Asymmetric Heat Conduction in Deformed Carbon Nanohorns

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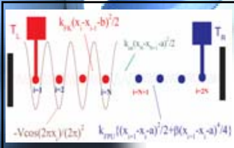
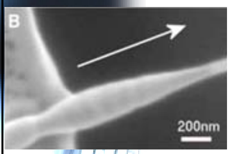
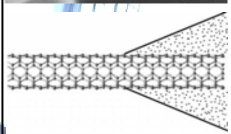
Abstract

Heat conduction in single-walled carbon nanohorns (SWNHs) is studied by using non-equilibrium molecular dynamics (MD) method. It is found that the heat conduction is asymmetric, which is called as thermal rectification. Mass gradient distribution is proven to be important for the rectification. This kind of gradient behavior can be further adjusted by applying external strain on the SWNHs. More importantly, the *negative differential thermal resistance* is observed in the deformed structure, which indicates that the carbon nanohorns might be used to construct the thermal transistor.

➤Background

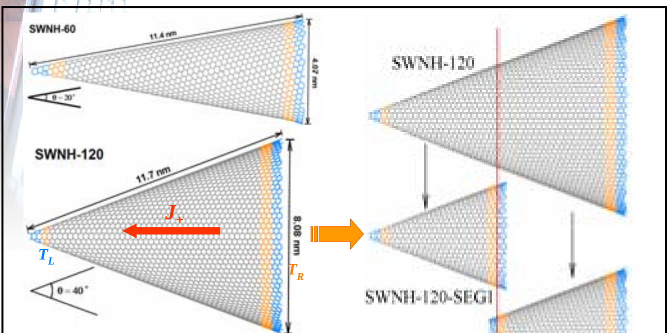


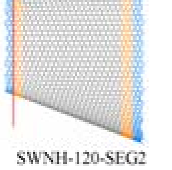




- **The heat conduction in nonlinear lattice models demonstrates rectification phenomenon, namely, heat flux can flow preferably in one direction.**
  [PRL 93, 184301 (2004); 95, 104302 (2005); PRB 74, 214305 (2006)]
- **Based on the *negative differential thermal resistance*, a thermal transistor model has been constructed.**
  [Appl. Phys. Lett. 88, 143501 (2006)]
- **The two segment model of thermal rectifier has been experimentally realized by using gradual mass-loaded carbon and boron nitride nanotubes.**
  [Science 314, 1121 (2006)]

➤Models



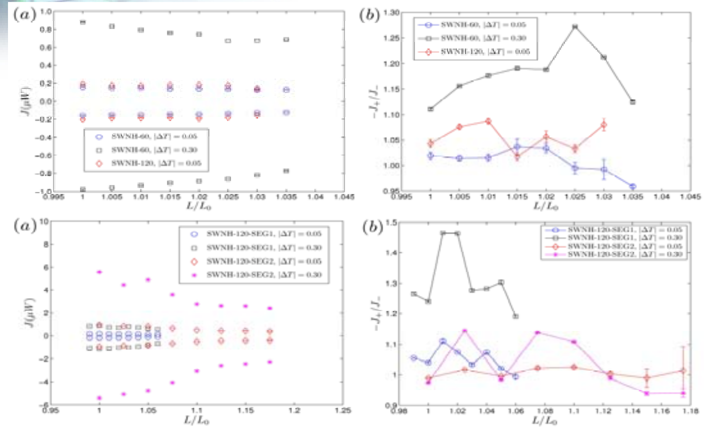


The SWNHs are obtained by cutting out 60° and 120° sectors from a graphene sheet and then gluing together the two cut sides of the sheet. They are named as SWNH-60 and SWNH-120. SWNH-120 structure can be further split into two segments, i.e., SEG1 & SEG2.

➤Methodology

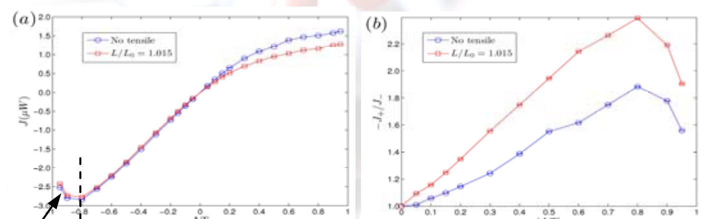
- ***The interaction between C atoms is simulated by the second-generation reactive empirical bond order potential, which is the new version of Tersoff-Brenner potential.*** **[J. Phys.: Condens. matter 14, 783 (2002)]**
- ***Fixed boundary conditions are assumed for the outmost region of each heads (colored by blue).***
- ***Then some atoms of each ends (illustrated by orange color) are subjected to heat bath at T_L and T_R, respectively, which is simulated by Nosé-Hoover thermostats.*** **[J. Chem. Phys. 81, 511 (1984); Phys. Rev. A 31, 1695 (1985)]**
- ***Two quantities are introduced for convenient: $\langle T\rangle = (T_L + T_R)/2$, $\Delta T = (T_L - T_R)/(2\langle T\rangle)$. In this work, $\langle T\rangle$ is always kept at 290 K.***
- ***The velocity Verlet method is adopted to solve the equations of motions.***
- ***The time step is chosen as 0.51 fs, and the total number of MD steps is taken as 5×10^6. 2.5×10^6 steps is used to relax the system to stationary state.***

➤Numerical Results and Discussions

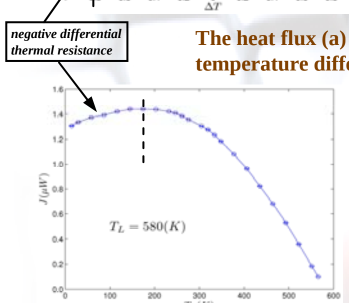


The heat flux (a) and the rectification (b) under different tensile strain versus top angle and temperature difference ΔT.

- **a.** **Temperature gradient $|\Delta T|$↑, heat flux J ↑.**
- **b.** **At same ΔT, J of SWNH-60 and SWNH-120 are almost same. ← Surface distances of SWNH-60 and SWNH-120 are almost same.**
- **c.** **J decreases in elongated structure. ← Bond length↑, interatomic force constants↓.**
- **d.** **$|\Delta T|$↑, the rectification $-J+/J-$ ↑. ← Larger temperature gradient can cause larger gradient of vibrational density of states along the tube.**
- **e.** **At the same $|\Delta T|$, rectification $-J+/J-$ of SWNH-120 is larger than that of SWNH-60. ← Top angle is an indicator of the structural asymmetry.**
- **f.** **The relation between rectification and tensile strain is not monotonous. ← Competition between the mass gradient and bond length (force constants) gradient.**
- **g.** **SEG2 can be elongated much more than SEG1. ← SEG1 has larger bond length (force constants) gradient.**
- **h.** **Rectification in SEG1 is larger than those in SEG2 and SWNH-120. ← SEG1 has largest structural asymmetry among the structures.**



The heat flux (a) and the rectification (b) versus temperature difference ΔT in SWNH-120-SEG1.



- **a.** **Elongated structure shows larger rectification. The overall maximum rectification is almost 2.4.**
- **b.** **When $\Delta T < -0.8$, a larger temperature difference $|\Delta T|$ can induce a smaller heat flux. This means the existence of the *negative differential thermal resistance*.**

It is shown from our work that SWNHs can be regarded as mass graded systems and used as thermal rectifier. And the *negative differential ther mal resistance* is also observed. This is essential for thermal transistors. Our work suggests a possible efficient heat control device, and the effici ency can be controlled by applying external stress. In this system, on-site potential is not requested to achieve asymmetric heat conduction.