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Structure of Calcite {10.4} / Artificial Seawater Interfaces

Hiroshi Sakuma[1,*] Henning O. Sørensen[2], Jun Kawano[3], Naoki Nishiyama[1], and Hironori Nakao[4]
[1]National Institute for Materials Science, Tsukuba 305-0044, Japan
[2]University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen, Denmark
[3]Hokkaido University, N21 W10 Kitaku, Sapporo, Hokkaido 001-0021, Japan
[4]Condensed Matter Research Center and Photon Factory, Tsukuba 305-0801, Japan

1 Introduction

Carbonate minerals are ubiquitous in the ocean. The incorporation and release of foreign ions during crystal growth, precipitation, and dissolution of carbonate minerals are critical for a range of research fields such as the estimation of temperatures of the sea in the past, biomineralization, and enhanced oil recovery.

Calcite is the major component in carbonate rocks. The structures of calcite/water interfaces have been extensively investigated by experiments and simulations for understanding reactions occurring at the interfaces. The structure contacted with seawater, however, is scarcely investigated by surface X-ray scattering measurements.

In this study, we conducted the crystal truncation rod (CTR) experiments for calcite {10.4}/artificial seawater interfaces.

2 Experiment

Sample preparation was described in our previous report [1]. Temperature of the sample was controlled from room temperature to 353 K. Specular X-ray CTR profiles of the cleaved {10.4} surface seawater interfaces were obtained by using the BL-4C beamline at the Photon Factory, KEK, Japan. The integrated CTR intensities were obtained by the rocking scans. The structure factors $|F|$ of the interfaces were derived by correcting for Lorentz, polarization, attenuation and area factors.

The electron density profiles of the interfaces were determined by the Fourier transform of a best-fit structural model to the experimental CTR curve. The model is composed by semi-infinite bulk calcite, relaxed surface, and liquid structures. The relaxed surface and liquid structures were constructed by the superposition of Gaussian distributions as conducted by previous research [2].

3 Results and Discussion

The specular CTR profiles of calcite/0.5 M NaCl solution interfaces are plotted in Fig. 1. Small differences upon increasing the temperature from 298 to 353 K was observed at the momentum transfer Q ~ 3.3 Å^{-1}. This reflects a change of the interfacial structure at 353 K. A best-fit structural model indeed indicates a small change of liquid structure going from 298 to 353 K.

The effect of temperature and dissolved ions in the solution will be discussed in a comparison with different experimental techniques and simulations in future works.

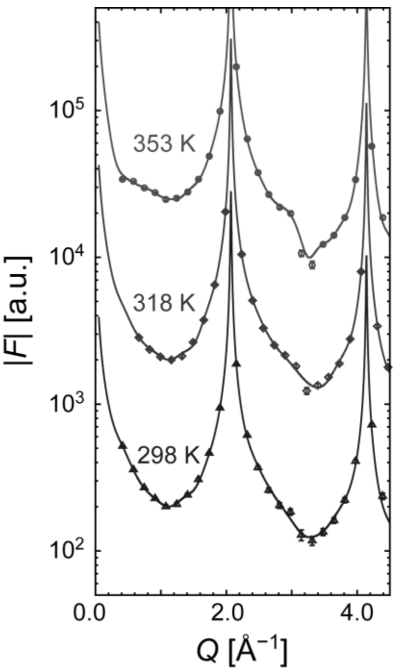

Fig. 1: Specular X-ray CTR profiles of calcite/0.5 M NaCl solution interfaces from 298 K to 353 K. Solid lines are best fit structural models. The profiles at 318 and 353 K are shifted for comparison on the same graph.

References

[1] H. Sakuma *et al.*, *Photon Factory Activity Report* 2014 #32 (2015) **B**.
[2] M.J.R. Magnussen *et al.*, *Phys. Rev. Lett.*, **74** (1995) 4444.

* SAKUMA.Hiroshi@nims.go.jp