Abstract Submitted
for the 4CF11 Meeting of
The American Physical Society

Modeling of Amorphous Calcium Carbonate SOURABH SINHA, PETER REZ, Arizona State University — Many species (e.g. sea urchin) form amorphous calcium carbonate (ACC) precursor phases that subsequently transform into crystalline $CaCO_3$. It is certainly possible that ACC might have up to 10 wt% Mg and ∼3 wt% of water. The structure of ACC and mechanisms by which it transforms to crystalline phase are still unknown. Our goal here is to determine an atomic structure model that is consistent with diffraction and IR measurements of ACC. For this purpose a calcite supercell with 24 formula units (120 atoms) was constructed. Various configurations with 6 Mg atoms substituting for Ca (6 wt%) and 3-5 H_2O molecules (2.25- 3.75 wt%) inserted in the spaces between Ca atoms, were relaxed using VASP. Most noticeable effects were the tilts of CO_3 groups and distortion of Ca sub-lattice, especially in the case of water. The distributions of nearest Ca-Ca distance and CO_3 tilts were extracted from those configurations. We also performed the same analysis starting with aragonite. Sampling from above distributions we built models for amorphous calcite/aragonite of size ∼1700 nm^3. We found that the induced distortions were not enough to generate a diffraction pattern typical of an amorphous material. Next we studied diffraction pattern of several nano-crystallites as recent studies suggest that amorphous calcite might be composed of nano- crystallites. We could then generate a diffraction pattern that appeared similar to that from ACC, for a nano-crystallite of size ∼2 nm^3.

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Date submitted: 16 Sep 2011 Electronic form version 1.4