Elastic constants of the 10 Å phase at high temperatures and pressures

Tararushkin E V

National Research University Higher School of Economics, Myasnitskaya 20, Moscow 101000, Russia

etararushkin@hse.ru

The 10 Å phase, $Mg_3Si_4O_{10}(OH)_2nH_2O$, is an important member of the family of dense hydrous magnesian silicates (DHMS) minerals is of great interest for fundamental geochemistry and geophysics, because they control mineral equilibria and balance of water under the conditions of the Earth's mantle in subduction zones at high temperatures and pressures. The ideal model of the 10 Å phase has already been successfully investigated by classical atomistic simulations [1]. However, more recent experiments show that tetrahedral silicate layers of real the 10 Å phase may contain a certain amount of hydrogarnet-type structural defects [2], which would affect its properties.

The ClayFF force field [3] has been originally developed for classical atomistic computer simulations of clays and other layered minerals and their hydrated interfaces. Here we are using the most recent modification of the force field [3], which can now more accurately account for the bending of Mg–O–H angles in the mineral layers and Si–O–H angles of the hydrogarnet-type defects.

The pressure and temperature dependencies of the 10 Å phase elastic constants are calculated in a series of classical molecular dynamics simulations using the ClayFF-MOH model and compared with a diverse set of available experimental data.

This research was funded by the HSE Basic Research Program.

[1] Wang J W, Kalinichev A G and Kirkpatrick R J 2004 *Earth Planet. Sci. Lett.* **222** 517–527

[2] Welch M D, Pawley A R, Ashbrook S E, Mason H E and Phillips B L 2006 *Am. Mineral.* **91** 1707–1710

[3] Cygan R T, Greathouse J A and Kalinichev A G 2021 *J. Phys. Chem. C* **121** 17573–17589