Crystal growth rate and prediction of particle shape for glycine in phase-field model

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Functionalities of final products fabricated in powder processes are determined by properties of consisted particles. Therefore, controlling of particle properties like particle morphology and size distribution is essential for developing products with higher quality. Crystallization is a useful technique for obtaining highly pure particles and is a process accompanied with nucleation and crystal growth at atomic level. However, it is hard to simultaneously observe nucleation and crystal growth by experimental approaches in the production processes. Then, predictions of crystallization by computer simulations has been mainstream. The conventional simulations of expressing crystallization are mainly Molecular Dynamics and Monte Carlo methods. These are good at expressing nano-scale, however, it is difficult to express micro-size as the same scale of experimental system because of heavy computational load. The development of simulations to be able to deal with crystallization up to macro-scale is required. Phase-field method recently focused in computational chemistry makes a remarkable progress and smoothly express interface by setting the interfacial region as an infinite thickness between different phases. In this paper, an application of the Phase-field method into crystallization processes was carried out.

Crystal growth simulations on the Phase-field model were performed for glycine as a model material which had the simplest structure in amino acids. The crystal growth was calculated with changing supersaturation of driving force. The validity of this simulation was evaluated by comparing the crystal morphology obtained by simulation results with another theoretical model. Moreover, an effect of operating conditions on morphology changes of anisotropic crystal particle was performed by a modeling anisotropy. By changing pH of solution, morphology changes of γ-form were expressed. Quantitative evaluation of crystal growth was possible by introducing calculation of crystal length. The relationship between crystal growth rate and supersaturation was illustrated in the case of constant and non-constant supersaturation. It is possible to determine the preferential growth direction of the crystal in the present simulation. Since crystal growth in various operating conditions can be predicted, the present simulation method helps to design operating conditions for obtaining the desired crystal morphology.