Relative stability and contrasting elastic properties of serpentine polymorphs from first-principles calculations

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We conduct first-principles calculations to determine the relative stability field and elasticity contrast of serpentine polymorphs at pressure and temperature conditions relevant to the oceanic lithosphere and subduction zone. At high pressures (> 4 GPa), the corrugated form of serpentine polymorph (antigorite, Atg) plus brucite (Brc) assemblage is thermodynamically more favorable compared to its planar counterpart (lizardite, Liz). The phase boundary between Liz and Atg + Brc exhibits a negative slope in the whole P-T range, indicating that this transition can be driven by increasing either pressure or temperature. Near 0 GPa, the slope is about –33 K/GPa. As pressure exceeds 1 GPa, the transition temperature starts to decrease more rapidly. Because of the corrugated nature of its constituent layers, Atg is more susceptible to intralayer deformations (7 to 36% smaller C_{11}, C_{22}, C_{12}, and C_{66} at ambient conditions) while more resistant to interlayer shear deformation (25% larger C_{44}, 36% larger C_{55}) than Liz. In contrast, their responses to the interlayer compressive deformation (C_{33}) are similar. For isotropic polycrystalline aggregates at pressures between 0 and 4 GPa, Atg exhibits a smaller bulk modulus (12 to 15%) and a larger shear modulus (6 to 11%) than Liz, while their density contrast is within 1%. Accordingly, a Liz/Atg transition is accompanied by a decrease in V_P (2 to 3%), an increase in V_S (3 to 5%), and a more pronounced drop in V_P/V_S (6 to 8%). These results may help to identify and characterize serpentine polymorphs produced under various geological settings.