

Study of structural and thermal properties of SiO₂ and Al₂O₃ in the Diatomite

K.Boubendira, K.LABIOD, S.BENAYACHE, A.BENFOUGHAL, N.SASSANE

Abstract: Diatomite, also known as diatomaceous earth, is the naturally occurring fossilized remains of diatoms. Diatoms are single-celled aquatic algae. They belong to the class of golden brown algae known as Bacillariophyceae. Diatomite is a near pure sedimentary deposit consisting almost entirely of silica. The Greeks first used diatomite over 2,000 years ago in pottery and brick. In this work we determine the structural and thermal properties of SiO₂ and Al₂O₃ in the diatomite using the plane wave method and linearized augmented (LAPW) in the functional theory of density (DFT). The potential for exchange and correlation is calculated by the generalized gradient approximation (GGA). Regarding thermal properties, we calculated the free enthalpy G, S entropy, specific heat C, thermal conductivity ? etc of SiO₂ and Al₂O₃ component. The temperatures used in this work are 1400, 1450 and 1500 respectively; The results are in good agreement with some experimental data.

Keywords : DFT1, diatomite, thermal proprieties