S. Fitzgerald

DE-FG05-93ER45507-FINAL

FINAL REPORT

DOE GRANT DE-FG05-93ER45507

15 September 1993 - 14 September 1997

Microstructural Evolution in Elastically Stressed Systems

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1 Overview

The purpose of our research program has been to understand the influence of alloy composition, elastic misfit strain, applied stress and stress gradients on microstructural evolution in multiphase structural alloys. The long-term goal of our research has been to identify those material parameters that promote microstructural stability against coarsening in multicomponent, multiphase systems at elevated temperatures.

Our efforts have been focussed primarily on two fronts. First, we developed a method and the corresponding code to simulate the *three-dimensional* coarsening behavior of elastically and diffusionally interacting spherical particles in an infinite matrix. Second, in continuing collaboration with Dr. Michael Fährmann and Prof. Teresa Pollock, we completed a set of experiments using model ternary Ni-Al-Mo alloys that were designed intentionally to provide quantitative data on symmetry-conserving and symmetry-breaking precipitate shape transitions and particle coarsening kinetics in order to obtain a critical check on the theory and computer simulations developed in this work. In addition, we have initiated a study involving the motion of nonequilibrium interfaces during diffusional phase transformations. These technical results are presented in more detail below, along with a list of publications resulting entirely from this Grant.

This program was initially funded for three years. However, as we were able to keep our expenditures low, we applied for and received a one-year, no-cost extension for the period September 15, 1996 to September 14, 1997. This extension enabled graduate student W. H. Hort to complete his Ph.D. and B. H. Hinderliter to initiate his Ph.D. research. We feel significant progress has been made in the last four years in understanding the effect of elastic stress on microstructural evolution and are grateful for the support, both financial and technical, provided us by the Department of Energy.

2 Technical Program

2.1 Computer Simulations

Assuming a spherical precipitate shape, we simulated the *three-dimensional* coarsening behavior of elastically and diffusionally interacting precipitates by solving simultaneously the elastic and diffusion field equations. Elastic stresses from misfit strains and applied stresses, including stress gradients, were considered along with elastic inhomogeneity (different elastic constants between precipitate and matrix). The simulation procedure required that the elastic field associated with a distribution of coherent, misfitting particles be determined first. The elastic field was then used to calculate the stress-dependent boundary conditions for diffusion obtained from the thermodynamics of stressed solids. The multiparticle diffusion problem was subsequently solved under the quasi-static approximation using the method of irreducible multipole tensors. Instantaneous radial growth rates and migration rates were obtained from mass balance at the interfaces and then time-integrated to follow the temporal evolution of the system. The influence of applied uniaxial loads and stress gradients as well as the sign and magnitude of the misfit strain on the coarsening behavior of soft and hard precipitates was investigated.

Our simulations indicated that particle misfit strains, the elastic interaction between precipitates, and the presence of an applied stress field can induce microstructures that are both qualitatively and quantitatively different from two-phase microstructures that develop during coarsening in the absence of stress. In particular, misfit strains were shown to lead to the development of strong spatial correlations between particles including the alignment of particles and the formation of precipitate clusters. Elastic interactions between precipitates and interaction between precipitate misfit strains and applied stresses resulted in significant precipitate migration and strong preferential coarsening of the particles. The preferential coarsening took the form of both inverse coarsening (smaller particles grow at the expense of larger particles) and accelerated coarsening where the elastic interaction between particles induces an accelerated growth or dissolution of certain particles in comparison to the unstressed case. Of particular interest was that a stressed coarsening system need not scale in a self-similar manner with time. This suggests that the temporal power laws describing microstructural evolution in unstressed systems are not necessarily applicable to stressed systems, so long as the system remains coherent. Such a deviation from the expected temporal power law for coarsening was observed in the simulations.

In our most recent work, we have begun to examine diffusion-induced, nonequilibrium interface motion in multicomponent stressed systems. We have obtained analytic approximations for the linear and parabolic growth rate constants, and for the time dependence of the interfacial compositions and interfacial velocity of a planar interface using a linearized gradient approximation. The results, which have been compared to numerical simulations and found to be in very good agreement, predict that deviations in composition on the order of several atomic percent (measured with respect to equilibrium compositions) are possible at the interface. Interfacial compositions are strongly time dependent and are also influenced by the stress state.

2.2 Experiments

Experimental work was conducted in collaboration with Dr. Michael Fährmann (now research scientist at INCO ALLOYS) and Prof. T. Pollock of Carnegie Mellon University. We examined the influence of the sign and magnitude of the misfit strain on particle shape evolution and microstructural evolution in five model Ni-Al-Mo ternary alloys ($\gamma - \gamma'$) using TEM and SAXS. Misfit strains were determined using x-ray diffraction at the aging temperature and the γ' volume fraction was approximately 10% in each alloy. The misfit strains varied from +0.6% to −0.3%. Particle shape changes, particle alignment, and coarsening kinetics were measured and quantified for all five alloys as a function of aging time and temperature.

Elastic misfit was shown to control both precipitate shape transitions and particle alignment. We observed both symmetry-conserving, sphere-to-cube transitions and the symmetry-breaking, cube-to-cuboid transitions with increasing particle size. These observations were quantified and compared with two-dimensional calculations of particle shape in a nickel matrix and a three-dimensional analysis of particle-shape transition sizes based on a bifurcation analysis (developed during a previous grant). General trends in particle shape evolution were found to be in excellent agreement with both theories.

It was also shown that the preferential partioning of the slow-diffusing Mo to the matrix phase resulted in a decrease in the coarsening rate with increasing Mo content rather than the decreased coarsening rate being a result of a change in the sign of the precipitate misfit, as had been argued in the literature. The experimental results were in good agreement with our theoretical calculations. We believe these experimental efforts to be one of the first attempts to compare systematically the effect of misfit strain on particle shape transitions and coarsening kinetics with theory in two-phase solid systems.

3 Personnel

W.H. Hort was a graduate student supported entirely by this grant. He earned his Ph.D. from CMU in December 1996, although he performed the last three years of his research at UVa. He is currently doing post-doctoral work at the University of Pittsburgh.

B.H. Hinderliter is a Ph.D. graduate student in the Engineering Physics Program at UVa. He has been supported by this grant for the past two years and has been actively involved with our efforts to look at interface motion in systems far from equilibrium. He has passed his Ph.D. comprehensive examination.

W.C. Johnson recently won the School of Engineering and Applied Sciences H. Morton Award for Undergraduate Teaching.

4 Publications from Grant

The following publications resulting from research supported entirely by this grant have been published or submitted since 1993:

1. T.A. Abinandanan and W. C. Johnson, "Coarsening of Elastically Interacting Coherent Particles: 1. Theoretical Formulation", *Acta metall. et mater.* **41**, 17-25 (1993).
2. T.A. Abinandanan and W. C. Johnson, "Coarsening of Elastically Interacting Coherent Particles: 2. Simulations of Preferential Coarsening and Particle Migrations", *Acta metall. et mater.* **41**, 26-39 (1993).
3. W. Hort and W. C. Johnson, "Diffusional Boundary Conditions During Coarsening of Elastically Interacting Precipitates", *Metall. Mater. Trans.* **25A**, pp. 2695-2703, 1994.
4. M. Fährmann, P. Fratzl, O. Paris, E. Fährmann and W. C. Johnson, "Misfit Strain-induced Shape Transitions of the γ' Phase in Model Ni-base Alloys", *Proc. Symp. on Alloy Phase Stability and Design*, eds; G. M. Stocks and P. E. A. Turchi, (TMS-AIME, 1994) pp. 157-163.
5. W. Hort and W. C. Johnson, "Coarsening of Tetragonally Misfitting Second-phase Particles: Domain Building and Applied Stress", *Proceedings of an International Conference on Solid-Solid Phase Transformations*, W. C. Johnson, J. M. Howe, D. E. Laughlin and W. A. Soffa, eds., (TMS-AIME, 1994) pp. 629-635.
6. M. Fährmann, P. Fratzl, O. Paris, E. Fährmann and W. C. Johnson, "Effect of Misfit Strain on Microstructural Evolution in Model Ni-Al-Mo Alloys", *Proceedings of an International Conference on Solid-Solid Phase Transformations*, W. C. Johnson, J. M. Howe, D. E. Laughlin and W. A. Soffa, eds., (TMS-AIME, 1994) pp. 593-99.
7. M. Fährmann, P. Fratzl, O. Paris, E. Fährmann and W. C. Johnson, "Influence of Coherency Stress on Microstructural Evolution in Model Ni-Al-Mo Alloys", *Acta metall. mater.* **43**, pp. 1007-1022, 1995.
8. T. A. Abinandanan and W. C. Johnson, "Development of Spatial Correlations During Coarsening", *Mater. Sci. Engr.*, **B32**, pp. 169-180, 1995.
9. W. Hort and W. C. Johnson, "Effect of Uniaxial Stress on Coarsening of Precipitate Clusters", *Metal. Mater. Trans.* **27A**, pp. 1460-1476, 1996.
10. W. Hort and W. C. Johnson, "Coarsening of Precipitate Clusters in Stress Gradients", *Scripta Metal. Mater.* **34**, pp. 1015-1020, 1996.
11. M. Fährmann, E. Fährmann, T. M. Pollock and W. C. Johnson, "Element Partitioning During Coarsening of $\gamma - \gamma'$ in Ni-Al-Mo Alloys", *Metal. Mater. Trans.* **28A**, pp. 1943-1946, 1997.
12. W. C. Johnson and B. H. Hinderliter, "Diffusion-Induced Interface Motion in Ternary Systems with Interfacial Kinetic Barriers", *Solidification 98*, in press.
13. W. Hort and W. C. Johnson, "Coarsening of Misfitting Precipitates in Low Volume Fraction Multicomponent Alloys", submitted.
14. W. C. Johnson and B. H. Hinderliter, "Nonequilibrium Evolution of Stressed Planar Interfaces", submitted.