Evolution of Local Microstructures: Spatial Instabilities of Coarsening Clusters

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Introduction

This work examines the diffusional growth of discrete phase particles dispersed within a matrix. Engineering materials are microstructurally heterogeneous, and the details of the microstructure determine how well that material performs in a given application. Critical to the development of designing multiphase microstructures with long–term stability is the process of Ostwald ripening. Ripening, or phase coarsening, is a diffusion–limited process which arises in *polydisperse* multiphase materials. Growth and dissolution occur because fluxes of solute, driven by chemical potential gradients at the interfaces of the dispersed phase material, depend on particle size. The kinetics of these processes are "competitive," dictating that larger particles grow at the expense of smaller ones, overall leading to an increase of the average particle size. The classical treatment of phase coarsening was done by Todes, Lifshitz, and Slyozov (TLS) in the limit of zero volume fraction, V_v, of the dispersed phase. Since the publication of TLS theory there have been numerous investigations, many of which sought to describe the kinetic scaling behavior over a range of volume fractions. Some studies in the literature report that the relative increase in coarsening rate at low (but not zero) volume fractions compared to that predicted by TLS is proportional to $V_v^{1/2}$, whereas others suggest $V_v^{1/3}$. This issue has been resolved recently by simulation studies at low volume fractions in three dimensions by members of the Rensselaer/NASA Marshall Space Flight Center team.

Background and Objectives

Our studies of ripening behavior using large–scale numerical simulations suggest that although there are different circumstances which can lead to either scaling law, the most important length scale at low volume fractions is the diffusional analog of the Debye screening length. The numerical simulations we employed exploit the use of a recently developed "snapshot" technique, and identifies the nature of the coarsening dynamics at various volume fractions. Preliminary results of numerical and experimental investigations, focused on the growth of finite particle clusters, provide important insight into the nature of the transition between the two scaling regimes. The companion microgravity experiment centers on the growth within finite particle clusters, and follows the temporal dynamics driving microstructural evolution, using holography.

This combined experimental and modeling approach also reveals the existence of spatial instabilities in microstructural homogeneity due to Debye screening, beyond which a particle within a cluster is not influenced by the presence of other particles. This screening length places limits on the extent and applicability of a mean-field description, and can result in local divergences from mean-field behavior. This research effort will extend our preliminary discoveries and develop a critical microgravity experiment to observe these phenomena in a suitably quiescent environment.

Work accomplished to date shows that the critical cross–over between the two scaling regimes ($V_v^{1/2}$ versus $V_v^{1/3}$) is a function of both the volume fraction, which, intuitively, affects this screening length, and the cluster size, *n*, where *n* is the number of particles comprising the cluster. Specifically, the cross–over occurs at a critical volume fraction for which $V_v \approx 1/(3n^2)$. One also expects that the volume fraction itself fluctuates from region–to–region, because the local size and distribution of particles vary. Thus, spatial variances should arise in the local kinetics. One of the scientific objectives of this work is to identify the nature of these microstructural fluctuations. This added level of understanding will be of importance in the development of more predictive models for microstructural evolution in heterogeneous materials.

Approach

Studies will continue on mixed–dimensional coarsening where three–dimensional particles grow via diffusion limited in two dimensions. This situation is of importance in the fabrication of thin–film microelectronic devices, where islands of deposited phase coarsen from surface diffusion of adsorbed atoms along the substrate. The dimensionality of the problem suggests that the growth law scaling should be $\langle R \rangle \approx t^{1/4}$, where $\langle R \rangle$ is the average radius of the island domains; this dependency is indeed observed experimentally.

We are also developing experiments to study three–dimensional coarsening in a finite cluster of droplets containing different volume fractions located at the central area of our holographic observation cell. This approach eliminates the influences of the container walls, and allows direct observation of the coarsening process. The goal is to confirm experimentally critical predictions about coarsening behavior in finite clusters, including the influence of local volume fraction on the kinetics. In mixed-dimensional a “new” length scale is expected – one set by the appropriate Debye screening and resultant local deviations from the mean field.

Holographic imaging is the optical tool selected for observing these phenomena. Holography provides more data than does conventional optical imaging techniques. A reconstructed hologram is amenable to various optical characterization techniques (e.g., *in situ* microscopy) and interferometry. An important aspect of the experimental study will include determining the extent of modifications required to allow incorporation of holography within operating envelope of the millikelvin thermostat (MITH) hardware.