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Systematic investigation of the misorientation- and temperature-dependent Kapitza resistance in CeO_2

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ABSTRACT

The misorientation- and temperature-dependent grain boundary thermal (Kapitza) resistance in CeO_2 is investigated using molecular dynamics simulations. A few empirical potentials for molecular dynamics simulations are evaluated for their predicted properties such as the phonon dispersion curves, bulk thermal conductivity, and grain boundary structures. Through the comparison of these properties with experimental results, the most reasonable potential (Gotte2007) is selected. The Kapitza resistances of tilt and twist grain boundaries with misorientation angles ranging from 3° to 87° are calculated and a clear transition angle at about 16° is observed. The Kapitza resistance is found to increase almost linearly with misorientation angle in the low-angle regime but remain nearly constant at the high-angle regime, a behavior very similar to the grain boundary energy. A nearly linear correlation between Kapitza resistance and grain boundary energy is thus obtained. Similar to the grain boundary energy, the Read–Shockley model can well describe the misorientation-dependent Kapitza resistance at low-angle regime. The Kapitza conductance (the inverse of Kapitza resistance) is found to increase almost linearly with temperature in our simulations.

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1. Introduction

Mass, charge and energy transport properties of a material system are intimately connected to the presence of interfaces, either homogenous type such as grain boundaries (GBs) or heterogeneous type such as interfaces between different materials or phases. In the context of the heat transfer, the effect of increased thermal resistance due to an interface was discovered by Kapitza in 1941 [1] in the liquid helium-metal system, but later has been demonstrated to be ever-present in any type of interfaces [2]. Therefore, an interface thermal resistance is termed as Kapitza resistance, and it plays an important role in many technological applications. For example, high density of heterogeneous interfaces in BiTe/SbTe superlattices and subsequent reduction of the thermal conductivity due to Kapitza resistance is the key in making these materials the most efficient thermoelectric to date [3]. In contrast, in applications where thermal conductivity has to be maximized interfaces might be detrimental to the performance of materials or devices. For example, interfacial resistance prevents efficient cooling of the high-power GaN electronics and is currently a bottleneck for harvesting their full potential [4].

In many ceramic materials, where phonons are the main thermal energy carriers, interfaces provide an additional phonon scattering mechanism which qualitatively explains the reduction of the thermal conductivity as the density of interfaces increases. The mechanism is applicable to not only the aforementioned heterogeneous interfaces, but also homogenous interfaces such as GBs. Yang et al. explicitly demonstrated the effect in the nanocrystalline ZrO_2 [5], by finding that thermal conductivity depends strongly on the grain size and decreases rapidly with the increased interfacial density. Quantitative prediction of the thermal conductivity reduction due to GBs is essential in many applications, such as nuclear fuel performance, or thermal barrier coatings. Unfortunately, quantitative theories developed in the past, so-called acoustic mismatch model (AMM) and diffuse mismatch model (DMM) [2] are not applicable in the context of GBs. Namely, AMM predicts zero thermal conductivity for any homogenous interface, while DMM predicts that GBs of any orientation will have the same Kapitza resistance. Thus, important details of the Kapitza resistance of GBs such as the dependence on misorientation, remain largely unexplored. Experimental measurements either focused on the averaged Kapitza resistance over a GB population [5,6], or studied

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the resistance in bicrystals that are laborious to fabricate and thus only a limited number of GB misorientations are sampled [7]. Molecular dynamics simulations have been employed to study misorientation dependence in symmetric $\langle 001 \rangle$ twist GB in diamond [8] and a limited sampling of the GBs in Si [9,10] and UO_2 [11]. While restricted to small number of GBs, these studies demonstrated that boundary conductance correlates strongly with the GB energy. In this work we address the thermal transport properties of a large number of twist and tilt GBs in ceria (CeO_2) of different misorientations via non-equilibrium molecular dynamics (NEMD) approach.

NEMD has been widely used for studying phonon-mediated thermal transport problems in semiconductors and oxides as outlined in a recent review [12]. Since MD can model much larger simulation systems than density functional theory (DFT) method can do, many microstructural features such as grain boundaries [8,11], voids [13,14], and dislocations [15] can be included in the simulation. However, the main disadvantage of the NEMD for the thermal transport simulations is the reliance on the empirical potentials, which typically are not fitted to reproduce those. We therefore first evaluate the quality of the available ceria potentials [16,17] with respect to bulk thermal conductivity and GB structures, both of which can be compared with experiments. For bulk thermal conductivity, we employ a fast and accurate approach based on the solution of the Boltzmann Transport Equation (BTE) for phonons as implemented in the PhonTS package [18]. For GB structures, we construct some special GBs in MD simulations and compare their minimum-energy structures with the published high-resolution transmission electron microscopy (TEM) images in literature. While accurate bulk thermal conductivity and GB structures do not guarantee an adequate representation of the interfacial resistance due to the integral nature of thermal conductivity [19], it is nevertheless a reasonable way to select the most appropriate potential for the simulations.

The paper is organized as follows: In the Section 2 we describe the computational methods employed in this work. Section 3 presents BTE calculations of the thermal conductivity in a bulk ceria predicted by various interatomic potentials available from the literature and motivates the potential choice for the GB studies. In Section 4 we present structural analysis of the GBs predicted by the selected potential and compare the GB structures with available experimental data, thus further validating the choice of potential. These results are discussed and related to other GB properties. In the next two sections we present our results of the Kapitza resistance for a large number of tilt and twist GBs of different orientations and at different temperatures. Finally, we discuss our results and present conclusions of this work.

2. Computational details

The quality of classical potentials of CeO_2 employed in this work has been surveyed previously with respect to their predicted surface properties by Galea et al. [16] and mechanical properties by Xu et al. [17] with some overlap in potentials tested. We maintain the designation of the potentials used in these two works and use the designation by Xu et al. [17] for overlapping potentials. Since these works a few additional potentials appeared in the literature [20,21]. Unfortunately, the parameters for the ceria potential developed by Walsh et al. [21] were not reported, while the potential developed by Burbano et al. [20] has not been implemented in PhonTS software. Therefore, we exclude these potentials from our discussion. All the potentials considered here employ the same functional form which includes a Coloumbic term that describes the electrostatic interaction between ionic charges q_i and q_j, and a Buckingham term that has both short-range repulsion and long range attraction

$$V(r_{ij}) = \frac{q_i q_j}{r_{ij}} + A e^{-\rho r_{ij}} - \frac{C}{r_{ij}^6}, \tag{1}$$

where r_{ij} is the distance between two ions i and j, A, ρ and C are Buckingham potential parameters. Nearly all potentials also include a core–shell model [22] which accounts for atomic polarizability. The essence of the core–shell model is to represent the negatively charged electron cloud around an ion (core) as a massless spherical shell. In the model, the shell is connected to the core by a harmonic potential so that it can move a distance relative to the ion core position to capture the polarization effect.

Thermal conductivity of bulk ceria is computed by BTE for phonon formalism, as described in details elsewhere [23]. In short, this approach calculates lattice thermal conductivity by considering lattice vibrations, or phonons, as heat carriers. In a harmonic picture, thermal conductivity by phonons is infinite, thus the leading anharmonic cubic term is considered using the perturbation theory. This leads to phonon–phonon scattering via 3-phonons processes. We further assume weak non-equilibrium and linearize BTE in terms of the function $\Phi_{\vec{k},n}$ which describes the deviation from the equilibrium Bose–Einstein distribution $f^0_{\vec{k},n}$ of the phonons in state with wave-vector $\vec{k}$ and branch n. BTE thus takes the form

$$\begin{aligned} -\vec{v}_{\vec{k},n} \cdot \frac{\partial f^0_{\vec{k},n}}{\partial T} \nabla T = \frac{1}{k_B T} \Bigg\{ \sum_{\vec{k}',n';\vec{k}'',n''} \Big[\Big(\Phi_{\vec{k},n} + \Phi_{\vec{k}',n'} - \Phi_{\vec{k}'',n''} \Big) \Lambda^{\vec{k}'',n''}_{\vec{k},n;\vec{k}',n'} \\ + \frac{1}{2} \Big(\Phi_{\vec{k},n} - \Phi_{\vec{k}',n'} - \Phi_{\vec{k}'',n''} \Big) \Lambda^{\vec{k}',n';\vec{k}'',n''}_{\vec{k},n} \Big] + \ldots \Bigg\} \end{aligned} \tag{2}$$

In this equation, $\vec{v}_{\vec{k},n}$ is the group velocity of the phonon; T is the temperature; k_b is a Boltzmann constant; Λ is the equilibrium transition rates for a specific process, computed on the basis of the perturbation theory. The first term on the right hand side describes the recombination process, where two phonons in the states k, n and k', n' combine to form a phonon in the state k'', n'', while the second term describes dissociation process for a phonon k, n into two phonons k', n' and k'', n''. Transition rates for these processes can be computed from the following expressions

$$\begin{aligned} \Lambda^{\vec{k}'';n''}_{\vec{k};n\vec{k}';n'} &= \frac{2\pi}{\hbar} \Gamma^2_{nn'n'';\vec{k}\vec{k}'\vec{k}''} f^0_{\vec{k};n} f^0_{\vec{k}';n'} (f^0_{-\vec{k}'';n''} + 1) \\ &\quad \delta(\hbar\omega_{\vec{k};n} + \hbar\omega_{\vec{k}';n'} - \hbar\omega_{-\vec{k}'';n''}) \\ \Lambda^{\vec{k}'';n''\vec{k}';n'}_{\vec{k};n} &= \frac{2\pi}{\hbar} \Gamma^2_{nn'n'';\vec{k}\vec{k}'\vec{k}''} f^0_{\vec{k};n} (f^0_{-\vec{k}';n'} + 1)(f^0_{-\vec{k}'';n''} + 1) \\ &\quad \delta(\hbar\omega_{\vec{k};n} - \hbar\omega_{-\vec{k}';n'} - \hbar\omega_{-\vec{k}'';n''}), \\ \Gamma_{nn'n'';\vec{k}\vec{k}'\vec{k}''} &= i \frac{(\hbar/2)^{3/2}}{V^{1/2}} \omega^{-1/2}_{\vec{k};n} \omega^{-1/2}_{\vec{k}';n'} \omega^{-1/2}_{\vec{k}'';n''} \\ &\quad \sum_{IJK} \frac{\bar{B}_{IJK;\vec{k}\vec{k}'\vec{k}''}}{m_I^{1/2} m_J^{1/2} m_K^{1/2}} \vec{e}^*_{I;\vec{k};n} \vec{e}^*_{J;\vec{k}';n'} \vec{e}^*_{K;\vec{k}'';n''}, \end{aligned} \tag{3}$$

here, $\hbar$ is the Plank's constant, I, J and K are indexes that count atoms of corresponding masses m in the primitive cell, V is the volume of the cell, while $\vec{e}_{I;\vec{k};n}$ is the eigenvector of the phonon with frequency $\omega_{\vec{k},n}$. $\bar{B}_{IJK;\vec{k}\vec{k}'\vec{k}''}$ is a Fourier-transform component of the cubic anharmonic term and δ-functions enforce conservation of energy in the corresponding 3-phonon process. Once transition rates are calculated, BTE in Eq. (2) can be solved for unknown deviation from equilibrium $\Phi_{\vec{k},n}$ thus allowing one to compute phonon heat current. Due to the assumption of weak non-equilibrium, or small temperature gradient, Fourier law is applicable and permits extraction of the thermal conductivity. All calculations in the Section 3 are performed using a six-atom orthorhombic primitive cell of CeO_2 with the k-mesh resolution for phonons calculations of $11 \times 11 \times 9$. Thermal expansion is taken into account within the quasiharmonic

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