INVESTIGATION OF THE ROLE OF POLYSACCHARIDE IN DOLOMITE GROWTH AT LOW TEMPERATURE BY USING ATOMISTIC SIMULATIONS. Z. SHEN[1], I. SZLUFARSKA[2], and H. XU[1], [1]Department of Geoscience, University of Wisconsin-Madison, 1215 W. Dayton Street, Madison, WI 53706 zshen@wisc.edu, [2] Department of Materials Science and Engineering, University of Wisconsin-Madison, 1509 University Ave., Madison, WI 53706 szlufarska@wisc.edu

It is well recognized in this community that the growth of dolomite at low temperature (<40°C) can't be accomplished without catalysts[1]. The rate-limiting step in the dolomite growth at low temperature is most likely to be the dehydration of water from surface Mg^{2+}. Regarding the role of catalysts in the this dehydration step, two hypotheses have been proposed. One is that catalysts (like hydrogen sulfide and polysaccharides) adsorbed to crystal surface can weaken the bonding between surface Mg(II) and water molecules[2-3]. Our previous work shows that adsorbed hydrogen sulfide will increase the bond distance the bonding between surface Mg(II) and water molecules, and enhance surface water removal[4].

Polysaccharides were chosen for our study because it is the major component in microbial exopolymeric substances (EPS). The effect of polysaccharide in this step has been investigated by using classical molecular dynamics (MD) calculations. Free energy (potential of mean force, PMF) calculations have been performed for water molecules leaving the first two hydration layers above dolomite (104) surface in the following three conditions: without catalyst, with monosaccharide (mannose) and with oligosaccharide (three units of mannose). The simulations have shown that there is no obvious effect of monosaccharide in lowering the dehydration barrier for surface Mg^{2+}. However, a bridge shape configuration of oligosaccharide lying relatively flat on the surface is able to decrease the dehydration barrier about 0.6~1.2 kcal/mol. This decrease is caused by the hydrophobic space near the surface created by the non-polar –CH groups of this bridge conformation, which is energetically metastable but kinetically stable at the temperature range of interest. Such kind of configuration could locally occur in polysaccharides adsorbed on mineral surfaces. Sedimentary dolomite and other low-temperature dolomite may indicate involvement of microbe during their formation.

References:

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