Molecular dynamics simulation of the T-P-V equation-of-states of the Mg2SiO4 polymorphs

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We have derived an accurate interatomic potential model which is applicable to the olivine, modified-spinel, and spinel forms of Mg2SiO4. Based on the molecular dynamics (MD) simulation technique, with the resulting potential model, we have succeeded in reproducing the observed structures, elastic constants, volume thermal expansivities, and volume compression data of the three Mg2SiO4 polymorphs very accurately. Here we present the MD values of the temperature-pressure-volume equation-of-states, bulk moduli, and rigidities of the three Mg2SiO4 polymorphs at temperatures and pressures up to 2000K and 30 GPa.