

How do ligands affect Mg partitioning in calcite formed via an amorphous precursor?

KATJA E. GOETSCHL¹, BETTINA PURGSTALLER¹,
MARTIN DIETZEL¹, VASILEIOS MAVROMATIS¹

¹Institute of Applied Geosciences, Graz University of
Technology, Rechbauerstraße 12, 8010 Graz, Austria

Calcium carbonate minerals are widely distributed on the Earth's surface and have been extensively studied for their chemical, structural and isotopic composition. The substitution of Ca by Mg in calcite has been the topic of a large body of studies investigating the impact of different physical and chemical parameters on the incorporation behaviour of Mg in marine and terrestrial calcite precipitates. In this context, the formation of Mg-calcite via the transformation of amorphous calcium carbonate (ACC) is a key process (e.g., in biomineralization), but still poorly understood. In natural calcite precipitation environments the presence of dissolved organic and inorganic ligands may affect the uptake of Mg into the calcite crystal lattice.

In order to assess the role of such ligands on Mg partitioning in calcite formed via an amorphous precursor we performed ACC transformation experiments under well defined physicochemical conditions in the presence and absence of distinct organic and inorganic molecules. Standardized ACC material was synthesized prior to the experimental runs in order to differentiate between formation and transformation mechanisms of the amorphous phase. The transformation of ACC in Mg-bearing solutions yielded up to 10 mol% Mg-calcite which was monitored *in situ* by Raman spectroscopy. The chemical evolution of the fluid and solid was analyzed throughout the experimental runs. First results indicate elevated Mg incorporation in calcite in the presence of dissolved organic ligands, e.g., citric acid, ethylenediaminetetra acetic acid (EDTA), etc.. However, in the presence of dissolved inorganic ligands, e.g., sulfate, we established lower Mg partitioning in calcite caused by the formation of MgSO_4^0 aquo complexes.

New insights on the formation of aquo complexes in the reactive fluid during the transformation process of ACC from the present study will shed light on ACC transformation mechanisms and may contribute to an enhanced picture of ongoing fluid-calcite interactions.