S01-2 **Crystallization mechanism from solution by molecular simulation**

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The mechanism of nucleation and crystal growth from solution in the process of particle formulation has not been clarified even in the field of inorganic substances. The crystallization of organic crystal at molecular level relies on the empirical trial and error in pharmaceutical fields. Classical nucleation theory, the theory describing nucleation proceeds as a one–step process, have been explained for the crystallization at the initial stage. However, recent studies on the experiments and simulations have been attracted from more complex mechanisms, which is two-step nucleation, especially in the high concentration. The cluster formation and its adsorption into crystal surface occurred in the crystal growth. The synergic study between experiments and simulations has been required to further understand the detailed mechanism of the particle formation in the solution at molecular level and its controlling technique. A particle formation of calcium carbonate ($CaCO_3$) using molecular simulation was shown in the present presentation. Molecular dynamic (MD) simulation is a well-known tool to investigate molecular behavior and makes it possible to simulate nano-scale phenomena in nano-seconds with exposing specific crystal faces. In order to reveal the aggregation mechanism of spindle $CaCO_3$, anisotropic phenomena at a molecular level of $CaCO_3$/water interfaces and solution structure should be taken into account the Monte Carlo simulation. In addition, particle formation on glycine of amino acids from solution have been studied by MD simulations.