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First-principles study of elastic properties and displacive phase transitions in MgSiO3 enstatites

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MgSiO3 enstatites belong to the pyroxene minerals, which constitute an important class of rock-forming minerals. Their basic structural units are single chains of SiO4 tetrahedra that are linked by M1 and M2 cations. Different stacking sequences of the chains and rotations of the tetrahedra within the chains (which depend on the size of the M1 and M2 cations) lead to a variety of pyroxene polymorphs. Recently, we studied the structural stability and mechanisms of pressure induced phase transitions in the enstatite system using both classical interaction potentials and first-principles methods [1]. Here, we discuss the relation of the displacive phase transitions, i.e. transitions without changing the stacking sequence of the chains, and the respective elastic properties. We concentrate on the orthoenstatite system, for which an anomalous elastic behavior was observed above 9 GPa experimentally [2] and for which two metastable high-pressure polymorphs were predicted from the previous simulations [1]. Using first-prinicles calculations in the framework of density functional theory we predict the pressure dependence of the elastic constants for the different polymorphs. The softening of specific constants provides insight into the mechanisms of the transitions and the sources of mechanical instability. The elastic wave velocities derived from the simulations are compared to the experimental data.

References

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