Molecular dynamics simulation of MgGeO3 polymorphs

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MgGeO3 is significantly important material because of the similar polymorphic relation to MgSiO3. In this study, mechanism of the high-pressure structural transformation from pyroxene-type to ilmenite-type and stability of perovskite form were investigated by means of the molecular dynamics (MD) simulation technique. In order to execute MD calculation, we optimized the two-body potential parameters by the static lattice energy minimization (WMIN) method. As results of MD calculation, the pyroxene-type transformed to a high-pressure state at 30 GPa and furthermore a mixed structure of the ilmenite-type and LiNbO3-type by shear stress. The perovskite-type structure had never transformed in a pressure range from ambient to 140 GPa.

[Introduction] MgGeO3 is significantly important material because of the similar polymorphic relation to MgSiO3. Many experimental works about high-pressure behavior of MgGeO3 have been executed. There are the orthpyroxene-type (Pbca), the clinopyroxene-type (C2/c), the ilmenite-type (R-3) and the LiNbO3-type (R3c) polymorph. A stable region of perovskite-type has never been determined.

[Molecular dynamics calculation] In this study, mechanism of the high-pressure structural transformation from pyroxene-type to ilmenite-type and stability of perovskite form were investigated by means of the molecular dynamics (MD) simulation technique. In order to execute MD calculation, The potential parameters of interatomic potential, which was described by the BMH-type two-body form containing the Coulombic, the exchange repulsive and the van deer Waals terms were optimized by the static lattice energy minimization (WMIN) method to reproduce the structures and the bulk moduli of MgGeO3 polymorphs.

[Results and discussion] As results of MD calculation, the clinopyroxene-type transformed to a high-pressure state at 30 GPa and furthermore a mixed structure of the ilmenite-type and LiNbO3-type by shear stress. The perovskite-type structure had never transformed in a pressure range from ambient to 140 GPa.