Japan Geoscience Union Meeting 2012
(May 20-25 2012 at Makuhari, Chiba, Japan)

MIS24-05 Room:202 Time:May 22 14:45-15:03

Dynamics of organic molecule adsorption on calcium carbonate calcite surface: a molecular dynamics study

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Crystal growth of $CaCO_3$ in organisms is controlled by organic molecules, such as polymers, proteins and peptides. Elucidating the mechanism of the $CaCO_3$ growth control by organic molecules is of particular importance for understanding of the mechanism of biomineralization, crystal morphology technologies and the development of novel organic/inorganic hybrid materials. However, it is quite difficult to analyze the structure and dynamics of water and organic molecules at a $CaCO_3$ crystal surface in detail by experimental means. Thus, our understanding of the mechanism of $CaCO_3$ crystal growth control by organic molecules is still poor.

Recently, we have started computer simulation studies on the mechanisms of $CaCO_3$ crystal growth and the control of it by impurities. One of them is a molecular dynamics (MD) simulation study of the adsorption of aspartic acid (ASP) on the surface of $CaCO_3$ calcite. At the presentation, I will talk mainly about this MD simulation study.

The simulation was carried out for both (104) and (110) faces of $CaCO_3$ calcite. Intermolecular interactions acting on $CaCO_3$ and H_2O are calculated using simple Ca^{2+}, ${CO_3}^{2-}$ and H2O models in which the Coulomb potentials between charges and the short-range interactions between atoms are assumed. The intermolecular interactions acting on ASP was calculated using the CHARMM force field. Temperature was set at 298 K.

Simulation results indicated the formation of a few H_2O molecular layers on the (104) face. In each layers, H_2O molecules were arranged in an ordered state. However, such layers did not appear on the (110) face. It proved that the formation of the layers strongly influences the adsorption conformation of ASP at the calcite surface. For the (104) face, ASP did not adsorb directly onto the face, but a H_2O molecular layer was sandwiched between the adsorbed ASP and the face. Moreover, careful analysis of the free energy of ASP adsorption suggested the existence of several metastable adsorption conformations at the face. Details of the results will be shown at the presentation.

This work was supported by a Grant-in-Aid for Scientific Research (No. 22107004) on Innovative Areas of ”Fusion Materials (Area No. 2206)” from the Ministry of Education, Culture, Sports, Science and Technology (MEXT).

Keywords: biomineralization, computer simulation, crystal growth, surface and interface, calcite, aspartic acid