THE THERMAL CONDUCTIVITY OF THIN INDIUM ARSENIDE NANOWIRES AND NANOTUBES

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Abstract: This paper reports the modeling, thermal conductivity, local heat flux analysis, and vibrational density of states of indium arsenide(InAs) nanowires(NWs) and nanotubes(NTs) theoretically using molecular dynamics(MD) simulations. The well-known idea of increasing surface to volume ratio(SVR) to decrease the thermal conductivity of nanostructures is applied. Major contribution of reduction in thermal conductivity arises from the localized phonons at the hole surface both in low frequency and high frequency range. By creating a tiny hole the lattice thermal conductivity decreases to 75% compared to that of the nanowire. Increased figure of merit ZT of 30% is expected stemming from the low thermal conductivity.

Keywords: Thermoelectrics, Thermal conductivity, InAs, Nanowire, Molecular dynamics

INTRODUCTION

Thermoelectric(TE) materials are promising candidates which convert heat to electricity directly. The efficiency is assessed as ZT=$S^2\frac{\sigma T}{\kappa}$, S, σ, κ, and T are Seebeck coefficient, electric conductivity, thermal conductivity, and absolute temperature, respectively. Recent study suggested InAs nanowires as an efficient TE material theoretically[1]. In this work we investigate the lattice thermal conductivity of InAs nanotubes(InAsNTs) to reduce further their lattice thermal conductivity from those of InAs nanowires(InAsNWs) and provide analysis containing inside mechanism which is responsible for the reduced thermal conductivity of InAs nanotubes.

METHOD

We use non equilibrium molecular dynamics(MD) simulation, direct method, to measure the thermal conductivity of InAsNWs and InAsNTs, which is one of two methods frequently used in MD simulations[2]. Because InAs is not a homogeneous system, the other method, Green-Kubo method, requires much effort such as using low pass filters with long simulation time[3]. Both of two methods yield the same results, therefore it is adequate to use direct method for binary alloy systems. We set [111] direction of InAs zinc-blend structure as longitudinal axis(z) of InAsNWs and InAsNTs.

RESULTS

The thermal conductivities of two InAsNWs and five InAsNTs are shown in Figure 1. By simply making a tiny hole of 0.3576nm^2, from (8,0) to (8,1), the thermal conductivity is reduced by 26%. Linear decrease of the thermal conductivity is shown as widening the hole size, which is consistent with the results of literature[4] as higher SVR induces more phonon localization at the surface. Comparing (6,0) and (8,5) of which cross sectional area is 6.715nm^2 and 6.675nm^2, respectively makes sure that the large amount of reduced thermal conductivity of 47% comes from not the decreased volume but the increased SVR of the InAsNW.

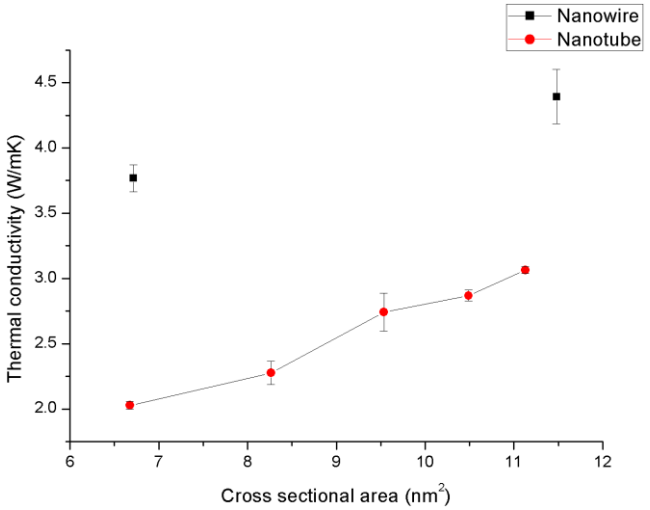

Figure 1. Thermal conductivities of two InAsNWs and five InAsNTs.

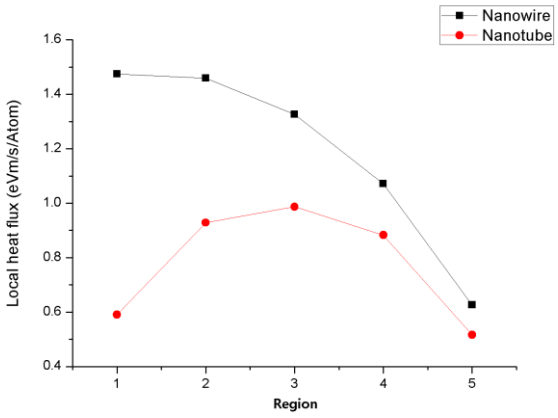

Figure 2. Local heat flux of NW (8,0) and NT (8,3) according to five divided regions. The values of the NW and NTs are normalized each other to have the identical temperature gradient.

Figure 2. shows local heat flux according to the region of five concentric circles from the center row of atoms. Numbers on x axis mean the local heat flux of each concentric circle. As the number increases, the radius of a concentric circle increases, too. Not surprisingly in the case of the InAsNW, atoms near the surface(Region 5) shows lower local heat flux than atoms at the smallest concentric circle(Region 1) as much as 58% because the phonon at the surface is localized and decreases the contribution of heat transport. Fitted curve has a wide parabolic shape with almost plat center in which adjacent two local areas(Region 1 and 2) have 1.475eVm/s/Atom and 1.459eVm/s/Atom, respectively. It is implied that most of the area except very close region to the surface has constant local heat flux and therefore phonon confinement effect becomes more significant for nano structures rather than bulk materials. The local heat flux scheme of the InAsNT is also predictable and consistent with the results of the silicon case in a previous study[4]. Additionally created surface due to the hole induces more phonons to be localized followed by thermal conductivity reduction whereas more negligible effects are shown as go further from the internal region to outside, though always does the local heat flux reduce.

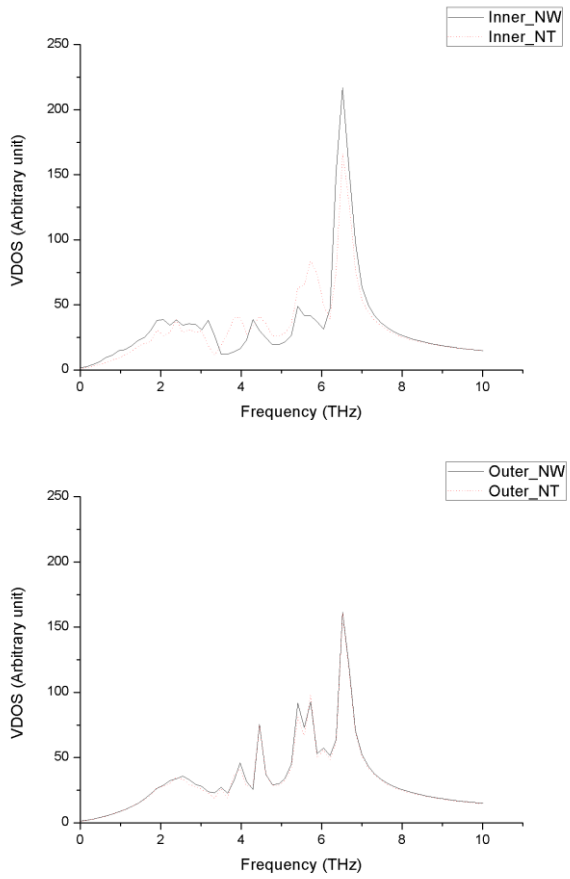

Figure 3. Local vibrational density of states on InAsNW and InAsNT at (a) Inner surface, (b) Outer surface.

Then what change can be expected in the behavior of phonons? The vibrational density of states can be derived through atom's velocity autocorrelation function followed by Fourier transform. In Figure 3, the inner surface and outer surface of InAsNW and InAsNT are analyzed separately to note how the existence of the hole makes differences for each region. First of all, the highest peak is observed in 6.5THz, which is quite lower than the frequency of the silicon nanowire's highest peak, 16.5THz[5]. Because of the heavier mass of indium and arsenic atoms than the mass of silicon atom, the maximum frequency of atoms constituting InAs is much lower than the case of silicon. Nevertheless quantitatively same trend which is responsible for the reduced thermal flow at the inner surface is shown in Figure 3.(a). Significant depression is exhibited both in low frequency and high frequency range, from 0 to 3.5THz and around 6.5THz, whereas the outer surface shows little change despite the generated inner hole, which supports the previous results of Figure 2. Several newly generated peaks at intermediate frequencies around 3.8THz and 5.8THz are also noticeable, as Ming Hu et al discovered for the silicon-germanium core/shell nanowire case[5]. Furthermore in Figure 3.(b), InAsNW has slightly larger values over some ranges than InAsNT does, which explains slightly reduced local heat flux of outer surface from NW to NT.

CONCLUSION

The MD simulations of InAs NWs and NTs show significant reduction of thermal conductivity by 25% for a tiny hole corresponding to a better performance by a factor of 1.3 for thermoelectric figure of merit. Heat flow reduction is significant at the surface surrounding a hole because of the depressed phonons of both long wavelength up to 3.5THz and high frequency around 6.5THz.

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