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Calculation of thermal conductivity of $\text{UO}_{2\pm 0.25}$ solving phonon Boltzmann equation

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Abstract

In this study, the effect of point defects on the thermal conductivity of UO_2 is investigated. Especially, the effects of oxygen vacancy and interstitial are considered. Thermal conductivity of UO_2 , $\text{UO}_{2+0.25}$ and $\text{UO}_{2-0.25}$ is calculated by solving the phonon Boltzmann equation (BTE) under the relaxation time approximation (RTA). The results show that introducing any defects to the lattice structure of UO_2 decreases thermal conductivity significantly. In addition, the results show that the variation of the thermal conductivity of $\text{UO}_{2-0.25}$ is much lower than that of $\text{UO}_{2+0.25}$ in the temperature interval of 300 to 1000 Kelvin.

Keywords: uranium dioxide, phonon Boltzmann equation, thermal conductivity, phonon lifetime, defect

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