

Molecular dynamics study of the interaction between water or ethanol and calcite

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Calcite is a common mineral at the Earth's surface and is interesting because of its role in biomineralization and because of its ability to fix CO₂. Adsorption of ethanol on calcite leads to changes of (re)crystallization rate and surface morphology as has been seen in AFM experiments¹. If we could define the mechanism for such behavior, it would provide a clue for understanding the way organisms control crystal growth. Cooke et al.² investigated the calcite {1 0 $\bar{1}$ 4} surface with molecular dynamics simulations and showed changes in surface energy after addition of ethanol. We extended that work with molecular dynamics simulations of the calcite cleavage plane {1 0 $\bar{1}$ 4}, a vicinal face with acute steps, {3 1 $\bar{4}$ 8} and a vicinal face with obtuse steps, {3 1 $\bar{4}$ 16} to investigate solvation with water or ethanol. The atomistic arrangement of the solvents is characterized by calculations of density profiles along the direction perpendicular to the surfaces and radial distribution function (RDF) calculations of various pairs of atoms from the solvents and the solid. Analysis of hydrogen bonds at the surfaces shows that water has (about 30%) higher hydrogen bond density on {3 1 $\bar{4}$ 8} and {3 1 $\bar{4}$ 16} than on {1 0 $\bar{1}$ 4}, while only slight variation (less than 5%) can be seen when the solvent is ethanol. The calculations of mean square displacement (MSD) of the solvents show that ethanol diffusion rate is much lower than water, suggesting a dramatic decrease in recrystallization when ethanol is present.

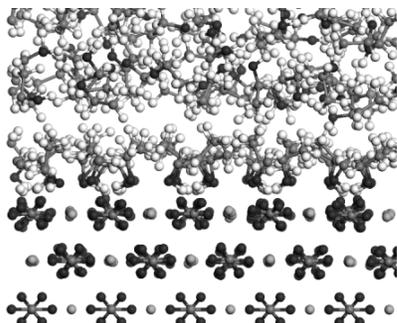


Figure 1: Ethanol arranges itself with the OH group toward calcite.

[1] K. Sand *et al.* this volume; [2] D. Cooke *et al.* in progress

Determination of dissolved Cu in Jiaozhou Bay by catalytic kinetic spectrophotometry

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A new method was developed to determine copper in seawater. It is based on reaction of Titan Yellow (MSDS) - H₂O₂ which is catalysed by Cu (II). It was found that Cu (II) catalyses the oxidation reaction of MSDS by hydrogen peroxide, the reaction speed linearly increasing with the concentration of Cu(II). The change of absorbency of MSDS was in a linear relationship with the concentration of Cu (II) in the range from 1.0 nM to 315.0 nM, indicating that the reaction catalysed by Cu is a first order reaction. And on this basis, the total concentration of dissolved Cu in sea water can be determined by the decrease of light absorption of MSDS. In the pre-concentration step, NH₃·H₂O was added to the system so that the dissolved Cu in sea water coprecipitated with magnesium hydrate. The recovery rate of copper was 99.04%. The result showed that the peak spectral response of MSDS appeared at 404 nm in ammoniacal media when pH=8.7, and iron did not interfere with the determination in the coexistence of a 4.0 mg/L KSCN. The optimum reaction conditions were established through single-factor experiment. The method precision was 96.80% and the detectability was 0.96nM at the fixed time of 10 min in 80-centigrade water bath, the concentration of MSDS was 0.8×10⁻⁴M, hydrogen peroxide was 1.2%, respectively. This method was used for analysing dissolved Cu in sea water from six stations in Jiaozhou Bay. It was found that the lowest and highest concentration of dissolved Cu were 15.6nM and 39.7nM, respectively. The average amount of dissolved Cu was 31.9nM, which was close to the result of 33.9nM by ICP-MS.