Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Phase stability and elasticity of $CaSiO_3$ perovskite at high pressure and high temperature from Ab inito molecular dynamic calculations
DONALD WEIDNER, LI LI, Stony Brook University, JOHN BRODHOLT, DARIO ALFE, DAVID PRICE, University College London, STONY BROOK UNIVERSITY COLLABORATION, UNIVERSITY COLLEGE LONDON COLLABORATION — We report the dynamics of the structure and elastic properties of CaSiO3 perovskite from *ab initio* molecular dynamics (AIMD) calculations at high pressure (P up to 130 GPa) and high temperature (T up to 5000K). Our calculations indicate three separate stability fields: metrically orthorhombic, tetragonal and cubic, with the tetragonal phase dominating the pressure and temperature region between room temperature and 4000K. The cubic phase is not entirely stabilized even at temperatures of the Earth's lower mantle. Calculated X-ray diffraction patterns indicate small super- lattice reflections that could result from the octahedral rotations throughout the P-T region investigated. The calculated elastic constants and velocities are independent of temperature at constant volume. Referenced to room pressure and 2000K, we find: Grûneisen parameter is $\gamma(V) = \gamma 0(V/V0)q$ with $\gamma 0 = 1.53$ and $q = 1.02(5)$, and the Anderson Grûneisen parameter is given by $(\alpha/\ \alpha 0) = (V/V0)\delta T$ in which $\alpha 0 = 2.89$ x 10-5 K-1 and $\delta T = 4.09(5)$. Using the third order Birch Murnaghan equation of state to fit our data, we have for ambient P and T, $K_0 = 236.6(8)$ GPa, $K_0' = 3.99(3)$, and $V_0 = 729.0(6)$ Å3.

Donald Weidner
Stony Brook University

Date submitted: 06 Dec 2005 Electronic form version 1.4