Geophysical Research Abstracts,
Vol. 10, EGU2008-A-05417, 2008
SRef-ID: 1607-7962/gra/EGU2008-A-05417
EGU General Assembly 2008

Molecular dynamics model of $CaSiO_3$ perovskite: insights into the ferroelastic transition

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Between 5 – 10% of the Earth's lower mantle is expected to be $CaSiO_3$ perovskite and the characterization of this material is challenging as this ferroelastic material is at most slightly distorted from the aristotypical cubic structure. In addition, this material can be produced at high pressure and temperature, but the perovskite phase reverts to a glass on pressure release thereby limiting experimental accessibility. The Earth science impact lies primarily in the elastic properties as a function of pressure and temperature as these properties will be sampled seismically. The phase relations among the possible space groups are relevant to this issue if the space group influences the elastic properties.

We have simulated the elastic properties and structure of $CaSiO_3$ perovskite using density functional theory coupled with molecular dynamics (AIMD). We calculate these properties at several pressures and temperatures to 5000K and 130 GPa. We analyze the structure in terms of coherent rotations of the octahedra over the 80 atom unit cell. We find that the octahedra oscillate between positive and negative rotations as temperature increases, but the rms value of the rotation remains almost constant over the entire temperature range. Thus, the spontaneous strain at any temperature reflects the time average of the octahedral rotations. We further find no elastic modulus signature of the ferroelastic phase transitions. Even in the tetragonal phase, the elastic moduli are quasi-cubic in their values. Thus, in contrast to some other studies, we predict that this is no observable seismic discontinuity associated with a ferroelastic phase transition in this material. However, we cannot rule out observable effects on Q

due to domain wall mobility.