 26–28           | 18                     | 40                  | 100–150                                  |

**Table 2.** Chemical composition of the low alloy steel (mass%).

| C   | Si  | Mn  | Ni  | Fe  | Mo  | P   | S   |
|-----|-----|-----|-----|-----|-----|-----|-----|
| 0.2 | 0.27| 1.47| 0.66| Bal.| 0.55| 0.01| 0.008|

**Table 3.** Chemical compositions of Alloy 82 (mass%).

| C   | Si  | Mn  | Ni  | Fe  | Cr  | Ti  | Cb+Ta |
|-----|-----|-----|-----|-----|-----|-----|-------|
| 0.012| 0.02| 3.45| 72.56| 0.83| 19.83| 0.61| 2.61  |
Figure 2. Geometry of the clad weld joint and location of the specimen for measuring the crystal orientation.

Figure 3. IPF map of the surface of the weld metal.

3. Numerical simulation model
Columnar grain shape models were generated with the same grain cross section on the surface and with different grain shapes in the Z direction. The grain cross section on the surface and the crystal orientation of each grain were based on the EBSD results.

In order to investigate the effect of the model thickness on the microscopic stress distribution at the surface of the metal, simulation models with different thicknesses were generated. The column axis was set parallel to the Z direction. The thicknesses of the simulation models were varied according to the following seven cases: 15, 75, 150, 450, 750, 1050, and 1500 µm. The simulation models with the different thickness are shown in Figure 4.

In order to investigate the effect of the column axis on the microscopic stress distribution at the surface of the metal, simulation models with different column axes were generated. The thickness of the simulation models was 750 µm. The column axis was defined by two angles: α and β. The angle between the column axis and the X direction was defined as α and the angle between the column axis and the Y direction was defined as β. These angles were varied according to the following five cases: (α, β) = (90°, 90°), (80°, 90°), (−80°, 90°), (90°, 80°), and (90°, −80°). The simulation models with the different column axes are shown in Figure 5.
A displacement corresponding to 5% macroscopic tensile strain was applied to each model in the $Y$ direction. At this strain level, stress in the $Y$ direction becomes comparable to the residual stress occurring in clad weld metal. The numerical simulation was performed using the commercial finite element software Abaqus and incorporated a UMAT subroutine to consider the crystal plasticity theory [1, 2]. In each simulation model, we confirmed that the characteristics of the microscopic stress distribution at the surface, for example, the location where stress concentration occurs, do not change qualitatively when the applied macroscopic tensile strain changes.

**Figure 4.** Columnar grain shape models with different thicknesses: (a) 15 µm, (b) 75 µm, (c) 150 µm, (d) 450 µm, (e) 750 µm, (f) 1050 µm, and (g) 1500 µm.

**Figure 5.** Columnar grain shape models with different column axes. The angles ($\alpha, \beta$) are: (a) (90º, 90º), (b) (80º, 90º), (c) (90º, 80º), (d) (90º, 90º), and (e) (90º, −80º).
4. Effect of grain shape modeling on the microscopic stress distribution at the surface

4.1. Effect of the model thickness on the microscopic stress distribution at the surface
The results of the series of simulations using models with different thicknesses are shown in Figure 6. When the thickness is less than 150 µm, the microscopic stresses near grain boundaries are greatly affected by the thickness of the simulation model. It is known that the surface of a thin plate is under a plane stress state. The more the thickness increases, the more the stress state at the surface deviates from a plane stress state. For a model thickness of less than 150 µm, it is considered that the model thickness greatly affects the microscopic stresses near grain boundaries at the surface due to the deviation from a plane stress state. This indicates that a sufficient thickness is required for the evaluation of IGSCC at the surface. The microscopic stress distribution becomes more similar as the model thickness increases. The threshold is approximately 750 µm, corresponding to three times the average width of the columnar grains.

4.2. Effect of the column axis on the microscopic stress distribution at the surface
The results of the series of simulations using the models with different column axes are shown in Figure 7. Although the column axes are different, the results are similar to each other. This indicates that the column axis has little effect on the microscopic stresses at the surface of the weld metal.

![Microscopic stress distributions at the surface of the metal calculated using simulation models with different thicknesses: (a) 15 µm, (b) 75 µm, (c) 150 µm, (d) 450 µm, (e) 750 µm, (f) 1050 µm, and (g) 1500 µm.](image-url)
5. Conclusions
In this paper, the microscopic stress distributions were calculated using CP-FEM with columnar grain shape models with different thicknesses and different column axes. Then, the effects of model thickness and column axis on the microscopic stress distribution at the surface of the clad weld metal of Ni base alloy were discussed. The conclusions of this paper are summarized as follows.
(1) When the column axis is perpendicular to the surface of the weld metal, a sufficient thickness is required for the evaluation of microscopic stress at the surface. Furthermore, the adequate model thickness for the simulation of microscopic stresses at the surface of the weld metal could be determined. This suggests that the adequate thicknesses of other grain models can also be determined by the proposed approach.
(2) The column axis had little effect on the microscopic stress distribution at the surface of the weld metal.

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