The Effect of the Groove on Grain Boundary Segregation during Colloidal Polycrystallization

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Grain boundary (GB) dynamics, in general, play a pivotal role in the fabrication of polycrystalline materials. Most researches assume that impurity segregation in GBs takes place after solidification, but recently, GB segregation during solidification of multicrystalline silicon was reported [1]. Impurity segregation at GBs is still under debate. Colloidal system has attracted considerable interest because of its promising analogy of phase transformation behaviors to that of atom or molecules on larger length and time scales down to one-particle resolution. In the present study, in-situ observation of colloidal polycrystal growth has been carried out to reveal how grooves affect GB segregation of impurity.

Polystyrene particle with a diameter of 500 nm was served as host, and polystyrene particles or fluorescent particles with diameter ranging from 560 to 700 nm 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 optical microscope.

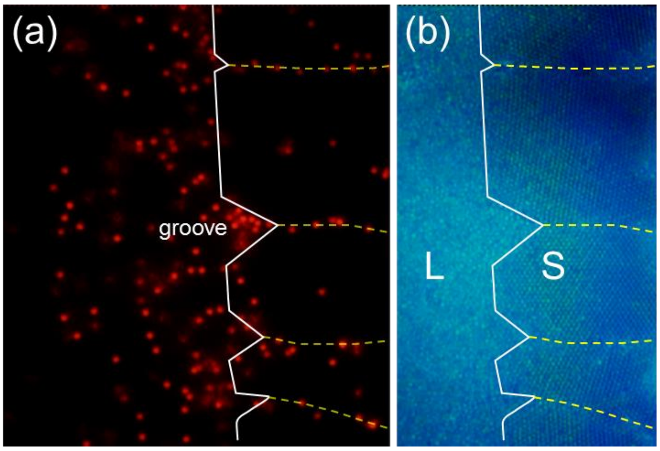

Figure 1. Optical microscopic images of growing colloidal polycrystal containing impurities (host: 500 nm, impurity: 700 nm, C_0 (initial impurity volume concentration): 0.005. The yellow dashed lines indicate the positions of GB, while the white lines show the positions of solid/liquid interface. (a) Fluorescence image of (b).

As can be seen in Figure 1, impurity particles (red) gather at GB rather than in the grain. Impurity concentration of GB (C_{GB}) for various misorientation angles (θ) and growth rates (V) have been investigated. C_{GB} is found to increase with either increasing of θ or V, and it also depends on the size of impurity. In-situ observations revealed three possible manners for impurity incorporation into GBs. We found that most of impurities that were incorporated into GB were supplied from the segregated impurities at solid-liquid interface, in which the relationship between C_{GB} and growth rate shows the BPS-like one.

In-situ observation revealed impurity distribution in the liquid during growth. Impurities gathered at the groove that formed at the solid-liquid interface (Figure 1 (a)). Grain boundary was exposed to liquid at the “bottom” of grooves. High value of C_{GB} was obtained when the area of the groove was large. It is assumed that impurity distributed homogeneously perpendicular to growth direction gathered in the groove as crystallization proceeded. This increases the opportunity of incorporation of impurity into GB. Our observation provides the experimental evidence of the relationship between the groove and segregation of impurity at GB during crystallization.

[1] Fujiwara K., Ishii M., Maeda K., et al., *Scripta Mater*. 69 (2013) 266–269.