Molecular Dynamics Simulations of Cubic $CaSiO_3$ at Lower Mantle Conditions

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First-principles projector-augmented wave (PAW) molecular dynamics was used to investigate structure and properties of what is thought to be the third most abundant phase in the Earth's lower mantle, $CaSiO_3$ perovskite. The commonly assumed cubic structure was found to be stable at high temperatures and unstable at low temperatures at all pressures. On the basis of these results, we predict that the low temperature structure of $CaSiO_3$ perovskite is tetragonal space group *I*4/*mcm*. This phase would transform into an orthorhombic *Imma* structure under non-hydrostatic conditions. It is also obtained by fast quenching of cubic $CaSiO_3$ perovskite. This *Imma* structure explains hitherto puzzling experimental X-ray powder diffraction patterns.

$CaSiO_3$ perovskite is thought to comprise between 6 and 12 wt% of the lower half of the Earth's transition zone and lower mantle. Its structure throughout this regime is generally assumed to be cubic [1,2] because temperature generally increases symmetry. At lower temperature deviations towards a tetragonal structure were found [1,4].

Using VASP code in the PAW frame the $CaSiO_3$ cubic structures were first optimized at 0 K for pressures of 0, 50, 100, 150 GPa . For MD simulations we used an *N*-*V*-*T*-ensemble with Nosé thermostat [5]. Temperatures of 500, 1500, 2500 and 3500 K were simulated. The lattice parameters were not relaxed but on the difference of stress in the three spacial directions we could observe a phase transition from the cubic phase at high temperatures to a tetragonal phase at low temperatures. As we observe a significant difference in stress components, we predict that transition takes place between 1500K and 500K.

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