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Equation of State and Elasticity of $MgSiO_3$ Perovskite at High Temperatures from Ab Initio Molecular Dynamics: Towards Interpreting Seismic Tomography

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We report on the first *ab initio* molecular dynamics simulations of thermoelastic properties of $MgSiO_3$ perovskite, the major mineral of the lower mantle, at lower mantle *P/T*-conditions. These are the first simulations of elastic constants to be ever performed for any material using finite-temperature *ab initio* molecular dynamics. Our simulations are based on density functional theory within the generalised gradient approximation, and yield excellent agreement with available experimental data. We resolve the long-standing controversy on the Grüneisen parameter and thermal expansion of $MgSiO_3$ perovskite, which are calculated to be equal to 1.49 and 1.86 $x10^{-5}$ K^{-1} at ambient conditions, respectively. Thermal equation of state of $MgSiO_3$ perovskite in the lower mantle is constructed, and upper and lower bounds for the lower mantle geotherm are derived. Notably, the standard geotherms of [1,2] meet our constraints. $MgSiO_3$ perovskite was found to remain orthorhombic throughout the lower mantle, with no evidence for the high-temperature phase transition into a cubic or tetragonal phase at relevant temperatures. From temperature derivatives of acoustic velocities, we find $\nu=(d\ln V_S/d\ln V_P)_P=1.5\pm0.2$ throughout the lower mantle. This is much smaller than the observed values (1.7 to 2.6 - [3]), suggesting significant anelasticity or large-scale lateral chemical heterogeneity of the lower mantle. From our temperature derivatives of seismic velocities and seismic tomography data [4] we obtain the lateral temperature contrast of 400 K between cold slabs and hot plume zones across most of the lower mantle.

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