American Mineralogist, Volume 98, pages 1881–1885, 2013

Determination of the melting temperature of kaolinite by means of the Z-method

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Abstract

The melting temperature of materials is an important thermodynamic property. Despite the importance of kaolinite, one of the most common clay minerals on the Earth's surface, its thermal and melting behavior is poorly understood.

We apply here the Z-method to determine the melting temperature (T_m) and the limit of superheating (T_{LS}) of kaolinite. The T_m is found at 1818 K (8.85 GPa), and T_{LS} at 1971 K (6.8 GPa). The diffusion coefficient for all atoms has been calculated in a broad temperature range. The calculated characteristics and, in particular, their dependence on temperature have confirmed the solid-liquid transition and strongly support the calculated melting point. In addition, some computed quantities, such as the radial distribution function, coordination numbers and mean-square displacement, were used to confirm the liquid state of kaolinite from the melting temperature as well as at other temperatures in the liquid branch. The diffusion coefficient for different atoms has been calculated throughout the isochore. These quantities and in particular their evolution under temperature have confirmed the solid-liquid states of kaolinite and the presence of the melting point. The latter quantity constitutes the first ever melting simulation of a clay mineral with close agreement to the experimental one.

Keywords: Kaolinite, melting, molecular dynamics, Z-method