Role of Dynamic Nucleation at Moving Boundaries in Phase and Microstructure Selection

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Objectives

Solidification microstructures that form under steady-state growth conditions (cells, dendrites, regular eutectics, etc.) are reasonably well understood in comparison to other, more complex microstructures, which form under intrinsically *non-steady-state* growth conditions due to the competition between the nucleation and growth of several phases. Some important practical examples in this latter class include microstructures forming in peritectic systems, in highly undercooled droplets, and in strip-cast stainless steels. In these systems, it is often difficult to predict which microstructure will form and which phases will be selected under prescribed processing conditions. This research addresses this critical role of nucleation at moving boundaries in the selection of phases and solidification microstructures through quantitative experiments and numerical modeling in peritectic systems. In order to create a well characterized system in which to study this problem, we focus on the directional solidification of hypo- and hyper-peritectic alloys in the two-phase region, imposing a large enough ratio of temperature gradient/growth rate to suppress the morphological instability of both the parent (α) and peritectic (β) phases (i.e., each phase alone would grow as a planar front). Already in this simplified case, the growth competition of these two phases leads to a rich variety of oscillatory microstructures that depend sensitively upon the relative importance of nucleation, diffusion, and convection.

Progress to Date

The first main finding is that the oscillating structures, with *seemingly* distinct isolated bands of α and β phases, which have been reported to date in the literature, are not discrete bands controlled by nucleation and diffusion. Successive polishing of directionally solidified hyper-peritectic Sn-Cd alloys clearly revealed that this type of structure is actually made up of two *continuous* interconnected phases in three dimensions. The microstructure consists of a large tree-like domain of primary α phase that is embedded inside the peritectic β phase. Moreover, an experimental technique was developed to directionally solidify several samples simultaneously in capillary tubes with a range of diameters, from 3.2 mm to 0.2 mm, to systematically reduce the effect of convection. In fine samples, the tree-like structure in hyper-peritectic alloy was found to disappear, indicating that this structure is the result of the convection present in the bulk liquid. A numerical model of convection was developed that confirms that the oscillatory microstructures observed in experiments in the hyper-peritectic region form due to the presence of oscillating convection in the melt. The simulated microstructure for a 0.6 mm diameter is diffusion controlled with a sharp

transition from α to β. In contrast, for a 6 mm diameter the convective flow drives an oscillating concentration profile at the interface, which gives rise to an oscillatory coupled growth of the two phases. This oscillatory growth, in turn, generates a tree-like microstructure that is in good agreement with the experimentally observed one.

The second main finding is that for a range of alloy composition in the hypo-peritectic region, where the purely diffusion model predicts *discrete* bands that grow by repeated nucleation of the primary and peritectic phases, discrete bands were indeed observed for the first time when the sample diameter was small enough (0.6 mm) for convection to be suppressed. Moreover, the experiments revealed that the microstructure in the diffusive regime is not unique, but depends on the size of the sample and the composition. These observations were confirmed by simulations of a peritectic alloy phase-field model which showed that, below a minimum sample size, discrete bands of the peritectic phase only fill the sample partially, whereas above this minimum they span its entire cross-section. The existence of this minimum size was explained by noting that partial bands are formed when the time for the excess solute rejected by the parent phase, which hinders the growth of the peritectic phase, to diffuse across the sample, is shorter than the time for the peritectic phase to spread across the sample.

Need for Microgravity

Ground-based experiments have clearly shown that convection effects preclude the formation of discrete nucleation-controlled bands and gives rise, instead, to the continuous growth of an oscillating tree-like structure of the two phases. Thus, microgravity experiments in bulk samples are required to investigate discrete band formation and other nucleation-controlled microstructures in a diffusive regime. These experiments will make it possible to determine accurately the nucleation undercoolings of the two phases under non-steady-state growth conditions and to obtain unambiguous results that can be compared accurately with the theoretical predictions developed for the diffusive regime.