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Monte Carlo simulations of phonon backscattering in low-sized nanowires

Zan Wang[1], Yunfei Chen[1,2], Jiapeng Li[1], Ruijie Zhao[1], Yanyan Zhao[1]

[1]School of Mechanical Engineering, University of Southeast, Nanjing, China 211189
[2]Key Laboratory of MEMS of Ministry of Education, Southeast University, Nanjing, China 211189

ABSTRACT

Monte Carlo model is used to study the roughness effects on lattice thermal conductivity of silicon nanowires. Based on the Matthiessen's rule, a roughness influence coefficient is adopted to amend the relaxation time. Individual silicon nanowires growing by vapour-liquid-solid method are different from those making by aqueous electroless etching method in the surface roughness, which are both simulated over a temperature range of 15-315K with various equivalent diameters. The results are close to the laboratory data, proving the validity of the MC model and showing the effects of surface roughness on thermal transport decrease with the increasing of equivalent diameter.

Keywords: Roughness, Monte Carlo, Thermal conductivity, Nanowire

1. INTRODUCTION

One-dimensional nanostructures, such as nanowires and single-walled carbon nanotubes, are the potential building blocks of next generation electronic and energy conversion devices. Thermal conductivities of the one dimensional nanostructures plays a crucial role in affecting the performance of those devices [1]. Phonons acting as main thermal transport carriers, are influenced greatly by quantum effects and boundary effects in the nanostructures. Li [2] synthesized nanowires by vapour-liquid-solid method and Hochbaum [3] used technique of aqueous electroless etching to generate nanowires, both of them measured the variation curve of thermal conductivities. Compared with the two group experimental data, the common point is, with reduction of diameter thermal conductivity decreases correspondly, from which it is easy to think the smaller the diameter, the more the boundary scattering. The different point is the thermal conductivities from the former experiment is as much as several times larger than those from the latter one. In that nanowires fabricated by different processes have different surface roughness, we have reasons to believe it is the backscattering that brings the difference. Backscattering is the collision between phonon and the lateral face of roughness. In the commonly used MC method [4] [5] [6] [7] [8] [9], the physical models are created by real shape geometrical bodies, the surfaces of nanowire are assumed totally flat and whether a phonon occurs to scattering by boundary just depends on its coordinates of position, which make the thermal transport of small radius nanowires hard to simulate. Additionally, there exist two difficulties in this kind of model to investigate thermal transport. One is how to identify the distribution density and shape of rough geometric feature in nonowires. Another is the increasing tremendous calculation time costs of solving backscattering, because the roughness complicates the boundary condition, only if its position goes beyond the limits of the physical model, will boundary scattering or backscattering take place.

2 MATHEMATICAL DEDUCTION

The aim of our work is to provide a method to clarify the boundary scattering effects on phonon transport in silicon nanowires. According to the Fourier law, $J_Q = -k_l \nabla T$, J_Q is the density of heat flux, ∇T is the gradient of temperature along nanowire and k_l is the thermal conductivity serving as a measure of the heat transport ability. Based on the Boltzmann transport equation, analytical methods [11] [12] are proposed by means of altering phonon relaxation time and dispersion relation. But, these studies do not provide much attention to surface roughness giving rise to phonons backscattering. Monte Carlo (MC) method is often used as a numerical approach to get statistical results. Klitsner [4] adopted MC to simulate phonon ballistic transport. Peterson [5] applied Debye Model to MC procedure. Mazumder and Majumdar [6] took phonon polarization and phonon dispersion into consideration. Chen [7] applied genetic algorithm to deal with N scattering and U scattering. Lacroix [8] [9] calculated the possibility and scattering rates of boundary scattering by tracking the total numbers of phonons colliding with boundary. Randrianalisoa [13] built a MC model to study steady-state microscale phonons transport. Jeng [14] utilized MC scheme study the phonon transport and the thermal conductivity of nanocomposites.

According to the experiment [3], surface of nanowire is not as flat as supposed. Owing to surface roughness, phonon mean free path is shortened by backscattering. Considering V-shape surface roughness, Saha [15] constructed a MC model for phonon backscattering with the 22nm diameter nanowire, but the results are still larger than the experimental values and proposed the future work is to investigate whether larger surface roughness or partially diffuse and partially specular scattering at the rough surface can lead to further suppression of the thermal conductivity.

According to Matthiessen's rule, for N scatter poses no thermal resistance directly, it is acceptable to neglect N scattering in the present simulation, the combined phonon relaxation time can be given as

$$\frac{1}{\tau_T} = \frac{1}{\tau_U} + \frac{1}{\tau_B} + \frac{1}{\tau_I} \tag{1}$$

where the total relaxation time τ_T counts on the U scattering relaxation time τ_U, the impurity and lattice defect scattering relaxation time τ_I and the boundary scattering relaxation time τ_B, details on τ_U and τ_I can be found in Ref. 6.

$$\frac{1}{\tau_B} = \frac{V}{D}(1-df) \tag{2}$$

where D is the equivalent diameter of nanowire, V is the group speed of phonons and df is the diffusing factor. For the sake of justifying the above regime of solving boundary scattering selection rule, a nanowire with different boundary diffusing factor is simulated. The physical intrinsic model has the total length of 550nm, with cross-section 50nm×50nm, and is divided into 11 cells averagely along the length. The first cell is regarded as hot part and the last cell is regarded as cold part.

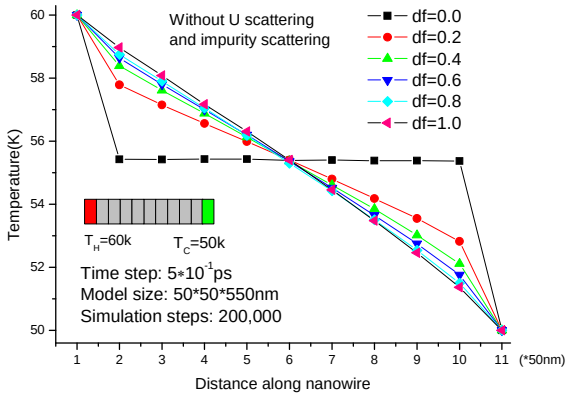

Fig.1 Temperature profile with different diffusing factor

From Figure 1, with the decreasing of diffusing factor, the gradient of temperature profile grows, which satisfies the two criterions: the effective thermal flux in each simulation cell should be nearly the same, and the temperature profiles should be reasonably close to linear.

From Figure 2, striking on a surface, a phonon may be scattered several times in one time scale by rough boundary.

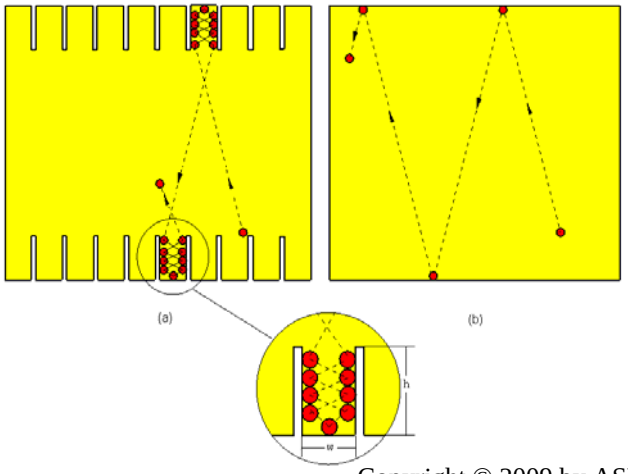

Fig.2 phonon transports in nanowire with different surface condition: (a) rough surface (b) flat surface

Since the value of its composite velocity keeps invariant, during the period of time T, distance traveled in the two kinds of wires drawn in Figure 2(a) and Figure 2(b) is equivalent, the following equations may be obtained

$$\frac{1}{\tau_B^a}=\frac{\eta}{\tau_B^b}=\frac{\eta V}{D} \tag{3}$$

The phonon relaxation time in Figure 2(a) is τ_B^a and τ_B^b is the phonon relaxation time in Figure 2(b), η is the roughness influence coefficient can be achieved by

$$\eta=\frac{D\ N_r}{D\ -2h} \tag{4}$$

where N_r is the number of backscattering when a phonon flies into the rectangular roughness region, h is the height of roughness, N_r can be given by

$$N_r=2\frac{v_x h}{v_y w}+1 \tag{5}$$

where w is the width, the velocity along x direction is v_x and v_y is the velocity along y direction. The mean roughness height of these nanowires varied from wire to wire, but was typically 1-5 nm with a roughness period of the order of several nanometers [14]. In order to enable η to be a constant, it is assumed v_x equals to v_y and w is always set by 1nm in the simulation. Through varying the value of h from 1nm to 5nm, diverse η can be calculated from equation (4) and (5) respectively. Additionally, by a lot of simulations, it is found that nanowires fabricated by the same method with different diameters have a distinct η, which is inversely proportional to the diameter of nanowire. Therefore, in order to determine the thermal conductivities of these nanowires, we just need to simulate one of them to obtain the most proper η_1 by trial-and-error process, based on experimental data. The η of other nanowires can be got by multiplying η_1 by the inverse ratio of their diameters.

3 SIMULATIONS AND DISCUSSION

In Figure 3, the nanowires grow by VLS method. The solid circle symbols represent experimental results [2] of diameters 22nm, 37nm, 56nm and the hollow symbols express the MC simulation results.

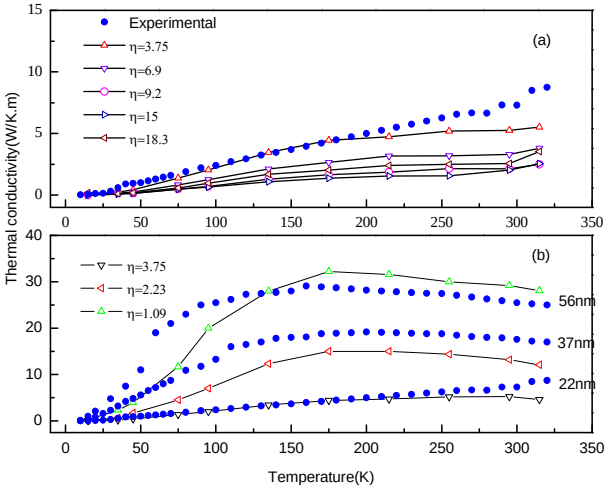

Fig.3 Thermal conductivity of different diameters Si nanowires (VLS):MC simulation results (hollow symbols) and experimental data (solid circle symbols)

Figure 3(a) shows the conductivities of Si nanowire with 22nm diameter by adjusting η. While η equals to 3.75, in the case h equals to 1nm, the simulation results get well with experimental values. Referring to 22nm diameter, the η of 37nm diameter equals to 3.75*22/37. The same solution is also used to compute the η of 56nm diameter nanowire. In Figure 3(b), for 37nm and 56nm diameter wire, the thermal conductivities are less than that of experimental results below 100K. Since heat conduction, at low temperature, is mostly dominated by boundary scattering, the reason maybe lies in the diffusing factor, which is set by the minimum value 0, in this scheme. In Figure4, the nanowires are synthesized by electroless etching (EE) method with the 10Ωcm etching wafer.

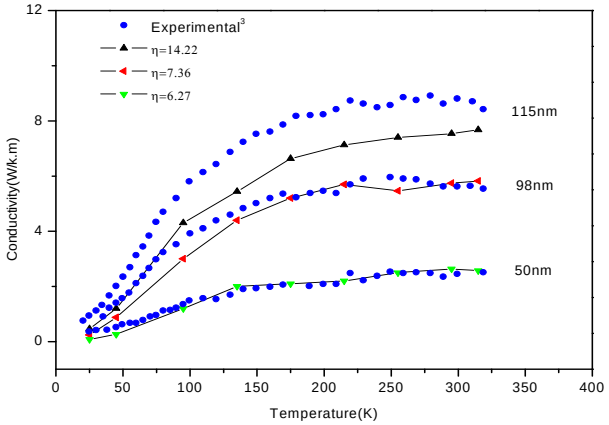

Fig.4. Thermal conductivity of different diameters Si nanowires:

MC simulation results (hollow symbols) and experimental data (solid circle symbols)

Taking 50nm diameter nanowire as reference object, the results are very close to the experimental data [3], while the h equals to 2.5nm. The η of 98nm and 115nm diameter wires can be achieved by the same approaches used in Figure 3. From simulation results, it can be shown that, in contrast to the smooth surfaces of typical vapour-liquid-solid (VLS)-grown, those of the EE Si nanowires are much rougher [3].

3. CONCLUSION

In conclusion, by using of the new MC model, we need not consider the distribution and real shape of surface roughness, there are two major advantages in this model. Firstly, assuming every phonon has a possibility of boundary scattering, without tallying the three-dimension coordinates, the calculation amount is reduced greatly. Additionally, the roughness influence coefficient η is applied to study the influence of roughness on thermal transport in nanowire, which has a reciprocal proportion to the diameter. The simulation shows that, surface roughness is the main reason to explain the sharp deduction of thermal conductivity of low-sized nanowires below room temperatures.

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