Impurity Partitioning of Grain Boundary during Polycrystalline Colloidal Crystallization

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Modeling of crystal growth by a colloidal system has attracted considerable interest because of theiranalogy to atomic or molecular system, and which enables us in-situ observation due to their intrinsic slowness of moving and larger size of colloidal particles.Recently, impurity partitioning of a single colloidal crystal was reported (J. Nozawa, et al., J. Phys. Chem. B, 2013), however, less understanding has been achieved on the partitioning of impurities during polycrystallization. In general, grain boundary (GB) dynamics play a pivotal role in the fabrication of polycrystalline materials. Hence, we investigate incorporation of impurities into GBs and grains during polycrystalline colloidal crystallization.

The monodisperse polystyrene spheresuspensions were used for experiments. The particle with a diameter of 500 nm was served as the host and spheres with diameter ranging from 560 to 700nm were added as an impurity.The experimental method is based on the convective self-assemble driven by evaporation. GB segregation of impurity during colloidal crystallization was directly observed by in-situ observation with optical microscopy.

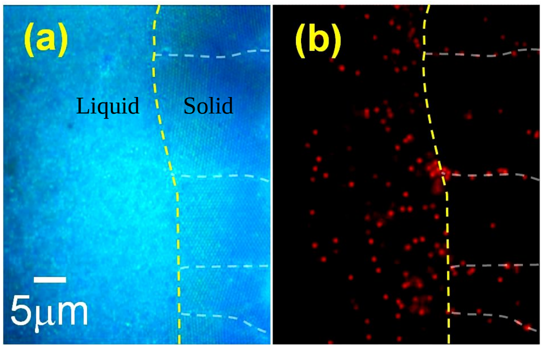

Figure1.(a) Image of growing of polycrystal containing impurities. Particle size of host and impurity is 500 and 700 nm, respectively. Initial impurity concentration, C_0, is0.01.(b) Fluorescent observation at the same place.

White dashed lines in Figure 1 indicate GB, while the yellow ones show the liquid/solid interface. In solid, impurity particles gather at GB rather than in the grain. The concentration of impurity at GB,C_{GB}, is characterized by V and θ (the difference of angle in crystallographic orientation of two adjacent grains that separated by GB) as shown in Figure 2. The effective partitioning coefficient, k_{eff}, ofGB (C_{GB}/C_0) is larger than unity. Plots in Figure 2 indicate that the segregation of impurity at GB is enhanced by the increasing of the θ. Dependency of V on C_{GB} is also found.

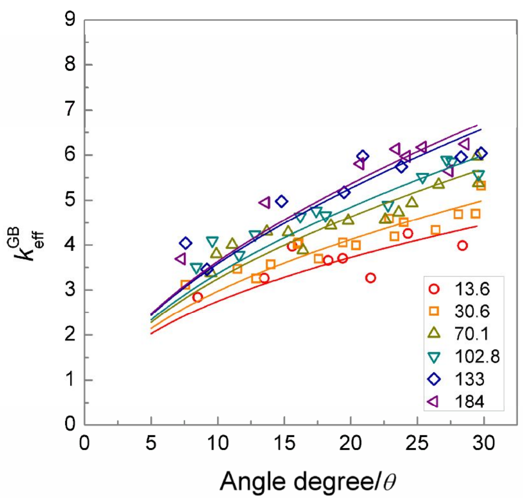

Figure 2. Plot of $k_{eff}$for 600 nm of impurity versus θ for GBswith different growth rates (µm/hr).

How impurity incorporates into GB is discussed. We infer that most of impurities existing at GB come from thoserepelled by grainsduring crystallization.That is as if GBs are diffusion layer of impurities at liquid/solid interface, which is accumulated as a result of segregation.Based on this concept and BPS theory, our data were analyzed.The results show that our experiment measurement are well fitted with this hypothesis, which indicates that our analysis is a reasonable model to explain the impurity partitioning of grain boundary during polycrystalline colloidal crystallization.