Full band Monte Carlo simulation of thermal transport in GaAs nanostructures based on ab initio calculation

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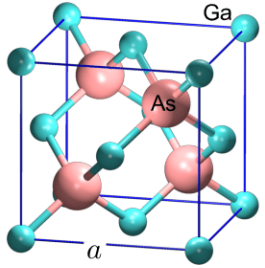
Introduction



2)

➢ Heat Transport at the Nanoscale

1)

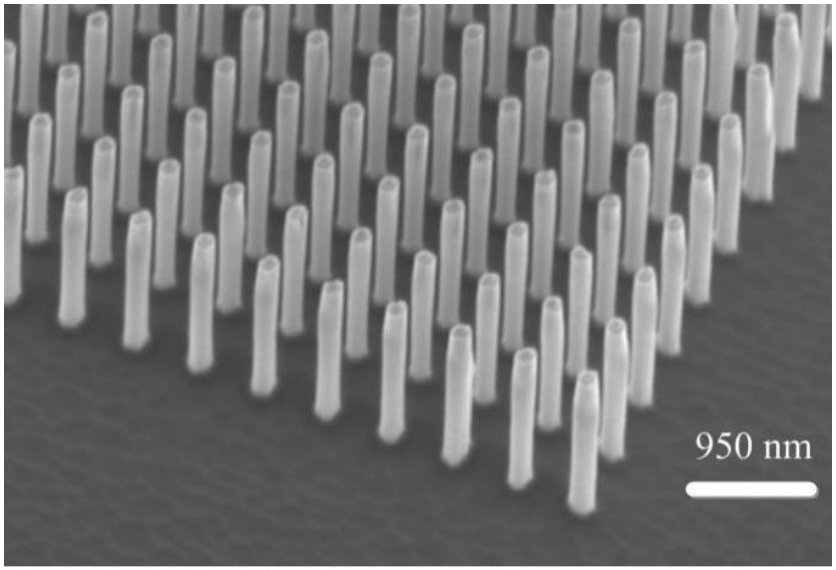


Figure 1. SEM image of vertically etched GaAs nanowire array

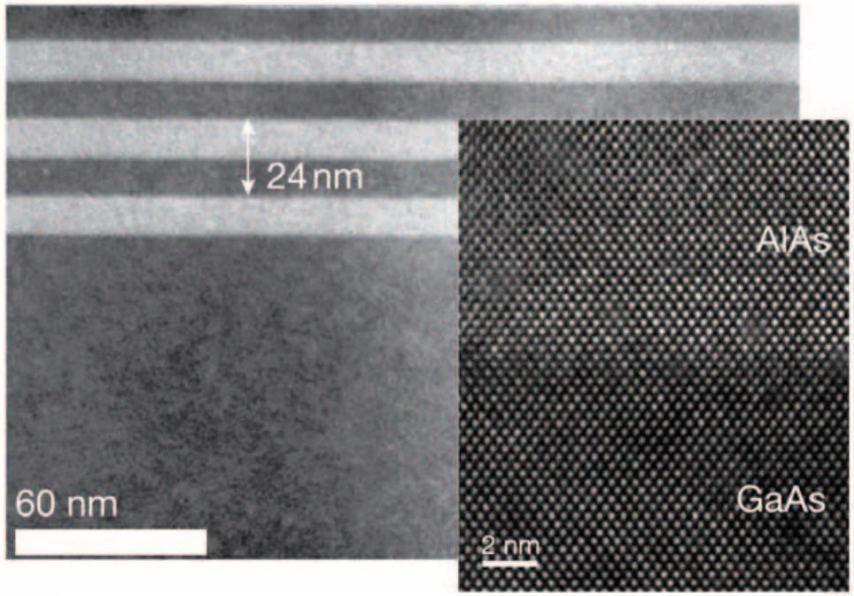


Fig. 1. (A) Cross-sectional TEM image of the 3-period (pd) SL.

✓ Semi-classical approaches by Fourier's law are no longer valid at the nanoscale

$$(q = -k\nabla T)$$

< Diffusive (Fourier) > < Intermediate > < Ballistic >

1) Walia, Jaspreet, et al. 14th IEEE International Conference on Nanotechnology. IEEE, 2014.
2) Luckyanova, Maria N., et al. *Science* 338.6109 (2012): 936-939.

Method

➢ Boltzmann transport equation for phonons

✓ The BTE is solved in the frame of the relaxation time approximation (RTA)

<BTE>

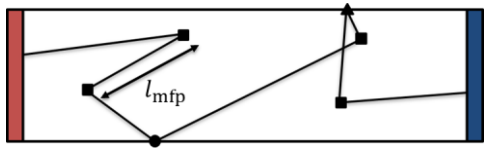
$$\overrightarrow{v_g}\frac{\partial f}{\partial r}+\frac{\partial f}{\partial t}=\left(\frac{\partial f}{\partial t}\right)_{coll}$$

<Relaxation time approximation>

$$\left(\frac{\partial f}{\partial t}\right)_{coll}=-\frac{f(\vec{r},\vec{k},t)-f_{BE}(\vec{r},\vec{k})}{\tau(\vec{k})}$$

➢ Stochastic solution of BTE by Monte Carlo method [3)]

- Phonons as pseudo-particles
- Random draw for free flights and scatterings
- Reconstruction of f from trajectories



➢ This work :

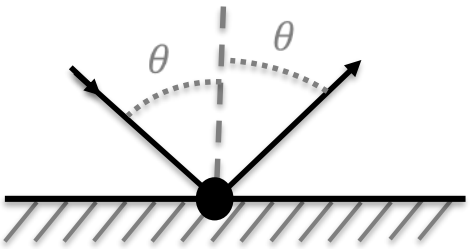
"Monte Carlo simulation parametrized by ab initio calculations"

3) Lacroix, David, Karl Joulain, and Denis Lemonnier. *Physical Review B* 72.6 (2005): 064305.

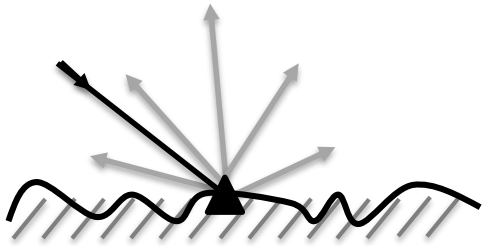
Method

➢ **Boundary condition** [4] Phonon collides with external boundaries ➡ Reflection!

Specular

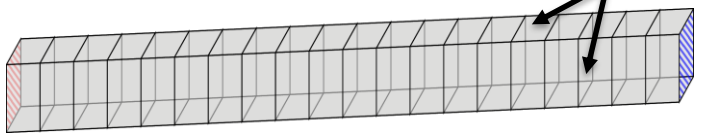


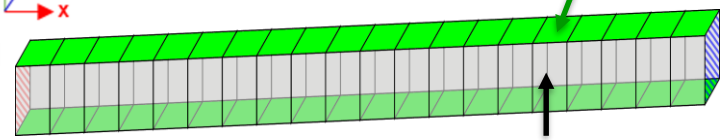
Diffusive



➢ **Device configuration** [5]

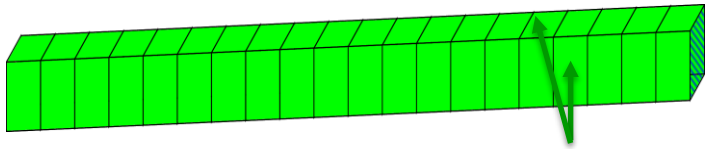
1) Nanofilm in cross-plane configuration (**CPNF**)





2) Nanofilm in in-plane configuration (**IPNF**)

3) Rough nanowire (**NW**)

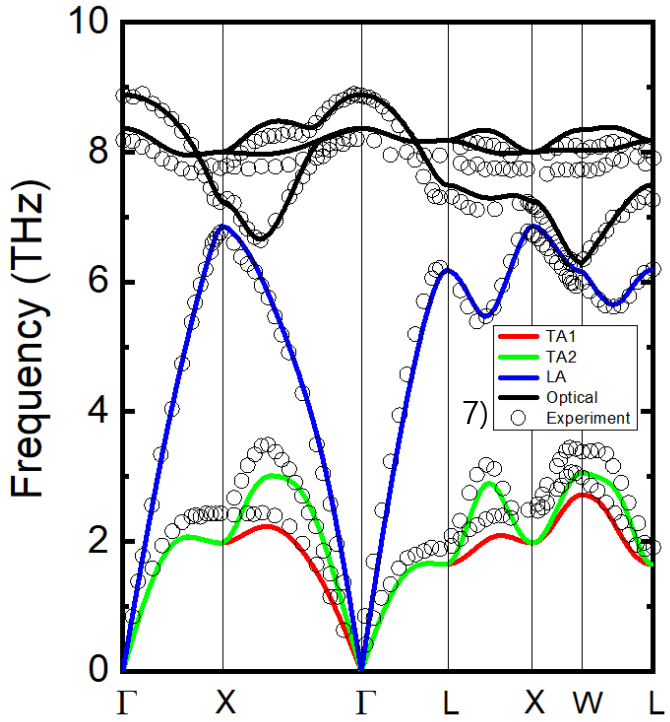


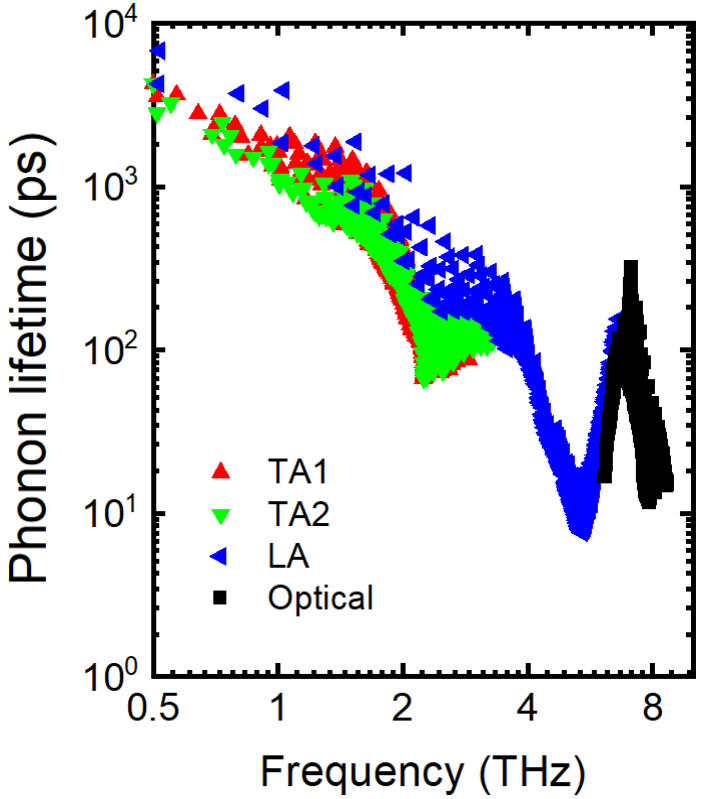
4) Soffer, Stephen B. *Journal of Applied Physics* 38.4 (1967): 1710-1715
5) Davier, B., et al. *Journal of Physics: Condensed Matter* 30.49 (2018): 495902

Results

➢ Full-band description of Bulk GaAs

6)



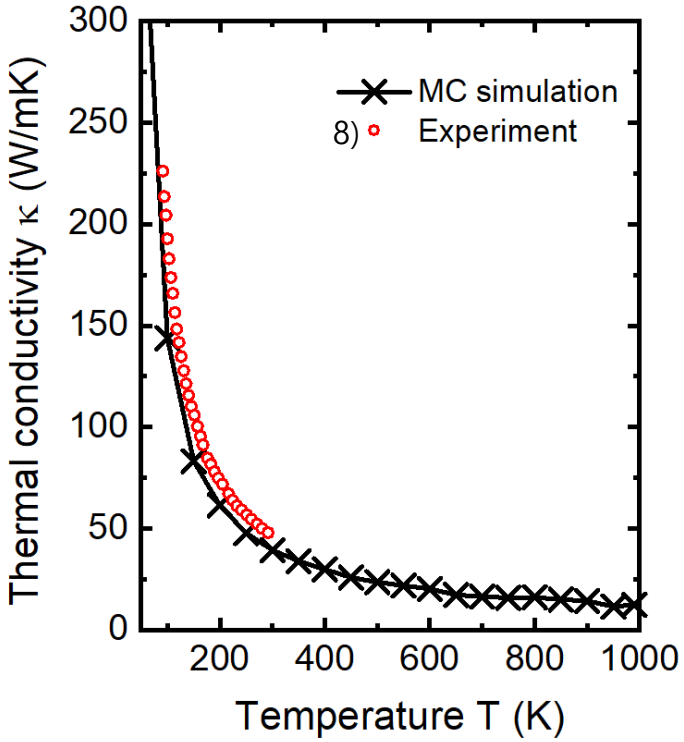


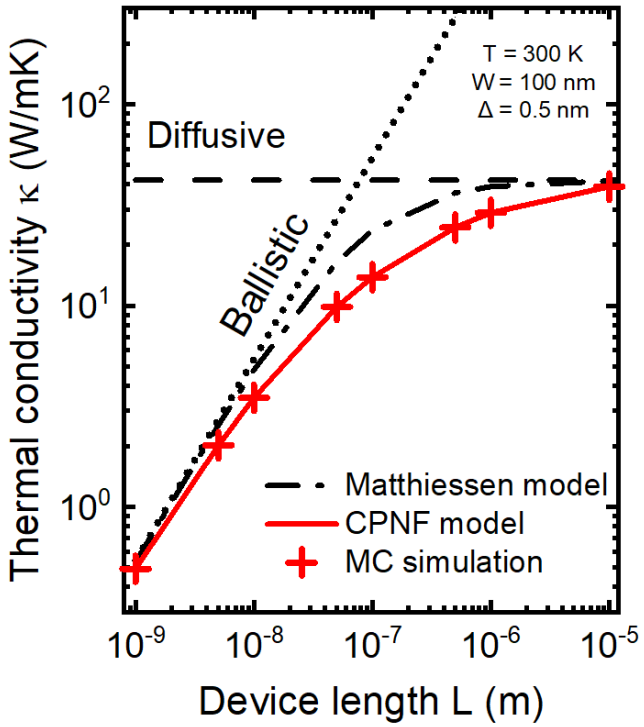
✓ Phonon dispersions and scattering rates was computed via ab initio methods

6) Giannozzi, Paolo, et al. *Journal of physics: Condensed matter* 29.46 (2017): 465901
7) Exp : Strauch, D., and B. Dorner. *Journal of Physics: Condensed Matter* 2.6 (1990): 1457.

Results

➢ Thermal conductivity of GaAs





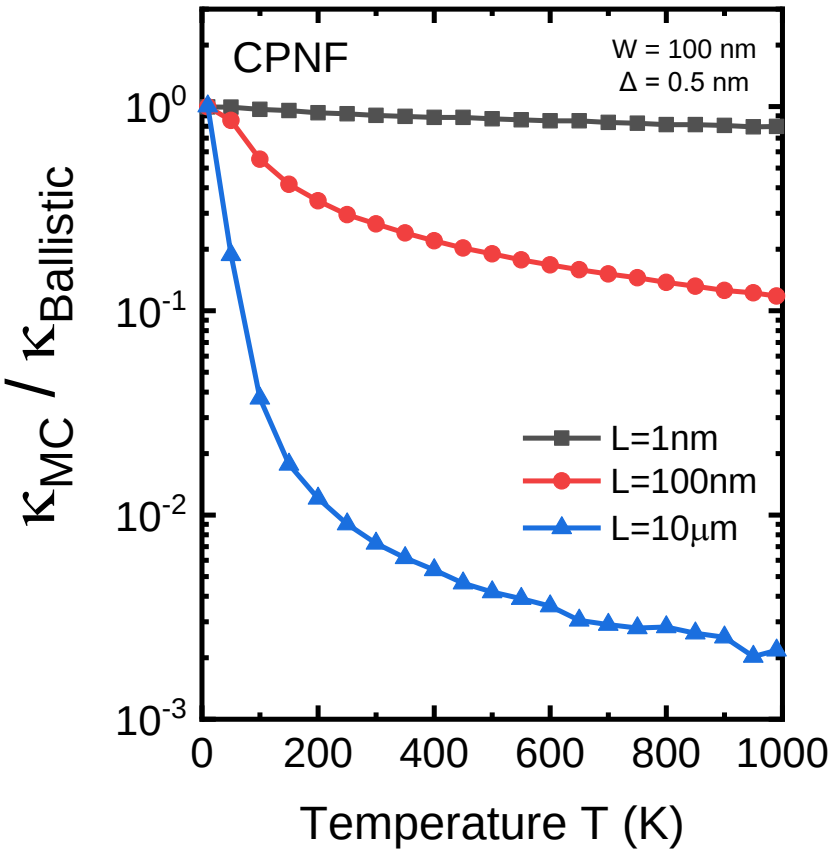
- ✓ MC results agree with the experiment data in the temperature range from 90 K to 300 K
- ✓ The Matthiessen model cannot properly capture the transition regime

8) Exp : Inyushkin, A. V., et al. Semiconductor science and technology 18.7 (2003): 685.

Results

➢ **The degree of ballistic transport**

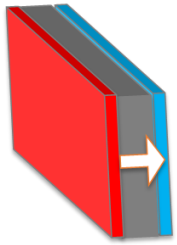
Knudsen number : $K_D = \frac{\kappa_{MC}}{\kappa_{Ballistic}}$



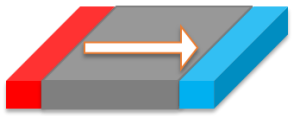
Results

➢ Thermal conductivity a function of length L and width W

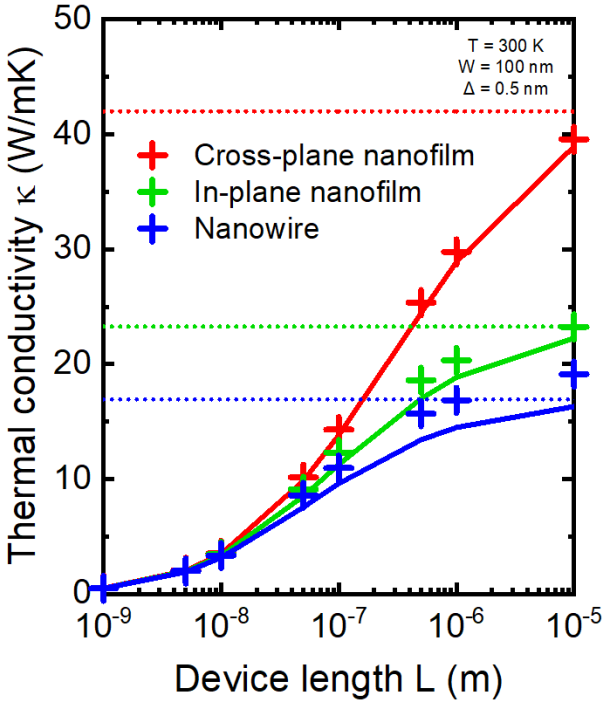
Cross plane

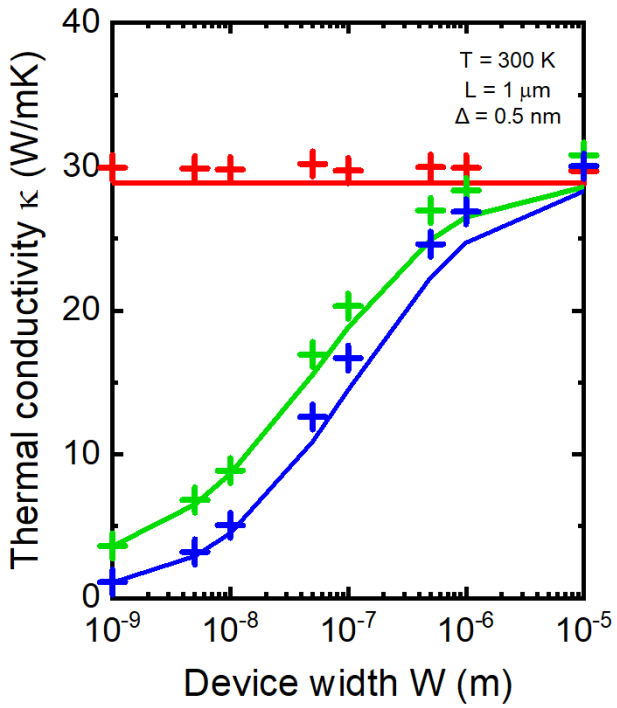


In plane



Nanowire

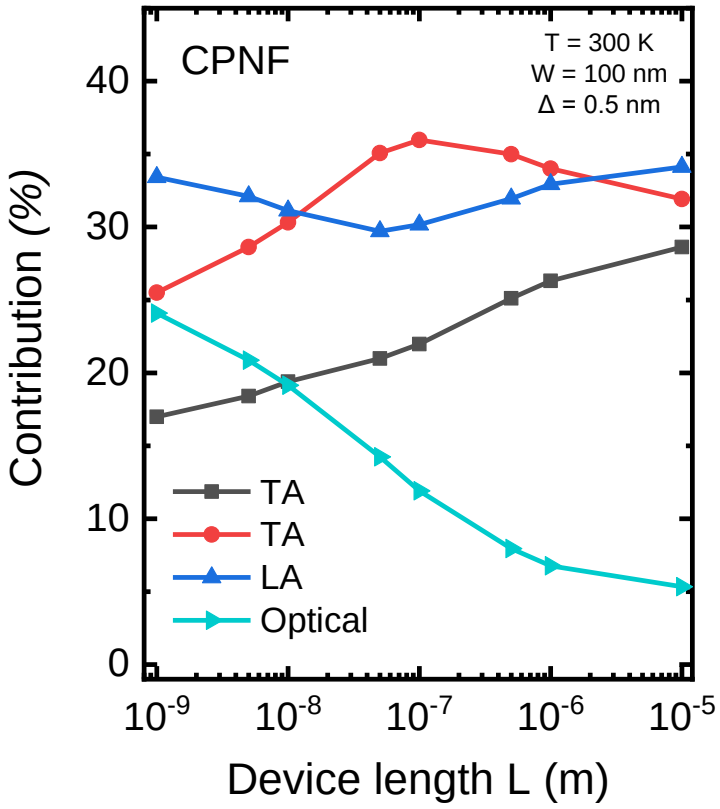




✓ The conductivity reduction is directly related to the number of rough boundaries when the heat transport is diffusive

Results

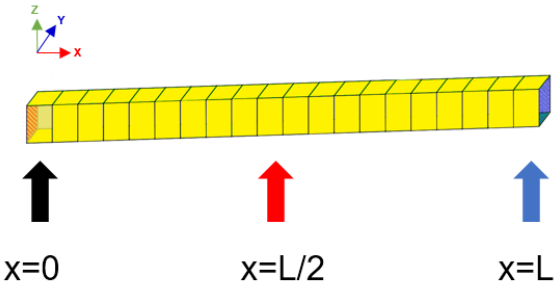
➢ **Contribution of each phonon mode as a function of length L**

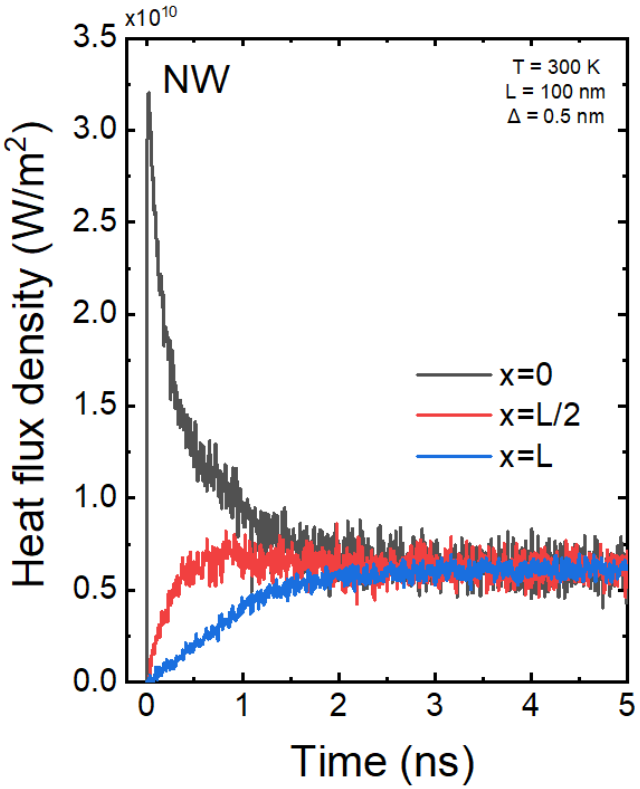


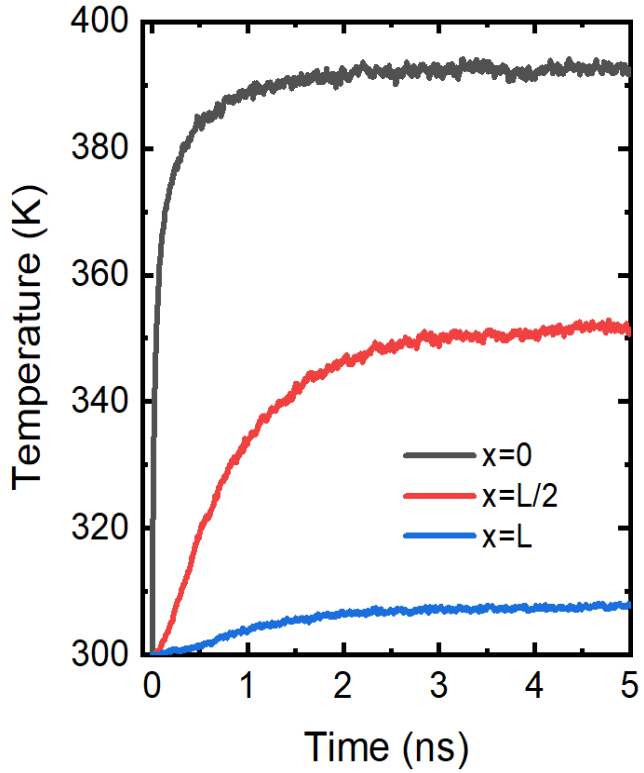
✓ Optical phonons can contribute over 20% to the thermal conductivity of nanostructures as compared to 5% in bulk.

Results

➢ Transient thermal response for NW



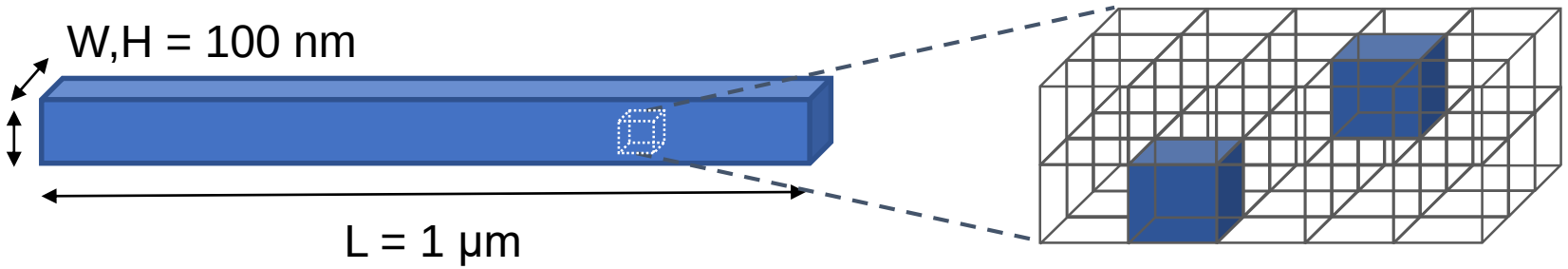




✓ The transient thermal response is investigated by analyzing the time evolution of heat flux density at different positions

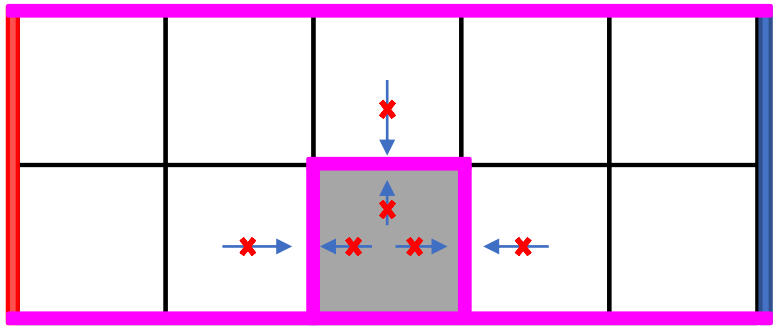
Results

➢ Porous nanowire (NW)



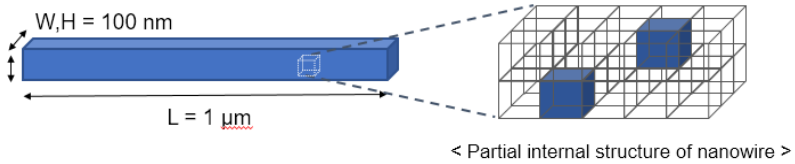
< Partial internal structure of nanowire >

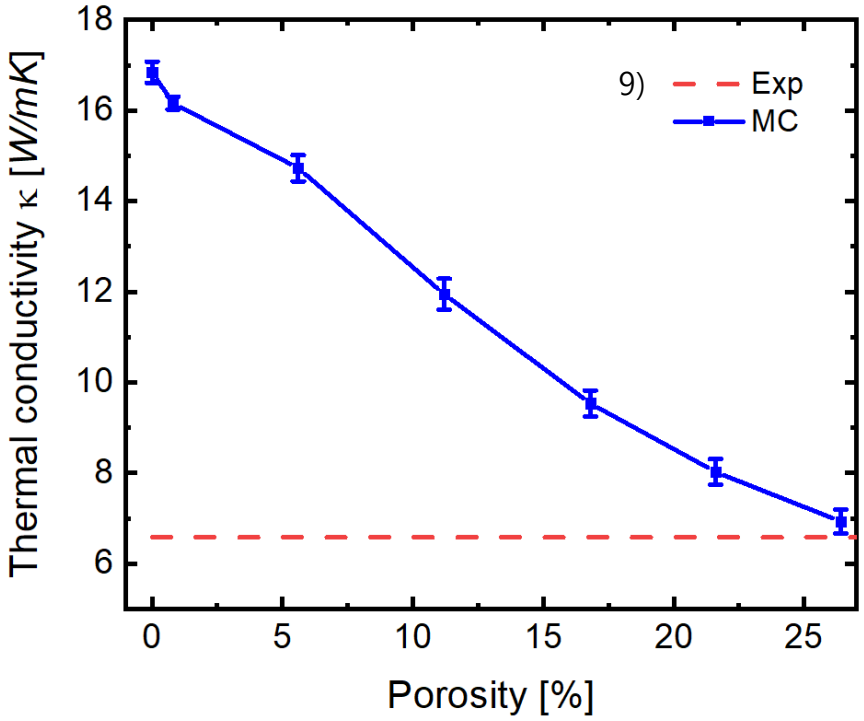
- To mimic the effect of nanopores, their boundaries are assumed to be diffusive boundaries



Results

➢ Thermal conductivity of porous NW





✓ Degradation effect of nanopores on the thermal conductivity according to the porosity of GaAs nanoiwres

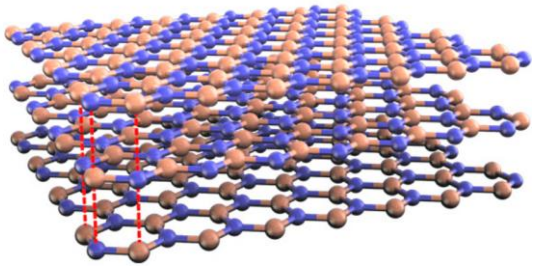
9) Exp : Ghukasyan, Ara, et al. *Nanomaterials* 12.8 (2022): 1288.

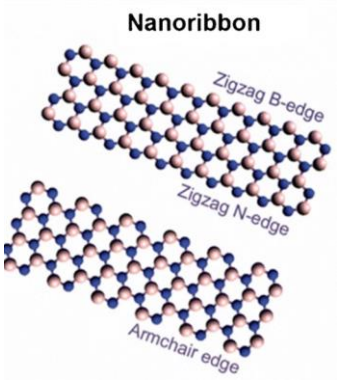
Conclusions

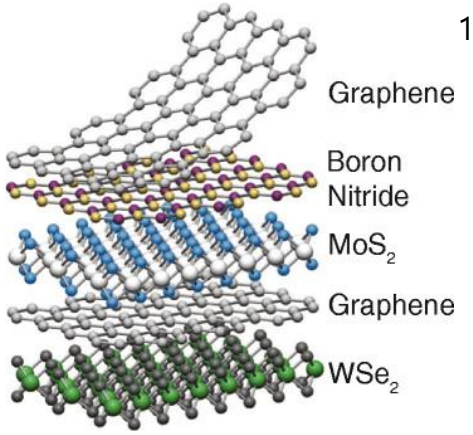
➢ Conclusions

- ✓ Theoretical investigations of nanostructures using the home-made Monte Carlo simulator using full-band DFT data for material (**Full band MC-DFT**)
- ✓ We investigate **the dependence of thermal conductivity** on several parameters and observe especially the transition between ballistic and diffusive transport regimes, and their optical contribution

➢ Prospective work







14)

14) Geim, Andre K., and Irina V. Grigorieva. *Nature* 499.7459 (2013): 419-425.

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Thank you for your attention