Protoenstatite at High Pressure and the Proto- to High-Pressure Clinoenstatite Transition Studied by Atomistic Simulations

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Pyroxenes are important rock-forming minerals with a general formula $XY(Si,Al)_2O_6$ and common structural features. While all pyroxenes are composed of single chains of SiO_4-tetrahedra, different stacking of these chains results either in an orthorhombic (ortho- or protopyroxene) or a monoclinic (clinopyroxene) crystal structure. Phase transitions between these three polytypes have a reconstructive character since the change in stacking sequence requires the breaking of bonds. Within each of these three pyroxene types, displacive phase transitions, mainly due to rotations of the chains, have been observed experimentally or predicted in theoretical work. This leads to a rather large number of possible crystal structures (e.g. Thomson and Downs, 2003). We are interested in the mechanisms and in the kinetics of the various phase transitions, which may have implications on the large scale physical properties of pyroxene-containing rocks but also on the understanding of geological processes that involve phase transformations. The phase diagram of the model system $MgSiO_3$ enstatite contains stability fields for five different pyroxene structures. Recently, additional phases have been observed as metastable phases, e.g. in in-situ high pressure and ambient temperature experiments (e.g. Kung et al, 2004) and in simulation studies. Here, we extend our previous studies of high pressure metastable orthoenstatite phases and the orthoenstatite to high-pressure clinoenstatite transition (Jahn, 2008; Jahn and Martoňák, 2008) to the protoenstatite system. Using a combined approach of first-principles static energy calculations and classical molecular-dynamics coupled to metadynamics, we find two possible metastable high-pressure polymorphs of protoenstatite. In addition, we provide a likely mechanism for the transition from proto- to high-pressure clinoenstatite, which we observe directly in the simulation as a sequence of slip deformations in the (100) planes of protoenstatite. From the energies of the intermediate structures estimates of the transformation barrier are obtained.

References

Jahn S (2008) High-pressure phase transitions in $MgSiO_3$ orthoenstatite studied by atomistic computer simulation. Am Mineral 93: 528-532

Jahn S, Martoňák R (2008) Plastic deformation of orthoenstatite and the ortho- to high-pressure clinoenstatite transition: A metadynamics simulation study. Phys Chem Minerals 35: 17-23

Kung J et al (2004) In situ measurements of sound velocities and densities across the orthopyroxene to high-pressure clinopyroxene transition in $MgSiO_3$ at high pressure. Phys Earth Planet Int 147: 27-44

Thompson RM, Downs RT (2003) Model pyroxenes I: Ideal pyroxene topologies. Am Mineral 88: 653-666

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