Theoretical investigation on crystallization mechanism of carbonate minerals using molecular dynamics simulation

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Mineral carbonation, which refers to the reaction of CO_2 with calcium or magnesium containing minerals to form a stable phase, is important CO_2 storage technology against greenhouse gas emission along with the industrial development. However, their crystallization mechanisms are still in dispute. Particularly for calcium carbonate, it has been reported that various crystallization mechanisms exist through the formation of pre-nucleation cluster (PNC) or dense liquid phase. In this work, we investigated the crystallization mechanisms of calcium carbonate involving PNCs depending on various control factors (i.e., pH, temperature, concentration) using molecular dynamics simulation. At the initial phase of the carbonate reaction, PNC was formed as dynamically ordered liquid like oxyanion polymer (DOLLOP), representing a mixture of Ca and carbonate ions as polymer chains. To scrutinize the PNC structure that varies depending on the control factor, the average coordination number and the average number of Ca ions in the cluster, radius of gyration and local density were analyzed. Also, the change in Gibbs free energy was compared to determine the spontaneity of the carbonation reaction.