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Phase Field Simulation of Stress Evolution during Grain Growth Process

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Summary

Stress evolution during grain growth in microstructure formation process are simulated by using the phase field model. Fundamental equations accounting for the coupling effects among phase transformation, temperature and stress/strain have been formulated based on thermodynamical laws, in which thermal expansion, transformation dilatation, and stress dependency on phase transformation are considered. An elasto-plastic constitutive relationship is applied so as to obtain the residual stresses. Based on these equations, numerical simulations are carried out by the finite element method. Results for two kinds of initial arrangement of nuclei are demonstrated in this paper. One model has four nuclei at the four corners of a square model resulting in cross-shaped grain boundaries, while another has nine internal nuclei incorporating polycrystalline structure. For both models, large stresses are generated at phase interfaces in the early stage when precipitated phase grow freely. Then remarkably higher stresses are observed at grain boundaries when grain collision occurs. The high-stress regions move as grains grow, and finally residual stress distribution along the grain boundaries is observed.

Introduction

Phase filed model has become one of the most promising tools for simulating microstructures of materials, such as dendrite [1,2], facet [3], directional cellular structure [4], and polycrystal [5,6]. In engineering viewpoint, macroscopic mechanical properties of materials are strongly dependent on the microstructure incorporated with phase transformation, which have been simulated by the phase field model. However, not only the morphology of the microstructure, but also the existence of residual stress affects the strength of the materials, as well as dynamic stress evolution causing crack formation and fracture during solidification. Therefore, the stress analyses have also been required. For this purpose, Inoue et al.[7] have formulated the coupling effects among phase transformation, temperature, and stress/strain from a classical continuum mechanical approach: i.e. volume fractions of every phase consisting the material are introduced as internal variable, and the mixture law is applied to represent the properties of entire material. In this method, however, the morphology and distribution of grains are inherently excluded. Meanwhile, the phase field model is considered to complementally overcome this weak point.

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Table 1: Parameters applied for simulations.

m	2.5×10^{5}	a, m^4	10	b, m^3/J	5.0×10^{-5}
L, J/m^3	3.0×10^{3}	T_m, K	400	ρ, kg/m^3	1.0×10^{3}
c, J/kg K	5.0×10^{2}	k, W/m K	150	α, 1/K	5.0×10^{-6}
β	1.5×10^{-3}	h, W/m^2 K	1.0×10^{4}	T_W, K	300
E, GPa	200	ν	0.3	σ_Y, MPa	250
H', MPa	250	n_1, MPa^{-1}	1.0×10^{-2}	n_2, MPa^{-2}	1.0×10^{-5}
Δx, m	1.0×10^{-2}	Δt, s	1.0×10^{-2}		

Fundamental equations for the phase field analyses of solidification process have been derived in thermodynamically consistent way by Wang, Sekerka et al.[2,8], and the effect of stress/strain can be appended by considering suitable energetic terms. Kassner et al.[9] and Hu et al.[10] have accounted for elastic strain energy to include the effect of strain on crystal growth. However, dynamic stress evolution by using the phase field model has not been fully investigated yet. One of the authors has derived a simplified model to show stress evolution during solidification by assuming liquid does not bear stress [11], and extended it to solid-solid transformation by applying the elasto-plastic constitutive relationship [12]. In this paper, the applied equations and the results of numerical simulations by using the finite element method are demonstrated.

Fundamental Equations

Fundamental equations are derived based on thermomechanical coupling, which is introduced in another literature[12]. The final formula of the equations is as follows.

Phase field equation:

$$m\dot{\phi} = a\nabla^2\phi + \phi(1-\phi)\left[\phi - \frac{1}{2} + M(\phi, T, \sigma_{ij})\right], \tag{1}$$

where,

$$M(\phi, T, \sigma_{ij}) = b\phi(1-\phi)\left(L\frac{T_m - T}{T_m} + f(\sigma_{ij})\right), \tag{2}$$

and

$$f(\sigma_{ij}) = n_1\sigma_{kk} + n_2\sigma_{ij}\sigma_{ij}. \tag{3}$$

Heat conduction equation:

$$\rho c\dot{T} = k\nabla^2 T + 30L\phi^2(1-\phi)^2\dot{\phi} - \alpha T\dot{\sigma}_{ij}\delta_{ij} + \sigma_{ij}\dot{\varepsilon}^{p}_{ij}. \tag{4}$$

Stress-strain relationship:

$$\dot{\varepsilon}_{ij} = \frac{1+\nu}{E}\dot{\sigma}_{ij} - \frac{\nu}{E}\dot{\sigma}_{kk}\delta_{ij} + \dot{\varepsilon}^{p}_{ij} + \alpha\dot{T}\delta_{ij} + 30\beta\phi^2(1-\phi)^2\dot{\phi}\delta_{ij}. \tag{5}$$

Here, ϕ is the phase field variable, m, a and b are the parameters depending on the interfacial thickness and energy, and L and T_m are latent heat and transformation temperature, respectively. A function $f(\sigma_{ij})$ expresses the stress dependency of phase transformation, and n_1 and n_2 are arbitrary parameters. The other parameters of ρ, c and k are mass density, specific heat and thermal conductivity, respectively. Variables for mechanical fields of σ_{ij}, ε_{ij} and $\varepsilon^{\mathrm{p}}_{ij}$ are stress, strain and plastic strain, respectively, and E, ν, α and β are Young's modulus, Poisson's ratio, thermal expansion coefficient and transformation dilatation modulus, respectively. δ_{ij} in Eqs (4) and (5) is Kronecker's delta. For the plastic constitutive relations, Mises yield function and kinematic hardening law are applied.

Model and Conditions

Based on the fundamental equations mentioned in the previous section, finite element analyses are carried out. In this paper, grain growth of precipitated phase is assumed, to examine the stress evolution during grain growth and residual stress distribution.

A two-dimensional square region divided with triangular mesh is prepared. Whole region is assumed to be uniformly in parent phase at a certain temperature with no initial stress distribution. The four boundaries are mechanically constrained, and thermally contacted to the surroundings of temperature T_{W} with heat transfer coefficient h. Parameters applied in the simulations are listed in Table 1, where σ_{Y} and H' are the initial yield stress and hardening coefficient, and Δx and Δt are the mesh size and time increment for numerical calculation, respectively. These values are determined based on those for typical steel but larger values for some parameters are applied so that the coupling effects clearly appear in the results.

Two kinds of simulations are demonstrated in this paper. One is for cross-shaped grain boundary formation, for which four nuclei of precipitation phase are set on every corner of the square region at the initial calculation step. The other one is for polycrystalline formation, for which nine nuclei are disposed randomly in the model.

Results I: Four-Nuclei Model

Figure 1 shows the variation of (a) phase field, (b) grain number, (c) temperature and (d) equivalent stress distribution, respectively, during grain growth from four nuclei. Grain numbers are independently assigned for each nucleus when they are disposed, and given to precipitated region to keep the number of the nucleus from which the corresponding gain initiated. The temperature $\bar{T}$ and equivalent stress $\bar{\sigma}_{\mathrm{eq}}$ are represented in normalized values so as to represent the qualitative results.

Grain growth processes from the nuclei are represented in Figs 1 (a) and (b). Since the anisotropy is not introduced in this model, the phase interfaces keep circular shape. The grains collide at the middle of four edges at t=10 s. After the collision of the grains, in-phase grain boundaries are formed, and finally, a mono-phase state with four grains are obtained. Temperature distribution is affected by

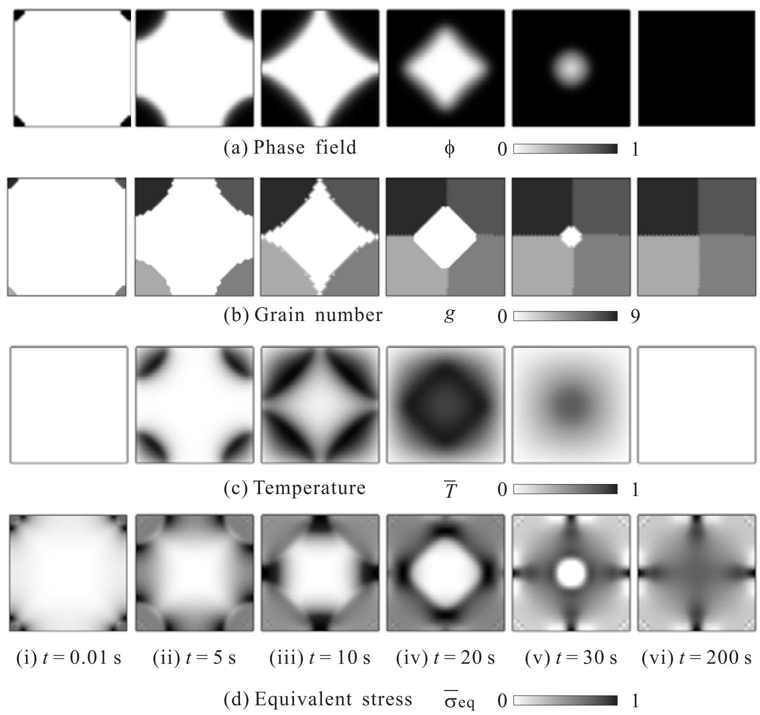

Figure 1: Variation of phase field, grain number, temperature and equivalent stress distribution during grain growth from four nuclei.

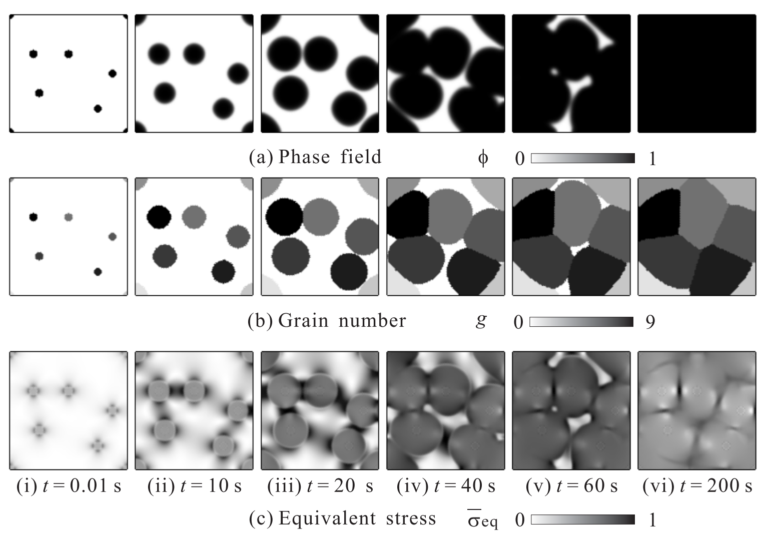

Figure 2: Variation of phase field, grain number and equivalent stress distribution during grain growth from nine nuclei, resulting in polycrystalline formation.

the phase transformation due to latent-heat generation, as shown in Fig. 1 (c). High temperature at the phase interface occasionally causes instability of transformation, and possibly incorporates dendritic growth, though it is not observed in this model.

Figure 1 (d) shows the stress evolution during grain growth. High stress regions are distributed around the phase interfaces by t=10 s before the grains collide. Since volumetric dilatation is assumed in this simulation, compressive stresses are generated when transformation occurs. After t=10 s when pairs of grains collide, significantly high stresses are observed at the collision sites as shown in Fig. 1 (d)(iii). The high-stress points move inside as grain boundary is formed toward inside the model as shown in Figs (iv) and (v), and a cross-shaped high-stress zone is generated. As a result, residual stress distribution is retained when transformation completes in the whole region.

Results II: Nine-Nuclei Model

Figure 2 exhibits (a) phase field, (b) grain number, and (c) equivalent stress distribution during grain growth from nine nuclei.

Precipitated grains start growing from nine nuclei as shown in Figs 2 (a) and (b). The shapes of grains are circular since no anisotropy is introduced in this paper. At around t=40 s, grains start colliding at several points, and grain boundaries are formed to result in polycrystalline structure with nine grains. Some of the grain boundaries have slight curvature. This reveals that the effect of stress dependency of phase transformation introduced in Eq.(3), since rather straight boundaries are formed without using $f(\sigma)$, though it is not discussed here in detail.

As shown in Figs 2 (c)(i)-(iii), high stress areas appear around the phase interface in the early stage when grains grow freely. Especially the regions where grains are closely located show higher stress in the parent phase. After t=40 s when grains collide with each other, grain boundaries present high stress, and finally residual stress distribution is remarkably observed along the grain boundaries. As shown in Fig. 2(c)(vi), the stress values on the grain boundaries are not identical, which might be caused by the timing of collision and spacing of nuclei.

Concluding Remarks

Phase field simulations of stress evolution during grain growth are carried out based on the fundamental equations considering the coupling effects among phase, temperature and stress/strain. As a result, it revealed that high stress is generated at the phase interface when the phase transformation proceeds freely. When the grains of precipitated phase collide and grain boundaries are formed, high stress regions are generated along the grain boundaries, and finally retained as the residual stresses. In this paper, the anisotropy of the grain growth and that of mechanical properties originating from the crystal orientation are not taken into account. The consideration of atomistic source of plasticity, such as dislocation and atomic shuffling at the grain boundary, is also a problem to be resolved for improving the current model.

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