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Study of Heat Conduction in Corrugated Si Nanowires Using Raman mapping

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Abstract

Thermal conductivity (*k*) reduction in Si nanostructures makes them promising thermoelectric materials. Recently, significant *k* reduction was obtained in 200 nm thick corrugated nanowires (NWs) at temperatures *T* < 5 K. For applications, increase in *T* is required. Here, we demonstrate ~ 70% *k* reduction in corrugated 55 nm thick Si NWs compared to straight ones with width equal to the average width of corrugated ones at *T* ~ 350 – 400 K. *k* measurement was done using Raman mapping of individual suspended Si NWs made from silicon-on-insulator. Our results are in agreement with theoretical predictions requiring sufficiently small NW diameter and large corrugation amplitude for significant *k* reduction at *T*~300 K. An important conclusion is that making asymmetric corrugations can lead to NW heat conduction asymmetry and new applications.

1. Introduction

Thermal properties of nanostructures have attracted growing interest, especially, in application in thermoelectricity. Thermoelectric figure of merit $ZT = S^2T/\rho k$, where S, ρ, k and T are the Seebeck coefficient, electrical resistivity, thermal conductivity and absolute temperature of thermoelectric material, respectively. Although bulk Si is a poor thermoelectric, by greatly reducing k without much affecting S and ρ, Si nanowires (NWs) show promise as high-performance thermoelectric materials. With size limitation in NWs, phonon mean free path (MFP) reduces due to phonon boundary scattering, therefore, k decreases. However, recently, even stronger reduction of MFP was obtained in corrugated 200 nm thick Si NWs at low temperatures $T < 5$ K [1] when only long-wavelength ballistic acoustic phonons contribute to the heat conductance. Nearly one order reduction of k in corrugated NWs compared to straight NW was demonstrated.

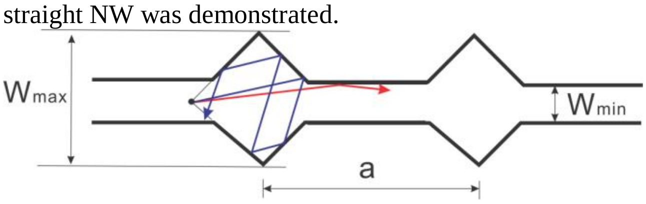

Fig. 1. Multiple phonon scattering in corrugated NW (top view). Red arrow shows forward scattering while blue arrow shows backscattering.

The effect of corrugation on k was attributed to multiple phonon scattering on corrugated surfaces (Fig. 1). As a result phonon MFP was dramatically reduced down to values smaller than so-called Casimir limit, MFP at completely diffusive phonon boundary scattering. For practical applications, it is important to study thermal conductivity of corrugated NWs at room and higher temperatures. Theoretical calculations showed significant k reduction in thin corrugated NWs at T ~300 K, namely, by factor of ~5 [2] and by factor of ~4 [3] compared to k of straight NWs with the same cross-section. Experimental realization of thin corrugated NWs with high corrugation amplitude is required for confirmation of these theoretical predictions.

2. Experimental

We study suspended Si NWs with length L = 5 and 10 μm made from silicon-on-insulator (SOI) structure with thickness H = 55 nm using electron beam lithography with subsequent removal of ~1 micron thick buried oxide layer (BOX) under NWs with HF. As a result, sets of parallel suspended NWs connecting two SOI islands were fabricated. We examined straight NWs with widths 40 – 150 nm, weakly corrugated NWs with minimal width W_{min} ~ 75 nm and maximal width W_{max} ~ 130 nm, strongly corrugated NWs with minimal width W_{min} ~ 50 nm and maximal width W_{max} ~ 150 nm, corrugation period a being ~150, 200 and 250 nm. Figure 2 shows a strongly corrugated NW with a = 150 nm.

Raman measurement was done using Nanofinder 30 confocal Raman system (Tokyo Instruments Inc.) equipped with a scanner and a 561 nm wavelength laser. Lens with 100× magnification and 0.95 numerical aperture focusing laser light into ~350 nm spot was utilized. The focused laser light was scanned along NW with ~300 nm step. Illuminated NW area displayed Raman downshift $\Delta\omega$ proportional to the laser-induced heating ΔT (ΔT (K) = $\Delta\omega$ (cm^{-1})/0.022).

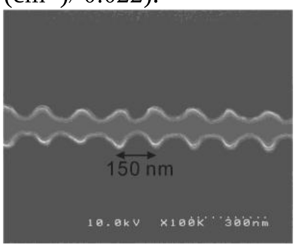

Fig. 2. SEM image of strongly corrugated NW (top view)

Figure 3 schematically illustrates an idea of experiment. It is easy to show that $\Delta T = Q(L/4 - x^2/L)/(HWk)$ (see, for example, Ref. [4], where k of straight GaAs NWs was studied using Raman mapping) when the NW thermal resistance is significantly larger than the contact thermal resistance, which is true for NWs made of SOI, Q standing for the heat generation rate. $Q = A\,P$, where P is incident light power while A stands for NW absorption. k can be found from maximal temperature increase in the middle of NW $\Delta T_{max} = APL/(4HWk)$ or from parabola curvature $B = AP/(LHWk)$. We used the first method that showed smaller experimental error than the second one. For corrugated NWs, we used averaged width W_{av}.

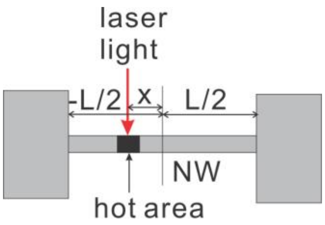

Fig. 3. Illustration for Raman mapping of suspended NW.

As our calculations show, ratio of NW absorption to the square root of its Raman efficiency is nearly independent of W for straight NWs with W = 40 – 150 nm. Assuminge that it is correct for corrugated NWs tool, we estimate the NW absorption as a square root of the NW Raman efficiency.

3. Results

Figure 4 demonstrates NW Raman spectrum, both NW and Si substrate bands contributing to the spectrum. However, as we see, they can be clearly distinguished due to the laser-induced-heating NW band downshift. Figure 5 shows dependence of temperature increase ΔT determined from temperature-induced NW Raman band downshift $\Delta\omega$ in laser-illuminated NW area on position along NW x. The dependence can be reasonably fit by parabola in agreement with theory.

Figure 6 shows dependence of k on W for straight (circles), weakly corrugated (triangles) and strongly corrugated (squares) NWs. The right axis shows thermal conductivity in W/m/K obtained by calibration of our data assuming equal thermal conductivities of straight nearly square NWs and circular ones with equal cross sections, data for circular NWs being taken from Ref. [5]. As expected, straight NWs display some increase in k with an increase in W. Weakly corrugated NWs show a slight decrease in k compared to straight ones while strongly corrugated NWs show considerable k reduction.

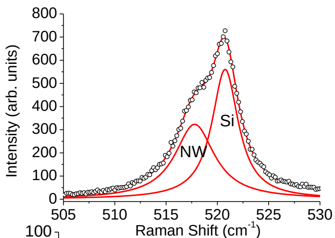

Fig. 4. Raman spectrum with downshifted NW band and unshifted Si substrate band

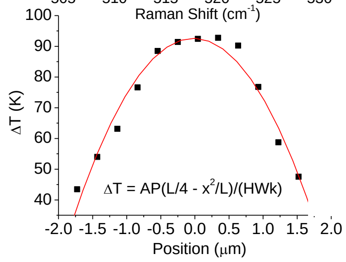

Fig. 5. Dependence of the laser-induced heating on the position along NW.

~70% reduction of k in strongly corrugated NWs (Fig. 6) suggests that the contribution of specularly scattered phonons to the heat transport at T = 350-400 K in 55 nm thick NWs is not small. On the other hand, corrugated surfaces can influence transport of diffusively scattered phonons as well. Anyway, large amplitude corrugations significantly affect k of NWs with sufficiently small cross-sections. Our calculations of corrugation impact on NW phonon dispersion, speed of sound and heat transport confirm this.

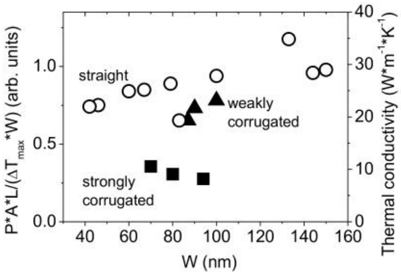

Fig. 6. NW thermal conductivity obtained from ΔT_{max}. Right axis scale is a result of calibration using reference data [5].

4. Conclusions

Using Raman mapping, we have measured thermal conductivity of 55 nm thick suspended straight and corrugated Si NWs at T = 350 – 400 K and observed ~70% k reduction for strongly corrugated NWs. The effect is attributed to corrugation-induced multiple reflections of specularly scattered phonons, reduced speed of sound and to enhanced resistance to the transport of diffusively scattered phonons. According to the obtained results, corrugated Si NWs can be considered as promising thermoelectric material. Moreover, strong effect of corrugations on NW k suggests that introduction of asymmetry to corrugations can lead to different k values in forward and backward directions. Such diode-like thermal conductor or thermal rectifier can be used for thermal regulation during energy harvesting and even in thermal logistics.

Acknowledgements

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