Molecular Dynamics Simulation of the Thermomechanical Properties of a Pyrophyllite Nanoplate

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Phyllosilicates are extensively used as constituents of polymer-clay nanocomposites; in this connection, the estimation of thermomechanical properties of nanoplates is one of the key problems in this field. We present the results of molecular dynamics simulations for a single nanoplate of pyrophyllite: 2:1 clay mineral consisting of two tetrahedral sheets of SiO_4 and an intervening octahedral sheet of AlO_6. The considered model consists of one crystallographic cell in the Z-direction under periodic boundary conditions in the XY-plane. There were 1800 atoms calculated in the cell. Simulations were performed in the temperature interval 100 to 700 K using ionic-type potentials [1]. The mechanical properties of the nanoplate were calculated from the force-displacement curve obtained at slow rates of deformation. Using different types of loading, we calculated the full elasticity tensor and the estimated temperature influence on its components. The thermal expansion coefficients were also found in a wide temperature interval. It turns out that the elastic stiffnesses in the unidirectional tension and compression cases are practically the same for both ionic- and covalent-type potentials [2].

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[1] R.T. Cygan, J.J. Liang, and A.G. Kalinichev, *Journal of Physical Chemistry* **108**, 1255 (2004).
[2] O.L.Manevitch and G.C. Rutledge, *J. Phys. Chem. B* **108**, 1428 (2004).