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Three-dimensional Phase field Simulations and Microstructural Reconstructions of Systems Undergoing Coarsening

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Coarsening or Ostwald ripening occurs in a vast array of two-phase systems. Coarsening results in a decrease in the interfacial area per unit volume and a concomitant increase in the size-scale of the interfacial morphology. Much is known about the coarsening process in two-phase mixtures consisting of a polydisperse array of spherical particles. In contrast, in many two-phase mixtures, such as those found in two-phase polymers, dendritic solid-liquid mixtures, and order-disorder transformations, the interfaces are both interconnected and have a spatially varying mean curvature.

Characterizing the interfacial morphology of such systems requires measurements of the three-dimensional microstructure. Using three-dimensional reconstructions, we characterize the morphology of the interfaces through measurements of the principle curvatures as a function of position along the interfaces, see [1-3] for related approaches. Using these data the interface shape distribution, the probability of finding a small patch of interface with principal curvatures was determined. This interface shape distribution is the counterpart for arbitrarily shaped interfaces of the particle size distribution for systems with spherical particles. We determined the principal curvatures of approximately 10^6 patches to characterize accurately the distribution.

In addition, we characterize the evolution of the topology of the interfaces during coarsening through measurements of the genus, the number of handles, and the number of independent bodies (liquid droplets) of the experimentally derived, three-dimensional reconstructions of dendritic samples. In order to remove the increase in size scale associated with the coarsening process, the genus, the number of handles, and the number of liquid droplets per volume are scaled by the inverse of the surface area per unit volume. The scaled genus decreased with coarsening time due to the simplification of the microstructure while the number of liquid droplets increased with coarsening time. We find that topological singularities are the route by which the genus changes with time during coarsening see figure 1.

Three-dimensional phase field simulations were used to provide insight into these experimental results. The experimentally measured microstructure was used as an input to a phase field calculation. Through these calculations and the predicted flow in curvature space it is possible to predict the evolution of the interfacial shape distribution [4]. The phase field calculations were also used to predict the interfacial velocity. Through these calculations it is shown that liquid droplet formation occurs through a number of different mechanisms, while liquid tubes were created through topological singularities that occur when two solid-liquid interfaces that compose the sides of large planar-like channels touch. The phase field simulations allows for different diffusivities between each of the phases. The effects of this difference in diffusivity on the evolution of the interfacial shape distribution and topological singularities will be discussed.

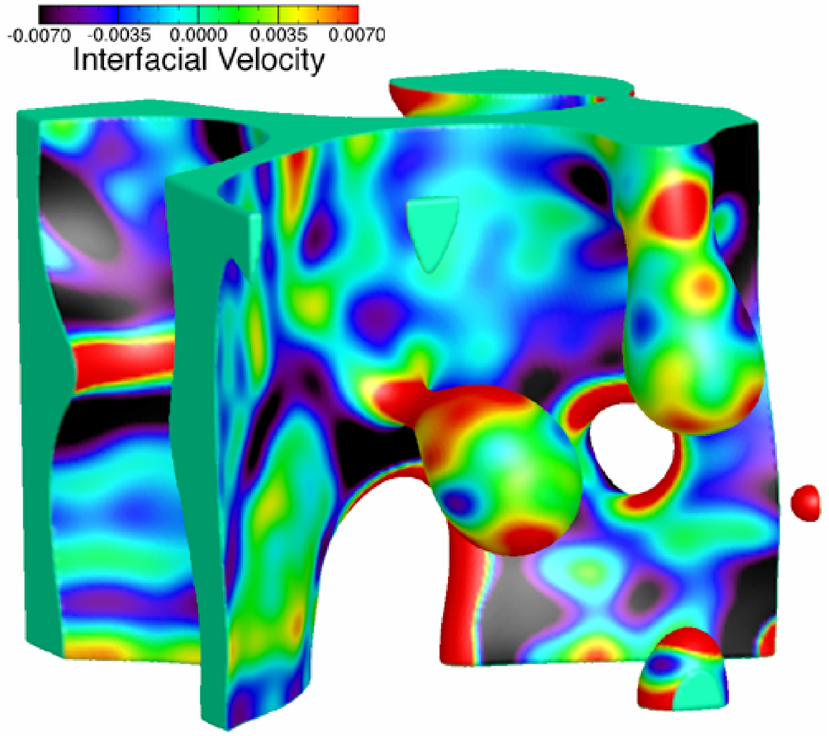

Figure 1. Interfacial velocity computed using a phase field model as a function of position along the solid-liquid interfaces. The liquid regions intersecting the outer box are solid. A positive velocity points towards the liquid. The red near the neck of the protuberance in the center of the figure indicates that this region will soon pinch off leaving behind a liquid droplet.

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