Phase Field Simulation of Precipitation Relevant to Imperfection of Crystal

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In the last two decades, the phase-field approach [1] has become a useful and powerful tool for understanding and modeling phase transformations and microstructure evolutions across many fields in materials science. The meaning of phase field is the spatial and temporal order-parameter field defined in a continuum diffused interface model. By using the phase-field order parameters, various types of complex microstructure changes observed in materials science can be efficiently described.

In this study, as typical examples of phase-field simulation applied to the precipitation behavior relevant to the imperfections of crystal such as the dislocation, the interface between different phases, and the grain boundary, the recent simulation results of the phase transformations and microstructure evolutions in Fe based alloys are demonstrated.

Figure 1 shows the simulation result of Cu precipitation on the edge dislocation during isothermal aging at 823K in Fe-10at%Cu. The local composition is represented in grayscale, so that the black part indicates high concentrations of Cu atoms. The numerical values in the upper-left corner of each figure indicate the dimensionless aging time. The white line at the center of each figure indicates the position where the extra half atomic plane exists, i.e. the edge dislocations are located at both ends of the white line. The direction of the edge dislocation line is perpendicular to the figure and the Burgers vector is along vertical direction. The initial state of the alloy is the supersaturated solid solution with bcc crystal structure. At the early stage of aging, Cu(bcc)-rich phase starts to nucleate preferentially at the outside region of the edge dislocation. This is because the stress field induced by the edge dislocation is relaxed by the lattice mismatch between Cu precipitate and matrix. Therefore, this precipitation behavior is mainly controlled by the elastic field relevant to both of the dislocation and the precipitate.

Figure 2 shows the two-dimensional simulation of the isothermal phase transformation of the supersaturated solid solution of α (bcc) phase at 873 K in an Fe-15 at.%Cu-1 at.%Mn-1 at.%Ni quaternary alloy [2], which is a base alloy of the light-water reactor pressure vessel. The upper two rows in Fig.2 indicate the crystal structure field and Cu composition field, respectively. The lower two rows show Ni and Mn composition fields. As for the crystal structure field, the brightness of the figure means the probability for finding fcc structure. On the other hand, the local composition is also indicated by the gray scale, where pure Cu, 10 at.%Mn and the 10 at.%Ni appear as white. In the early stage, Cu-rich zones appear, and Ni and Mn atoms are partitioned in the Cu-rich phase (Fig.2(a)). As aging progresses, the Ni atoms inside the precipitates move to the interface region between the precipitate and matrix. Mn atoms do not move to the surface of the Cu particle, and the Mn concentration in the center of the Cu particle is increased. In the later stage of aging, the Cu-rich α (bcc) phase eventually transforms to the γ (fcc) phase (Fig.2(c)), and the segregation of Ni atoms at the surface of the Cu particle is enhanced. Segregation of Mn atoms also takes place, and then the shell structure appears (Fig.2(d)).
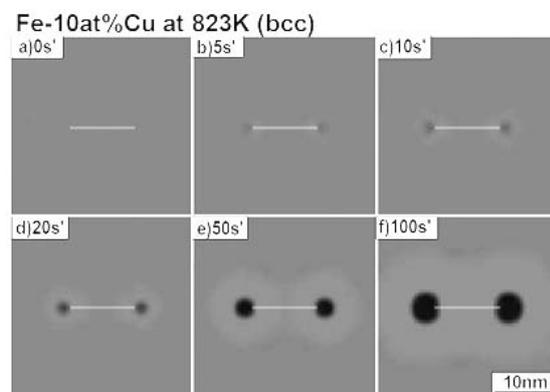

FIG.1 Simulation of Cu precipitation on edge dislocation during isothermal aging at 823K in Fe-10 at.%Cu.

Figure 3 shows the two-dimensional simulation of phase transformation and microstructure development in Fe-0.4 mass.%C at 1023K with an external magnetic field along the vertical direction [3]. The microstructure change in the upper row in Fig. 3 demonstrates the temporal evolution of the phase field that represents the polycrystalline grain microstructure. The gray and white regions indicate α-ferrite and γ-austenite phases, respectively. The lower row of Fig. 3 shows the temporal development of the carbon composition field. The local composition value in the microstructure is represented in grayscale, and a dark shade means a high concentration of carbon atoms, i.e., pure Fe and Fe-1 mass.%C correspond to white and black, respectively.

At the initial stage of aging (Fig. 3(a)), carbon atoms begin to segregate in the grain boundary region of the polycrystalline α phase, and the carbon-enriched part becomes slightly elongated along the vertical direction. This tendency is enhanced with aging and the γ phase nucleates at the grain boundary region with high carbon concentration (See Fig. 3(b)). As shown in Figs. 3 (b) and (c), the γ phases grow along the vertical direction so as to follow the carbon-enriched region at the grain boundary, and the volume fraction of the γ phase increases. Finally, it is seen in Fig. 3(d) that the (α+γ) two-phase structure elongated along the external magnetic field. Since the scale of microstructure covered by the phase-field method is mostly the mesoscopic scale, the phase-field method is used as a buffer simulation between the first-principals atomistic calculation and the macroscopic computer-aided process simulation such as the finite-element method, and the continuum phase-field model can be applied to any microstructure changes in alloys, ceramics, and polymer systems. Therefore, the phase-field method will be a suitable simulation method for understanding the mesoscopic and multiscale complex microstructure formations in materials science.
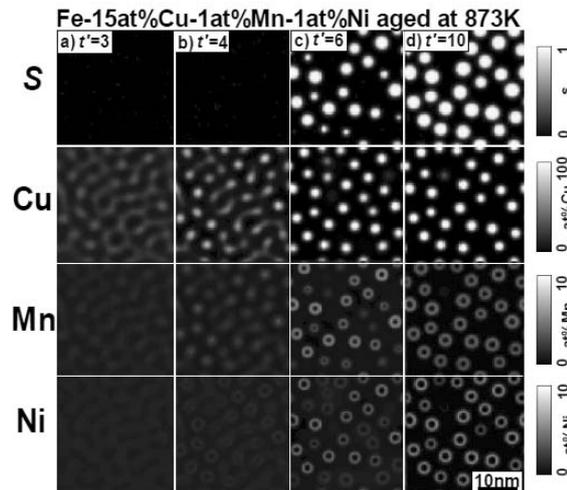

FIG.2 Simulation of the isothermal phase transformation of α phase in an Fe-15 at.%Cu-1 at.%Mn-1 at.%Ni ternary alloy at 873K [2].

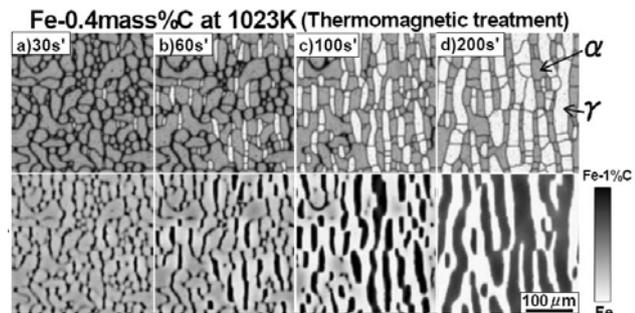FIG.3 Simulation of microstructure development in Fe-0.4 mass.%C at 1023K with external magnetic field along vertical direction [3].

References
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