Japan Geoscience Union Meeting 2015
(May 24th - 28th at Makuhari, Chiba, Japan)

BPT03-14 会場:104 時間:5 月 26 日 14:55-15:10

無機的環境下における炭酸カルシウム多形の形成過程とその前駆物質
Inorganic precipitation mechanism of calcium carbonate polymorphs and their precursors

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Calcium carbonate, $CaCO_3$, occurs in six different forms: three crystalline polymorphs (calcite, aragonite, and vaterite), two hydrate phases, and amorphous calcium carbonate (ACC). These polymorphs are important both in life and material sciences, especially the occurrence of $CaCO_3$ in living organisms has received considerable attention. As a basis for understanding biomineralization, inorganic precipitation mechamism of these polymorphs has been extensively investigated for over a hundred years. Recently, crystallization pathway through non-classical mechanism such as stable prenucletaion cluster aggregation has been proposed, which give a new picture of the early stages of calcium carbonate growth. However our knowledge of formation process of $CaCO_3$, especially that of the mechanism of polymorph selection, is far from complete.

We have investigated experimentally and theoretically the metastable formation of $CaCO_3$ polymorphs and their precursors. In particular, the effect of Mg^{2+} on the nucleation and growth of $CaCO_3$ polymorphs has been focused and the quantum chemical calculations of Mg-containing $CaCO_3$ surfaces and clusters appearing in the early stages of $CaCO_3$ formation have been performed. As a result, Mg^{2+} substituted for Ca^{2+} affects the structure of surfaces and clusters, and may have significant effect on the polymorph selection of $CaCO_3$. In this presentation, we will report our results in detail based on the recent progress in this field.

Keywords: calcium carbonate, metastable phase, precursor