Elucidating Mechanisms of Phonon Transport in the Vicinity of Dislocations by Perturbed Molecular Dynamics

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Abstract

Recently, the impact of dislocations on phonon transport has begun to be studied, but its microscopic mechanism is still unclear. In this study, we carry out perturbed molecular dynamics simulations for MgO to analyze how phonon thermal conduction is suppressed by dislocations at atomic level, especially by core structures and bond strains. It is found that dislocations scatter different phonon modes at different regions around dislocation cores, resulting in a significant decrease in the phonon thermal conductivity. This result suggests that, through controlling slip systems of dislocation in materials and separately controlling the different phonon modes, it is possible to control phonon thermal conduction, for thermoelectric energy conversion, for example.

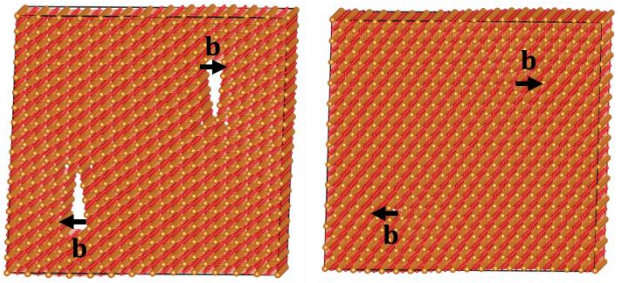
1. Introduction

To improve thermoelectric figure of merit, it is necessary for materials to simultaneously achieve high electrical conductivity and low thermal conductivity. To meet with these conflicting demands, it is important to understand the mechanisms of thermal conduction and its dominant factors. Recently, dislocations, which are often used to control mechanical properties, have attracted much attention as a means of manipulating thermal conductivity. In experiments[1)], the impact of dislocations on phonon thermal conductivity was evaluated by controlling the stress direction and the slip system of dislocations. However, it is difficult to quantitatively understand the underlying mechanisms behind the observed phenomena because of the complex dislocation textures and interactions with other lattice defects in real materials. On the other hand, an analytical model based on theories of nonlinear elasticity and discrete lattice model[2)] allow us to gain a basic understanding of the impacts of dislocations on thermal conduction. However, such analytical model is not sufficient to apply to real materials because it simplifies dislocation core structures and interactions of dislocations in exchange for generality.

2. Experiment

In this study, perturbed molecular dynamics calculations[2)3)] have been performed, which can generate a heat flux by applying perturbations to each atom and calculate the thermal conductivity at the atomic level. MgO was chosen as a model material because it has FCC sublattice of O atoms which is shared by many materials, not only metals but also various oxides. Therefore, the findings of this study can be applied to a variety of important materials.

A pair of dislocation core with the antiparallel Burgers vector was introduced into a supercell at most stable positions at an angle 45 degrees between two dislocation cores according to the Peach-Koehler equation (Fig. 1).



(a) $\mathbf{b} = a[001]$ (b) $\mathbf{b} = a/2[110]$

Fig. 1 dislocation models with antiparallel Burgers vector

3. Results and discussion

Figure 2 shows the dependence of thermal conductivity on dislocation density in different slip system of dislocations. The thermal conductivity was significantly reduced from that of the perfect crystal due to dislocations. In addition, the crystallographic anisotropy of the lattice thermal conductivity is altered by dislocations due to the different dislocation core structures. In order to understand this complex impact of dislocation on lattice thermal conductivity, we analyzed the lattice thermal conductivity at the atomic level and the contributions of longitudinal and two types of transverse phonon modes to lattice thermal conductivity. The magnitude of decrease in lattice thermal conductivity varies with the relative position from the dislocation core. In addition, it is found that different phonon modes are scattered or transformed into another phonon in different regions. These results suggest that those phonons are selectively scattered by the elastic strain in each direction of the dislocation, resulting in a reduction of the lattice thermal conductivity at atomic level.

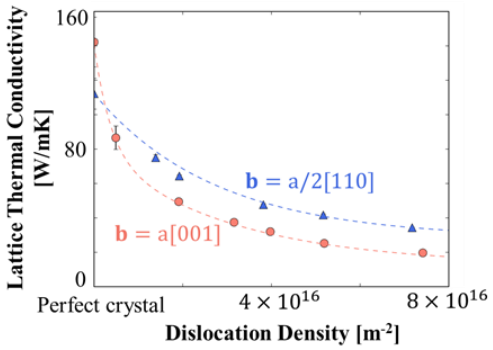


Fig. 2 Dependence of thermal conductivity on dislocation density[5)]

4. Conclusions

From this study, it is suggested that phonon transport can be controlled by selectively introducing slip systems of dislocations and separately controlling different phonon modes, which are highly orientation dependent.

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