



Theoretical and experimental research of thermal conductivity of silver(Ag) nanowires in mesoporous substrate

Jing Li^{a,*}, Yanhui Feng^b, Xinxin Zhang^b, Ge Wang^c

^a Key Laboratory of Low-grade Energy Utilization Technologies and Systems (Chongqing University), Ministry of Education, Chongqing 400044, China

^b School of Energy and Environmental Engineering, University of Science and Technology Beijing, Beijing 100083, China

^c School of Materials Science and Engineering, University of Science and Technology Beijing, Beijing 100083, China

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ABSTRACT

Thermal conductivities of Ag nanowires with different sizes and temperatures were studied theoretically. The lattice and electronic thermal conductivities of Ag nanowires include contributions from interface scattering and grain boundary scattering. While the molecular dynamic simulation was used to get the contribution of interface scattering to the lattice thermal conductivity of Ag nanowires along the axial direction, a model derived from Boltzmann transport equation and the Wiedemann-Franz relation were applied to calculate electronic thermal conductivities of Ag nanowires along the axial direction. And then coupling with the lattice and electronic thermal conductivities, the effective thermal conductivity of Ag nanowire along the axial direction was obtained. Furthermore, Kubo linear-response formalism was used to approximately predict the thermal conductivity in the plane perpendicular to the axis of the Ag nanowire. It turns out that effective thermal conductivities of Ag nanowire in the r - θ plane and along the Z direction show a great anisotropy. Finally, by measuring the thermal conductivities of Ag/SBA-15, the thermal conductivity of a single Ag nanowire can be obtained by using PWD model, and the theoretical thermal conductivities of Ag nanowire were compared with the experimental results.

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0. Introduction

It is known that the effects of surface and grain boundary scattering reduce the thermal conductivity of nanowire, which has great difference from the bulk material [1]. It has been attracted great interest in recent years. Thermal conduction is mainly due to electrons in bulk metals. In nanoscale, the total thermal conductivity k in metals is the sum of the electronic thermal conductivity k_e and the phonon thermal conductivity k_{ph} , $k = k_e + k_{ph}$, since scattering of electrons and phonons at surfaces and grain boundaries will reduce the thermal conductivity.

So far, the methods used to calculate the phonon thermal conductivity were the Boltzmann transport equation [2,3], molecular dynamics simulations [4,5], Monte Carlo simulations [6,7]. Zou and Balandin [2] used Boltzmann transport equation to study the phonon heat transfer of semiconductor nanowires. Volz and Chen [5] researched the phonon thermal conductivity of Si nanowires by molecular dynamics simulations. Dames and Chen [8] studied the phonon thermal conductivity of Si/Ge superlattice nanowires by theoretical analysis. The methods to calculate the electronic

thermal conductivity were the Boltzmann transport equation [9,10], and Wiedemann-Franz law [11].

In this paper, we focus on thermal conductivity of Ag nanowires incorporated in ordered mesoporous substrate SiO₂ (Ag/SBA-15 [12,13]). And the present work is expected to provide some useful data for mesoporous composites applications. In the first part, the lattice and the electronic thermal conductivities of Ag nanowires with different size, length and temperature, including contributions from interface scattering and grain boundary scattering, were studied respectively. While a molecular dynamic simulation was taken to get the lattice thermal conductivity of Ag nanowires along axial direction (Z direction), a model derived from Boltzmann transport equation and the Wiedemann-Franz relation were applied to calculate electronic thermal conductivities of Ag nanowires along the axial direction. And then coupling with the lattice and electronic thermal conductivities, the effective thermal conductivity of Ag nanowire along the axial direction was obtained. Furthermore, Kubo linear-response formalism was used to approximately predict the thermal conductivity in the plane perpendicular to the axis of the Ag nanowire. It turns out that effective thermal conductivities of Ag nanowire in the r - θ plane and along the Z direction show a great anisotropy. Finally, the structures of Ag/SBA-15 were introduced, and the thermal conductivities of

* Corresponding author.

E-mail address: lj202740@cqu.edu.cn (J. Li).

Ag/SBA-15 were measured by using the heat stack method. The thermal conductivity of a single Ag nanowire can be obtained by using PWDMM model and the experimental results of Ag/SBA-15, and the theoretical thermal conductivities of Ag nanowire were compared with the experimental results.

1. Lattice thermal conductivity of Ag nanowire along the Z direction

It is known that the thermal conductivity of nanowire includes contributions from surface boundary scattering and grain boundary scattering [14], as shown in Fig. 1.

1.1. Surface boundary scattering simulation of lattice thermal conductivity

Although Ag nanowires filled in mesoporous substrate (SBA-15) mesochannels are cylindrical nanowires, cube nanowires were used to study the lattice thermal conductivity of Ag nanowires along the Z direction while approximating a cylindrical nanowire as a cube nanowire with equal cross-sectional area is a preferred approximation [15]. In this paper, face-centered cubic (FCC) was built as the basic unit to construct microstructure of Ag nanowires.

Lattice thermal conductivities of Ag nanowires were numerically predicted by equilibrium molecular dynamics (EMD) method with frequently used embedded atom method (EAM) and many-body potential [16]. Embedding energy of atoms in local electron density background was considered in this potential. The potential energy of the i th atom is given by [16]:

$$E_{Pi} = \frac{1}{2} \sum_{j \neq i} \Phi(r_{ij}) + U(\rho_i) \quad (1)$$

$U(\rho_i)$ is the embedding energy of atom into electron density ρ_i . $\Phi(r_{ij})$ is the two body central potential between atoms i and j separated by r_{ij} and is an repulsive term.

The total energy of the i th atom is the summation of the potential energy and kinetic energy, $E_i = \frac{1}{2} m v_i^2 + E_{Pi}$, where v_i is the velocity associated with atom i , m is the atom mass.

The Kubo method was used to relate equilibrium current-current autocorrelation function with lattice thermal conductivity via the Green-Kubo expression [17,18]. $k_{ph,Z}$ is an element of the thermal conductivity tensor along the Z direction,

$$k_{ph,Z} = \frac{1}{3Vk_B T^2} \int_0^\infty \langle J(0)J(t) \rangle dt \quad (2)$$

where V is the system volume, k_B is the Boltzmann constant, T is the system temperature, and the angular brackets denote an ensemble average. $J(t)$ is heat current expressed as $J(t) = \frac{d}{dt} \sum_i r_i(t) E_i(t)$, r_i is the position vector of i atom.

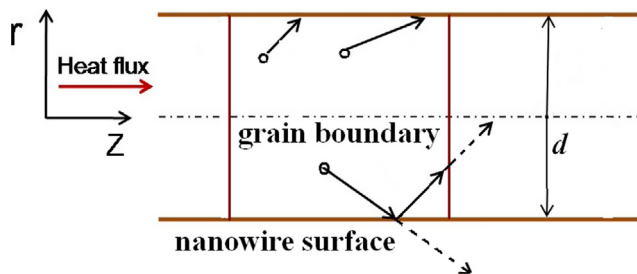


Fig. 1. Interface scattering and grain boundary scattering of nanowire.

1.2. Grain boundary scattering model of lattice thermal conductivity

For low dimensional structures, such as films, superlattices, nanowires, reducing the grain size significantly leads to further lattice thermal conductivity reduction [19–21].

Diffuse Mismatch Model (DMM) [22] is used to describe transmission characteristics of phonons at the interface and to predict the thermal resistance of the grain boundary R_{int} , which is derived from heat flow barrier through the grain boundary.

$$R_{int} = \left[\frac{k_B^4 \pi^2}{30h^3} c_1^{-2} \alpha_{1-2} \right]^{-1} T_2^{-3} \quad (3)$$

where T_2 is the temperature of the second side, $\alpha_{1-2} = \frac{c_1^2}{c_1^2 + c_2^2}$, c_i is the sound velocity of the material at the i th side. Then we can obtain the lattice thermal conductivity of nanowire modified by R_{int} :

$$k'_{ph,Z} = \frac{d_g}{\frac{d_g}{k_{ph,Z}} + R_{int}} \quad (4)$$

where d_g is the average in-plane grain diameter. It is difficult to obtain the exact value of grain size. Some papers have shown that grain size is linear with width for nanowire. Therefore, we can write $d_g = \beta d$, where β is close to 1 [23], where d is the diameter of the nanowire.

1.3. Results of lattice thermal conductivity of Ag nanowire along the Z direction

Lattice thermal conductivities of Ag nanowires with different cross section areas and period lengths at temperature $T = 300$ K were studied. Results are shown in Fig. 2(a) and (b).

From Fig. 2(a), it can be drawn that: With increasing diameter of nanowire, the lattice thermal conductivity of Ag nanowires becomes larger. The similar phenomenon was reported in N. Mingo's work [24]. It is understood that the surface scattering, grain boundary scattering of phonons are the main causes of the thermal resistance in nanoscale structure. It can be concluded that the boundary scattering of phonons becomes less important on lattice thermal conductivity as the cross-section area becomes larger. Since the characteristic length increases, the ratio of the surface area and volume of the structure significantly decreases, which will result in the exaltation in the mean free path of the phonons. Therefore, lattice thermal conductivity of nanowire increases since the phonon relaxation time is evaluated.

In Fig. 2(b), the lattice thermal conductivity of the Ag nanowire increases with increasing period length, which illustrates that particle number of simulation system is not enough in this situation, similar to the result of Gang Wu's work [25]. Increasing the particle number can solve the "finite size effect", which is consistent with the low dimensional heat conduction theory. When the period length of the Ag nanowire reaches 6.5376 nm, its lattice thermal conductivity approaches constant, which means that the size effect generated by the calculation of the period length has basically disappeared. Thermal conductivities of nanowires with period length of 6.5376 nm were employed for further study in this article. Other studies show that the lattice thermal conductivity of a nanowire is much lower than that of bulk, sometimes, only 1–10% of the bulk value [26–28]. The result of our study is consistent with those.

In Fig. 2(c), it can be seen that the lattice thermal conductivity of Ag nanowire becomes lower with increasing temperature. It is understood that the surface scattering, grain boundary scattering of phonons are increasing with increasing temperature. Since the random thermal motion of micro particles increase with increasing

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