Dislocation Controlled Segregation-Assisted Precipitation and Pinning Grain Growth: A Phase-Field Study

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Abstract: Based on the grain growth model and dislocation stress field model, we investigated the dynamic processes of grain growth and nucleation and growth of CRPs, with the combined effect of dislocations and grain boundaries. Meanwhile, CRPs can pin grain growth to maintain smaller grain sizes. Simulation results reveal that both grain boundaries and dislocations promote the nucleation and growth of Cu phase, hindering grain growth. The precipitate is a dual core-shell structure of Mn/NiAl/Cu at the grain boundary in the middle stage of aging. The precipitate at the grain boundary is a co precipitate of MnNiAl and Cu rich, while the intragranular precipitate is a dual core-shell structure of Mn/NiAl/Cu in the later stage of aging. The precipitation at the grain boundary undergoes a process of strip→spherical→strip with increasing dislocation density. On the whole, this modeling framework provides an avenue to explore the role of dislocation on the grain growth and microstructural evolution of Cu-rich precipitates.

Keywords: Grain growth, Dislocation, Phase-field method, Cu-rich precipitates.

1 Introduction

Fu-Cu alloy—as a typical nanocrystalline metal, its high-density grain boundaries exhibit a unique combination of characteristics, which also constitute a huge driving force for grain growth [1]. The ability to stagnate grain growth and retain the nano-crystalinity of Fu-Cu alloy under high temperature and for extended time scales is arguably one of the enormous challenges to the RPVs [2]. Several studies, such as recrystallization, pore or bubble drag, precipitate pinning and solute segregation have been shown to mitigate grain growth [3]. In recent years, GBs segregation-assisted precipitates has been the subject of active research as it has been proposed as important route to stagnate grain growth in Fu-Cu alloy. However, coarse precipitates and strip/needle shaped precipitates at GBs lead to stress concentration, increasing the risk of catastrophic failure. Ensuring the pinning of GBs segregation-assisted precipitates and the fine distribution of precipitation dispersion is one of the important issues that still need to be addressed. Although the precipitation process of multi-component Fe-Cu-based alloys has been studied, the effect of dislocations on the morphology of precipitates at grain boundaries and precipitates at grain boundaries pinned grains growth have not been reported. On this basis, a phase field model was established by coupling grain growth, multi-component field, and dislocation elastic field. The simulation model and results in this work were integrated into the EasyPhase software package developed by Professor Zhao. The purpose is to study the process of grain boundary precipitation, dislocation-controlled grain boundary precipitation, and precipitation pinning grain growth.

2 Phase field model

Our phase field model is built upon the incorporation of structural order parameters (OPs) $\phi_p(\boldsymbol{r},t)(p=1,\dots,m)$ ($\phi_p(\boldsymbol{r},t)$ characterizes the grains present in the alloy, each possessing distinct crystal orientations) and compositional field $c_i(\boldsymbol{r},t)$ $(i=2,3,4,5$ are Cu, Mn, Ni and Al atoms, respectively). We propose the expression for the overall free energy F, which can be written as

$$F = \int \begin{bmatrix} f_{ch}(c_i,T) + \frac{1}{2}\sum k_{c_i}^2(\nabla c_i)^2 + \frac{1}{2}\sum k_{\phi_p}^2\left(\nabla\phi_p\right)^2 \\ + f_{\text{grain}}\left(\phi_p\right) + f_{inter}\left(c_i,\phi_p\right) + f_{el}\left(c_i,\phi_p\right) \end{bmatrix} dV \quad (1)$$

According to Khachaturyan' micromechanical theory, the elastic stress $\sigma_{ij}^{el}(\boldsymbol{r})$ can be expressed as:

$$\sigma_{ij}^{el}(r) = C_{ijkl}\varepsilon_{kl}^{el}(r) = \left(C_{ijkl}^0 + \Delta C_{ijkl}\Delta c\right)\left(\delta\varepsilon_{ij} - \varepsilon_{ij}^0 - \varepsilon_{ij}^d\right) \# (2)$$

The governing equations for the evolution of the concentration field c and OPs ϕ_i, can be stated respectively as

$$\frac{\partial c_i(\boldsymbol{r},t)}{\partial t} = \nabla\cdot M\cdot\nabla\frac{\delta F}{\delta c_i(\boldsymbol{r},t)} + \xi_{c_i}(\boldsymbol{r},t)$$
$$\frac{\partial \phi_i}{\partial t} = -L_i\frac{\delta F}{\delta \phi} \qquad \#(3)$$

3 Result and discussion

The simulation results in Fig. 1 show that solute atoms preferentially aggregate at the triple intersections. Subsequently, solute atoms aggregate at grain boundaries and gradually form granular CRPs. Meanwhile, granular CRPs absorb solute atoms near grain boundaries to connect as strips of CRPs (a Cu/Mn/NiAl double core-shell structure), leading to the formation of solute-poor and solute-rich regions. Mn, Ni and Al atoms continue to aggregate at the shells of the CRPs gradually forming co-precipitates of Cu-rich and MnNiAl.

Fig. 1. 2D element distribution diagram of polycrystalline grain boundaries and intra particle precipitation

While the intracrystalline randomly formed spherical CRPs of double core-shell structure. There is a competitive mechanism between the nucleation and growth of CRPs within the grains and the growth of CRPs at the grain boundaries, that is, the nucleation and growth of CRPs within the grains leads to the refinement of CRPs at the grain boundaries. The equivalent stress result in Fig. 1 (b) shows that the strip-shaped CRPs lead to stress concentration at grain boundaries. The 2D results in Fig. 2 indicate that solute atoms preferentially aggregate at dislocations of grain boundaries. Solute atoms continue to aggregate at dislocation to form spherical CRPs, leading to an increase in solute poor regions around grain boundaries. Subsequently, a small portion of spherical CRPs at the grain boundaries gradually connects to form short rod-shaped CRPs, while spherical CRPs form gradually within the grain. Competition between precipitation within the grain and at the grain boundaries leads to the refinement of spherical and short rod-shaped Cu-rich cores at the grain boundaries. The equivalent stress in Fig. 2(b) shows almost no stress concentration. This indicates that a $3.43\times10^{13}/m^2$ dislocation density can significantly regulate the morphology of CRPs at the grain boundaries, thereby resulting in a more uniform stress distribution.

Fig. 2 Dislocation of $3.43\times10^{13}/\mathrm{m}^2$ regulates the process of polycrystalline precipitation

4 Conclusion

This study investigates the process of grain growth, grain boundary precipitation and pinning, as well as the regulation of grain boundary precipitation and pinning of grains by dislocations of grains in Fe-Cu-Mn-Ni-Al alloys. The segregation of solute atoms near grain boundaries forms CRPs that can effectively pin grain growth. But the strip-shaped CRPs lead to significant stress concentration. A uniformly distributed dislocation with a density of $3.43\times10^{13}/m^2$ at the grain boundary can effectively regulate the morphology of precipitated phases at the grain boundary. The precipitates at the grain boundaries are double core-shell structures of Cu/NiAl/Mn in the middle stage of aging, which are co-precipitates of Cu-rich and NiAl/Mn in the late stage of aging.

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