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Metadynamics simulation study of the olivine-ringwoodite phase transition

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A combination of molecular dynamics and metadynamics is used to study the martensitic-like phase transition between olivine and ringwoodite. This process is expected to be especially important in subduction zones where olivine may persist as a metastable phase to depths of 600-700 km. The actual phase transition is accompanied by an increase in density and seismic velocities and has been related to the occurrence of deep earthquakes. As a model system for the simulations, the pure Mg2SiO4 composition is chosen for simplicity. The particle interactions are described by an advanced ionic potential that accounts for ion polarization and shape deformations. Simulations are performed at different temperatures and pressures up to 1500 K and 25 GPa, respectively. When olivine (forsterite) is used as starting configuration, the application of high pressure and external strain either leads to shear deformations with the system essentially remaining in the olivine structure or to amorphization. This underlines the high structural stability of the olivine structure. On the reverse path, ringwoodite becomes unstable under pressure release and transforms either into an amorphous phase or into a defect olivine structure. The defects are annealed in the course of the respective simulation such that the final structure is almost perfect forsterite. The transition mechanism we observe will be compared to experimental observations.