Study of spatial heterogeneity and molecular aggregation dynamics during evaporative crystallization by hyperspectral camera imaging

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The initial stage of crystal nucleation is important in determining the morphology, size distribution, and properties. We have reported the aggregation dynamics of fluorescent molecules during the evaporative crystallization process. In the case of BF_2DBMb (Figure. 1), fluorescence color changes from purple to blue via orange. This phenomenon reflects the process of transition from the monomeric state in solution to crystal via high-density intermediate states called the liquid-like cluster[1],[2], which supports the two-step nucleation mechanism proposed as a crystal nucleation model[3]. According to several reports, the precipitates after evaporation have structures that reflect Marangoni convection and capillary flow[4]. It is implied that the evaporative crystallization reflects the spatial and temporal heterogeneity. Therefore, it is important to evaluate the heterogeneity to understand the molecular aggregation mechanism in the process of forming the final products from the liquid-like cluster. In this study, to clarify the effect of heterogeneity, we used a hyperspectral camera (HSC) which can simultaneously obtain spatial photography and spectroscopic information. An example of results from HSC imaging is shown in Figure 1. We successfully revealed the relationship between the liquid-like cluster and the final products and the importance of the liquid-like cluster for crystallization. We have demonstrated that fluorescence spectrum imaging by HSC is useful for investigating self-assembly process in heterogeneous systems.

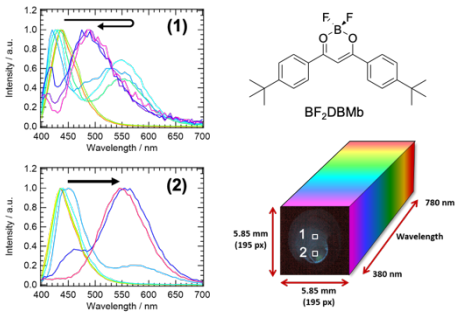

Figure 1. Molecular structure of BF_2DBMb and fluorescence spectral changes in each region observed by hyperspectral camera as a function of time.

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