§32. Dissolution of Ordered Precipitates Due to Local Disordering and Atomic Mixing under Irradiation

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Stability of ordered precipitates under particle irradiation is recognized as a relevant subject in the application of intermetallic alloys to nuclear technology. When an alloy is exposed to irradiation with energetic particles, the external forces due to the particles act directly on the constituent atoms, and often induce disordering and dissolution of initially ordered precipitates. Matsumura, *et al.* [1,2] have proposed a mesoscopic description on kinetics of the phase change induced by the external forces and/or the thermally activated atomic motions based on a time-dependent Ginzburg-Landau (TDGL) model for local degree of order $S(\boldsymbol{r},t)$ and compositional modulation $X(\boldsymbol{r},t)$. In the present study, the TDGL equations of S and X were employed to simulate the microstructural change due to stochastic local disordering and atomic mixing in precipitated alloys under irradiation.

If particle irradiation produces local damaged areas, the temporal change of local composition X and degree of order S can be described as follows:

$$\frac{\partial X}{\partial t} = \theta(\boldsymbol{r},\phi,t)D^{mix}\nabla^2 X + L(T,\phi)\left(\frac{\delta F}{\delta X} - \mu\right), \qquad (1)$$

and

$$\frac{\partial S}{\partial t} = -\theta(\boldsymbol{r},\phi,t)M^{bal}S - M(T,\phi)\frac{\delta F}{\delta X}, \qquad (2)$$

where ϕ is the atomic displacement rate due to the irradiation, F is the free energy, μ is the chemical potential, and L, M, D^{mix} and M^{bal} are positive constants for the thermal mobility of atoms, the ordering rate, the ballistic mixing coefficient and the ballistic disordering rate, respectively. The first terms in the right hand side of eqs. (1) and (2) express ballistic mixing and disordering of atoms as local events within cascade damaged regions under irradiation. The shape function θ defines the damaged regions formed at a time t, taking unity within these areas but otherwise zero. On the other hand, the second terms in eqs. (1) and (2) represent thermal processes of atomic motion approaching the equilibrium state. The free energy is expressed by a Ginzburg-Landau form,

$$F = \int \left\{ f(X,S,T) + \frac{H}{2}(\nabla X)^2 + \frac{K}{2}(\nabla S)^2 \right\} d\boldsymbol{r}, \qquad (3)$$

and the bulk free energy density $f(X,S,T)$ is given by

$$f = X^2 + b(T)\left\{x_0(T)^2 - X^2\right\}S^2 + b(T)^2 x_1(T)^2 S^4. \qquad (4)$$

Here, H and K are the interfacial energy coefficients for local fluctuation in X and S, and a, b and x_1^2 are positive constants depending on temperature T. The parameter x_0 determines the ordering phase field. For simplicity, the thermal and the ballistic parts of atomic motion were handled separately in the simulation. In a unit time interval Δt, the irradiation at first produces damaged regions with a given probability. The positions of the regions were determined stochastically with an array of random numbers. We assumed that the complete disordering and the homogenization in concentration occur within the damaged regions at the same time as their formation. Following the production of damaged regions, the thermal relaxation proceeds for the finite time interval Δt, according to the second terms in eqs. (1) and (2). The above procedure of simulation was repeated given times I.

Fig. 1 shows an example of partial dissolution of a precipitate due to random formation of the damaged regions. Here, the upper and lower rows give temporal changes in X and S, respectively. One can see that the initially ordered precipitate located at the center shrinks and splits into finer particles. We are now studying the disordering and dissolution process as a function of damage rate and size of damaged regions. The results will be reported elsewhere in near future.

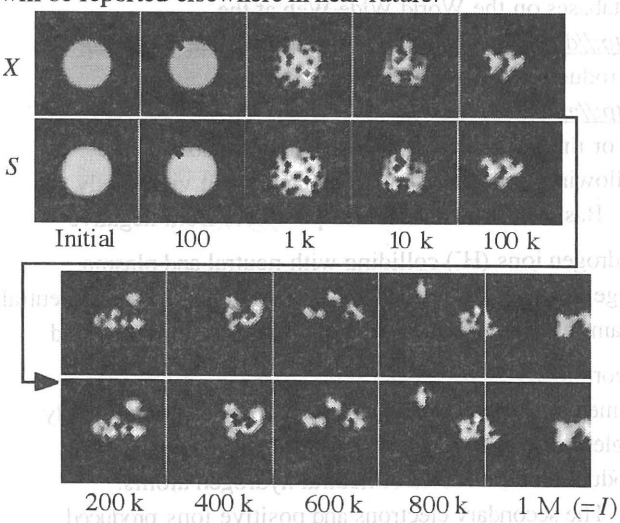

Fig. 1. Time evolution of partial dissolution of an ordered precipitate.

References

(1) Matsumura, S., Müller, S. , and Abromeit, C., Phys. Rev. B **54**,(1996) 6184.

(2) Matsumura, S., Tanaka, Y., Müller, S., and Abromeit, C., J. Nucl. Mater. **239**, (1996) 42.