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Mechanism of ice nucleation on (100) plane of calcium oxalate monohydrate: a molecular dynamics simulation study

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Calcium oxalate monohydrate (COM) is the most thermodynamically stable polymorph of calcium oxalate. COM is known as an organic mineral formed on the surface of the Earth, under the bottom of sea, in atmosphere, in meteorites, in plants and in kidney stones. So far, COM has been studied in fields of mineralogy, biology and medical science.

Recently, Ishikawa et al. suggested that COM plays as an ice nucleation promoter, like silver iodide and ice nucleation-active bacteria. They speculated that the structure of COM (100) plane induces ice nucleation. Studies on the mechanism of ice nucleation promotion by COM are important, because the studies may help provide development of new materials to make artificial snow. Molecular dynamics (MD) simulation is a helpful method to investigate the mechanism of ice nucleation at the molecular scale. Thus, we performed a MD simulation to elucidate the mechanism of ice nucleation on the (100) plane of COM.

In the simulation, the intermolecular interaction between a pair of water molecules was estimated using a six-site model. The water-COM interaction was estimated using a COM potential model proposed by Tommaso et al. In the <100>direction of COM, two different molecular layers are piled up by turns; one is positively-charged Ox-1 layer consisting of calcium ions and oxalate ions, and the other is negatively-charged Ox-2 layer consisting of oxalate ions and water molecules. In this study, the simulation was performed for a rectangular parallelepiped system in which supercooled water consisting of 4000 water molecules was sandwiched by Ox-1 and Ox-2 layers. Temperature was set to 268 K. Total run was 4 ns or longer. The simulation indicated the formation of a polar cubic ice structure near the Ox-2 layer. However, the formation of a hexagonal ice structure was not observed. Details of the simulation results will be shown at the presentation.

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