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Investigation of the phonon properties and thermal behavior of UO_2 crystal using density-functional theory

S Sheykhi and M Payami Shabestar

Physics and Accelerators Research School, Nuclear Science and Technology Research Institute, AEOI, Tehran, Iran

E-mail: mpayami@aeoi.org.ir

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Abstract

Understanding thermal behavior and processes underlying the heat transport of UO_2 nuclear fuel in nuclear reactor plays a key role in predicting the efficiency of the fuel. If the heat transport, which is an important parameter in temperature distribution of the fuel, does not occur properly, the continuous increase of temperature would lead to the melting of the fuel and therefore, environmental hazards. In this work, by using a non-spin-polarized calculation for the simple description of the paramagnetic state and ignoring the Hubbard correction, the thermal properties and phonon properties of bulk UO_2 are calculated. These calculations are based on the density-functional theory (DFT) and density-functional perturbation theory (DFPT). To determine the lattice-vibration properties by the finite-displacement method, we have calculated the second-order and third-order force constants based on which such quantities as constant-volume specific heat, Gruneisen parameter, three-phonon scattering rate, scattering rate due to different levels of isotopic enrichment, and cumulative thermal conductivity are calculated. The results of the calculated specific heat based on the harmonic approximation show a good agreement with the experimental values, specifically for temperatures lower than 400 Kelvin. The results obtained for three-phonon scattering rate reveal that the scattering rate increases with temperature, thereby leading to the decrease of thermal conductivity. The results related to different levels of isotopic enrichments do not show any sensible changes in the scattering rates.

Keywords: uranium dioxide, phonon, phonon scattering rate, phonon mean free path, Boltzmann transport equation

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