PhD defense:
Quantum Thermal Transport in Semiconductor Nanostructure with Diffusion

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Outline

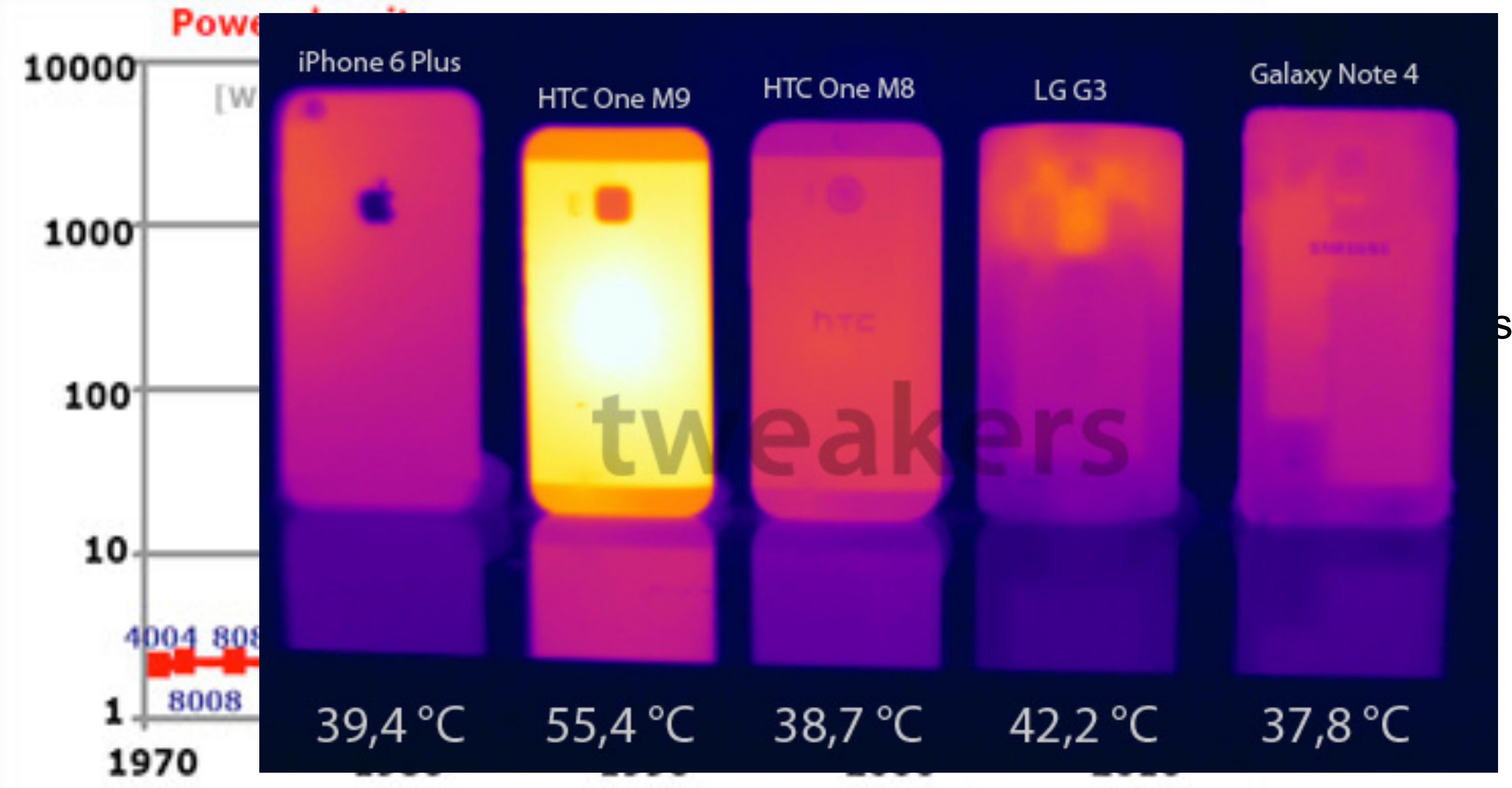
- Motivation
- Methodology
- Thermal Transport in Homogeneous Structure
- Thermal Transport in Heterostructure
- Transport with Electron-Phonon Coupling

Outline

Motivation for Thermal Transport

Increasing power density a great concern in downscaling trends

Question1: Why are we interested in the heat transfer?



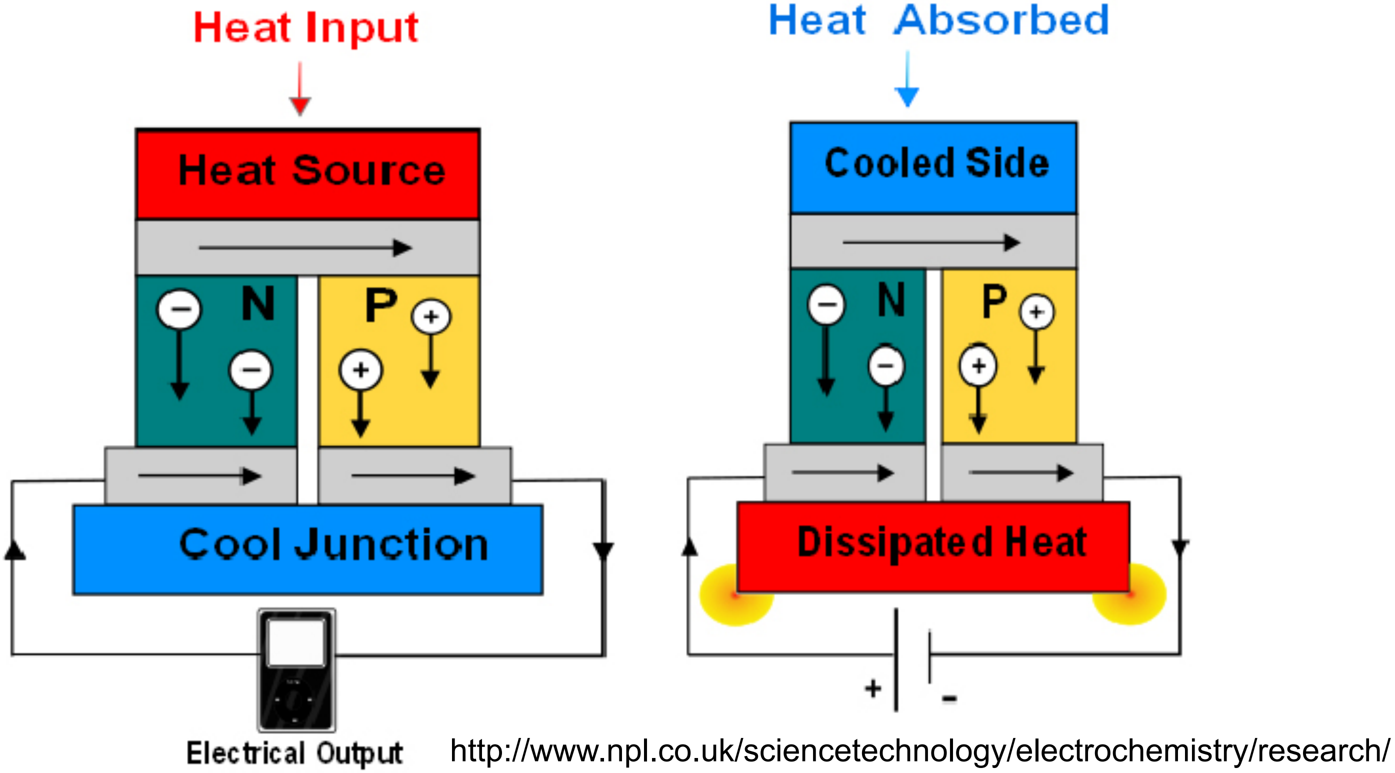
sity vs time
Intel

Nanometer-scale device -> huge heat generation -> High power density

Bad thermal treatment -> Heating up issue

Heat dissipation is critical.
Keyword: Temperature

Application of thermoelectric device

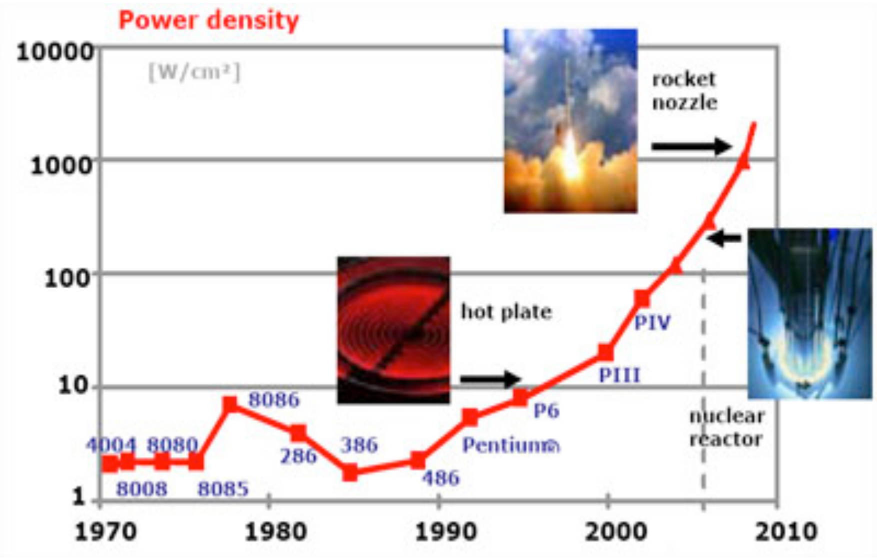


http://www.npl.co.uk/sciencetechnology/electrochemistry/research/nanostructured-thermoelectrics

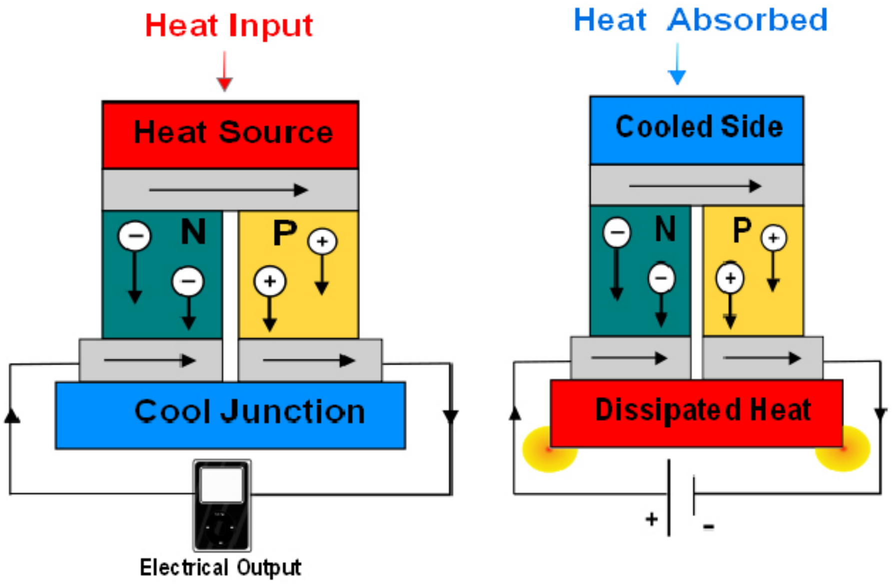
$$ZT = S^2\sigma T/\kappa$$

Low thermal conductivity is critical to enhance the performance of thermoelectric device.

High thermal conductivity is needed.

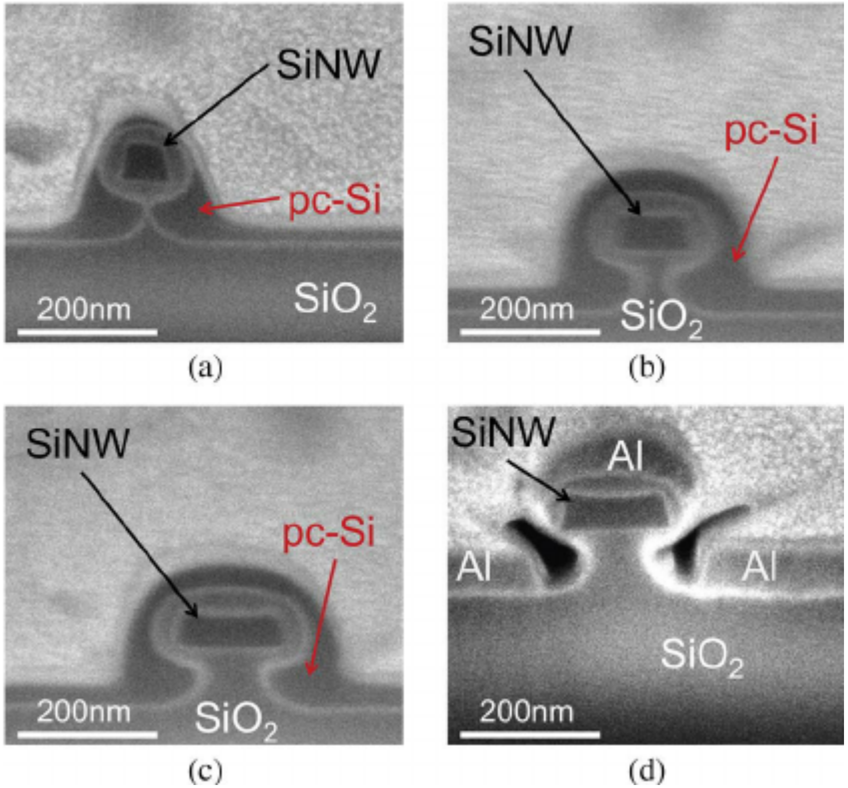


Low thermal conductivity is needed.



The thermal transport should be modeled accurately.

Challenges of device level simulations



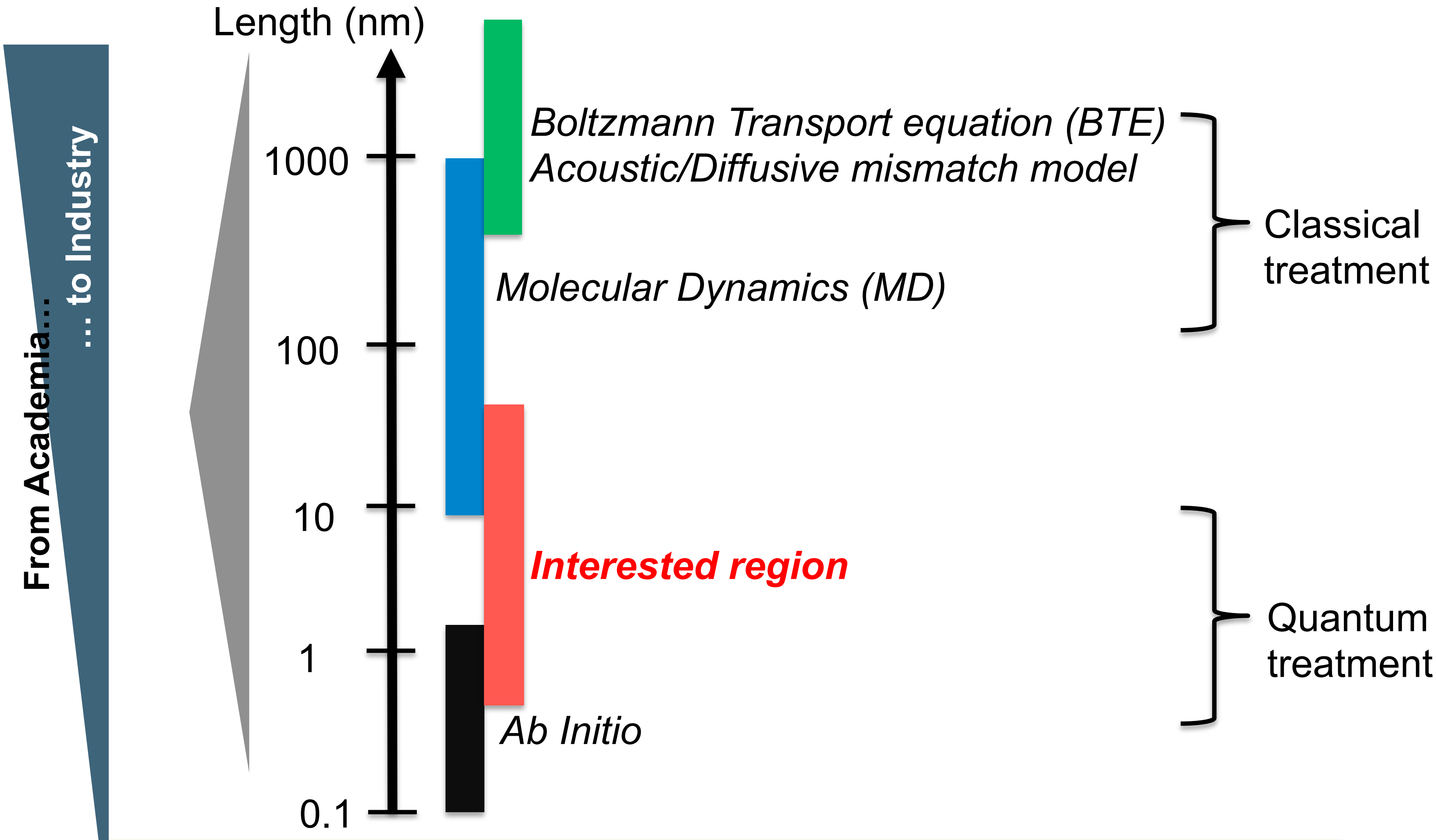
D. Sacchetto et. al. Proceedings of the IEEE, Volume: 100, Issue: 6, June 2012

Complicated systems

- ➢ Complicated geometries
- ➢ Multiple materials
- ➢ Strain/Relaxation
- ➢ Interfaces
- ➢ Boundary confinement
- ➢ Challenging simulation domain

Atomistic model to target complicated systems is necessary for realistic device modeling.

Thermal transport: from academia to industry

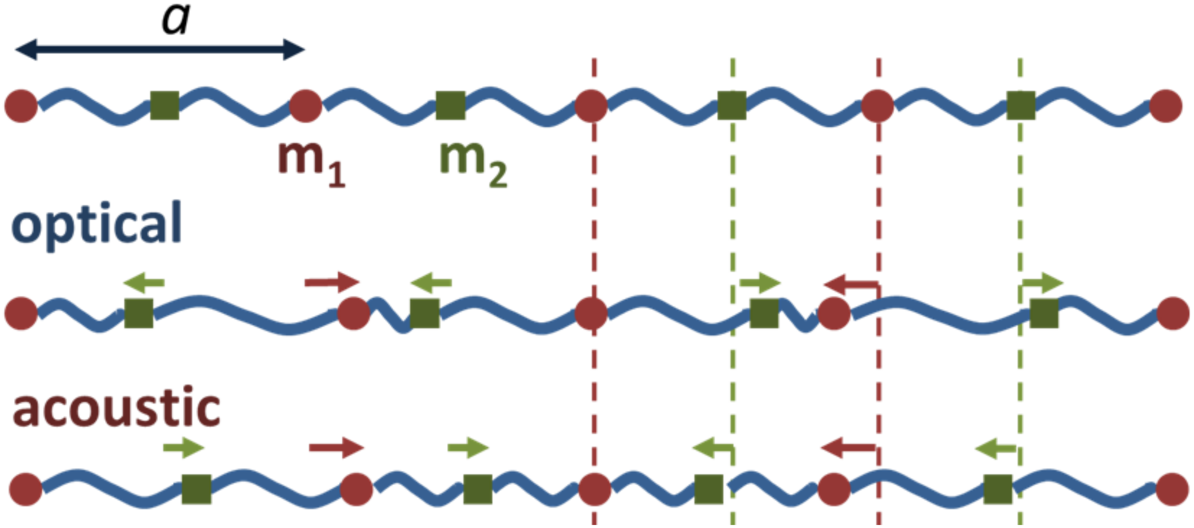


An atomistic model with quantum treatment is preferred to close the gap from academia to industry.

Quantum treatment for heat transport

Devices are now in sub-20nm regime→
Quantum treatment of heat flow: Phonon transport

one-dimensional quantum mechanical *harmonic chain*



By Brews Ohare (http://creativecommons.org/licenses/by-sa/3.0), via Wikimedia Commons

Phonon frequency ω and wave vector *k* → Phonon dispersion

Phonon transport includes two parts: Non-equilibrium Green's function and Bose-Einstein distribution.

Thermal transport calculations in real devices/materials

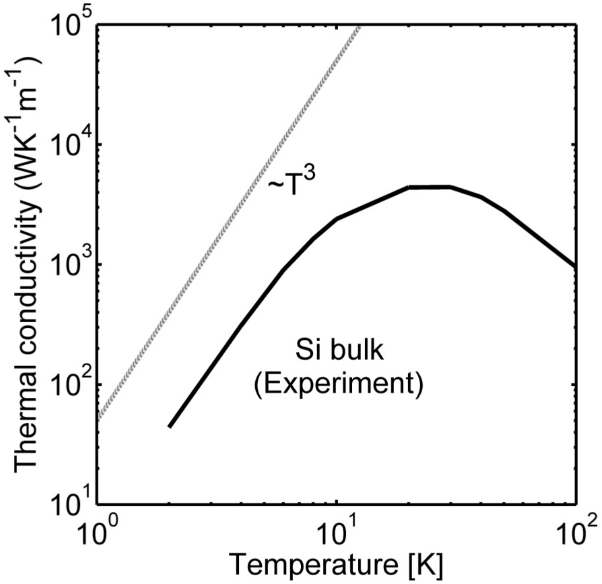
Question: Is it enough to have a correct phonon dispersion?

Thermal conductivity extraction:

$$\kappa = \frac{I_Q \cdot L}{\Delta T \cdot S}$$

This equation fails in the ballistic case!
→Phonon scattering model is needed

Experimental result

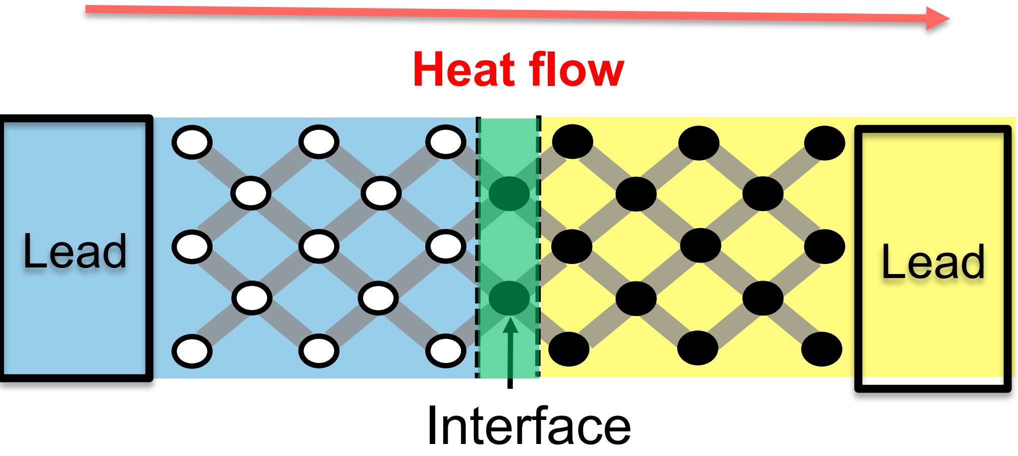


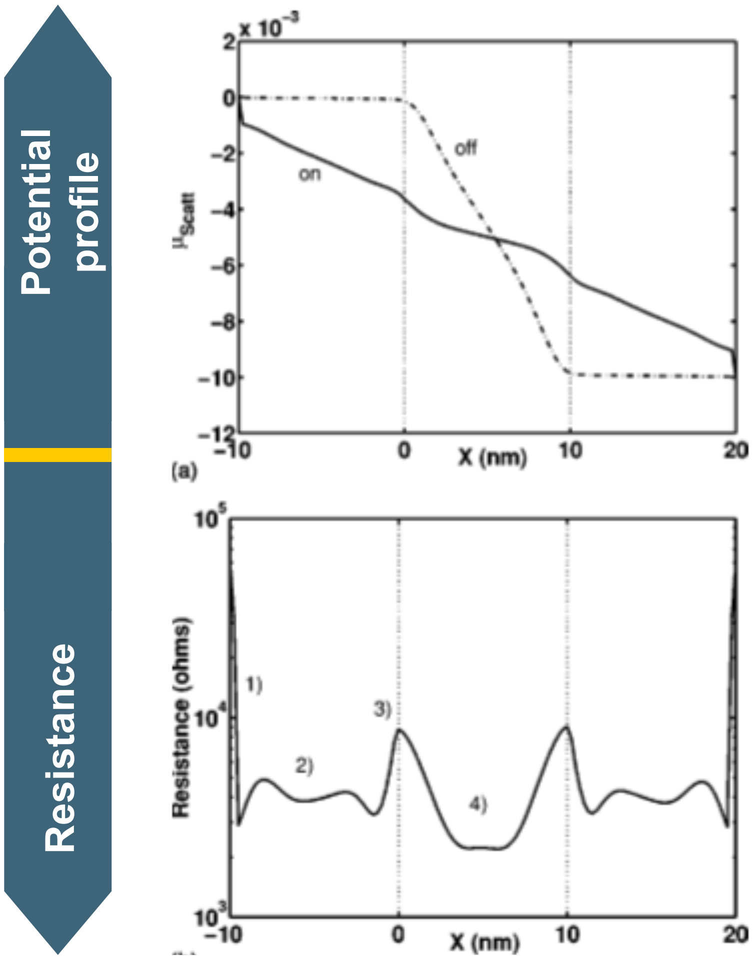
R.Berman, *Thermal conduction in Solids*, Clarendon, Oxford, 1974.

Need to capture the behaviors of thermal conductivity

Proper phonon scattering model should be chosen.
Keyword: scattering.

Temperature analysis should be included

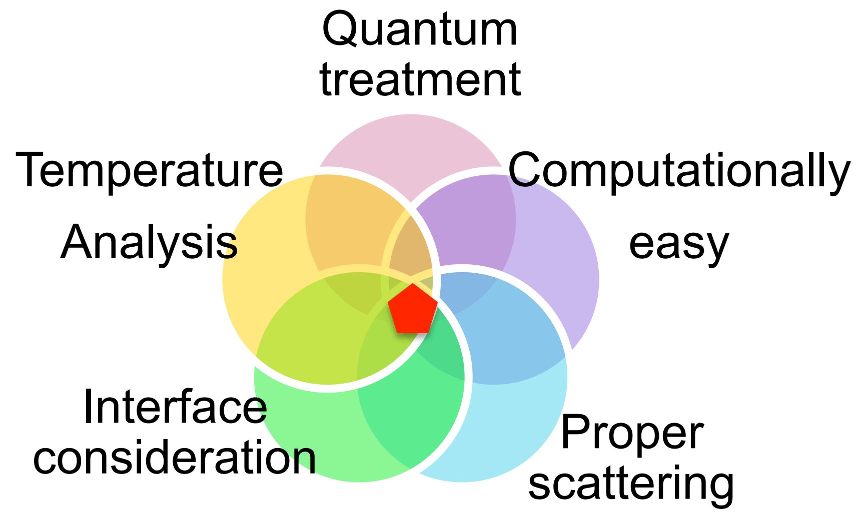




R. Venugopal et al. J. Appl. Phys., Vol. 93, No. 9, 2003

What does the temperature picture look like in thermal transport?

Summary: Key ingredients for a good heat transport model
Quantum, interface, scattering, temperature, and efficient



Question:
Can we find a method that can balance all these 5 aspects?

Introduction of Quantum Thermal Transport

Overview of heat transport models: Pros and Cons

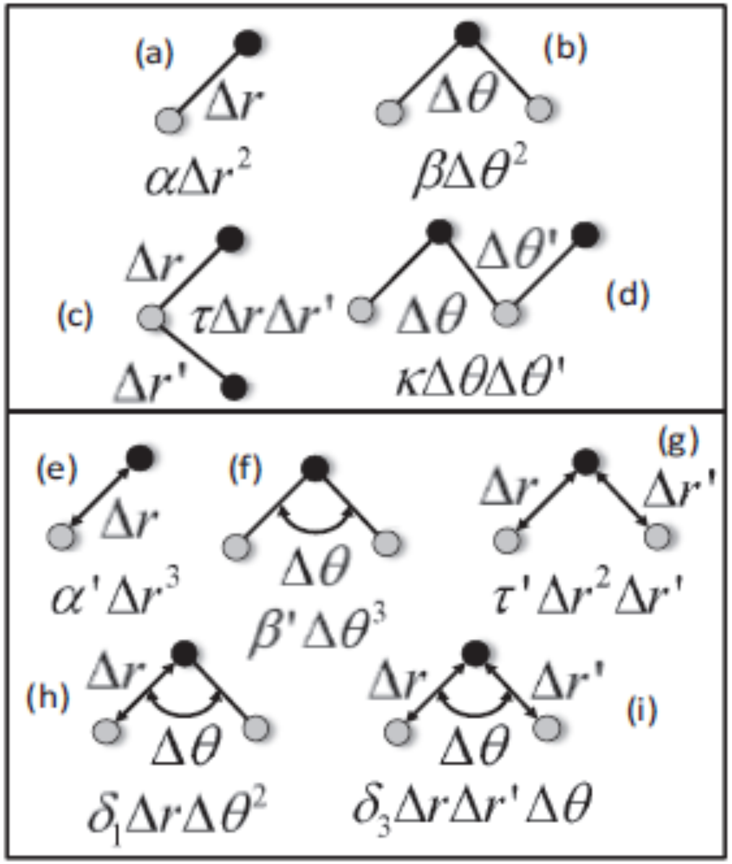
	Quantum	Interface	Scattering	Temperature	Efficient
DMM	✗	✓	✗	✗	✓
BTE	✗	✓	✓	✓	✓
MD	✗	✓	✓	✓	✗
GF(Anharmonic)	✓	✓	✓	✗	✗
Landauer	✓	✗	✓	✗	✓

DMM: Diffusive mismatch model; **BTE**: Boltzmann transport equation;
MD: Molecular dynamics; **Laudauer** approach: Landauer approach with full dispersion
GF(Anharmonic): Green's function with anharmonic phonon-phonon scattering

Quantum transport models are our main interest.

VFF + NEGF with anharmonic phonon-phonon scattering

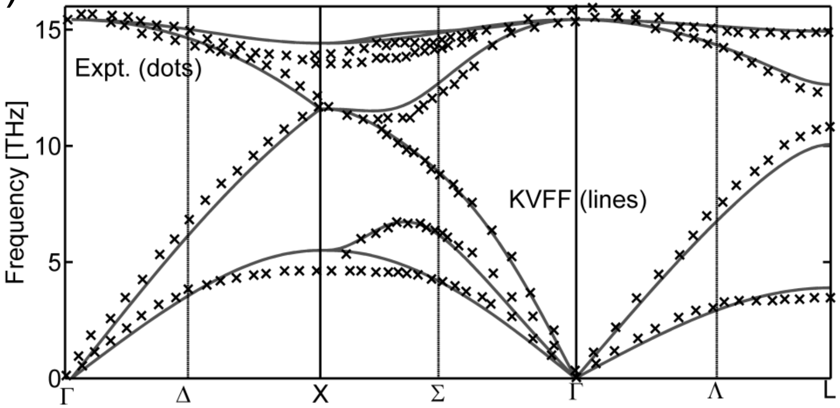
Valence force field model



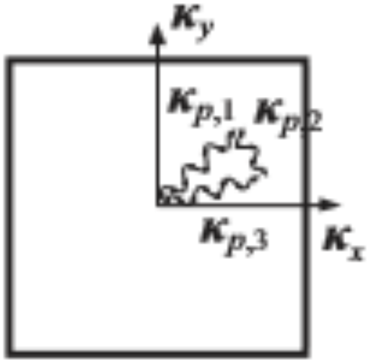
M. Luisier, Phys. Rev. B 86, 245407 (2012).

(Harmonic)

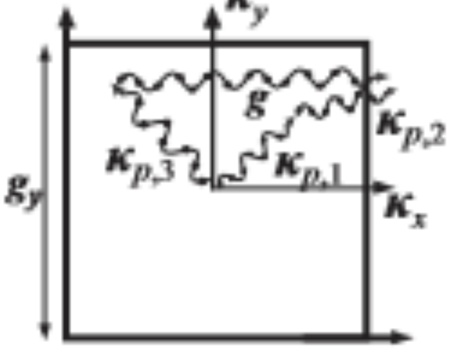
Physical properties



(Anharmonic)



N process

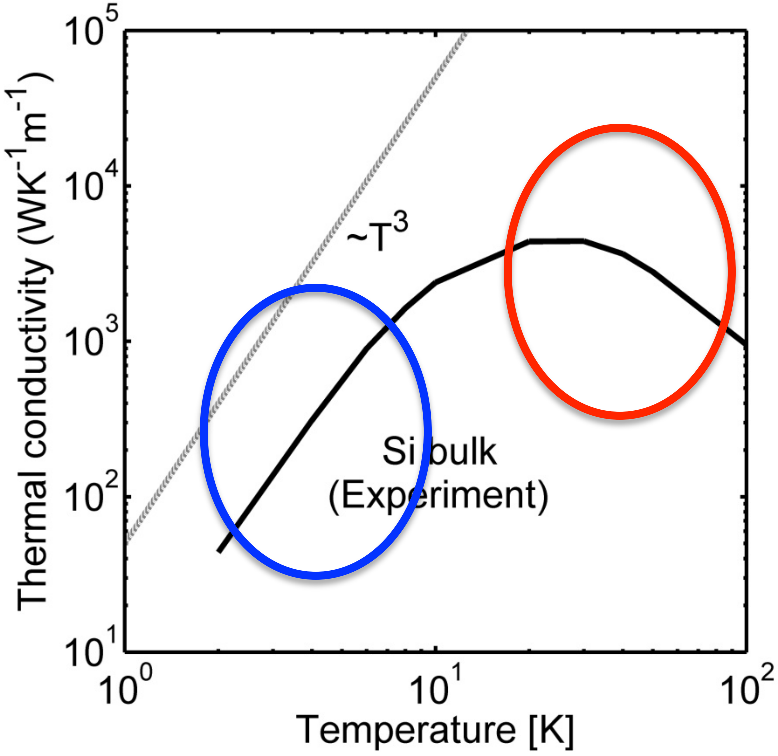


U process

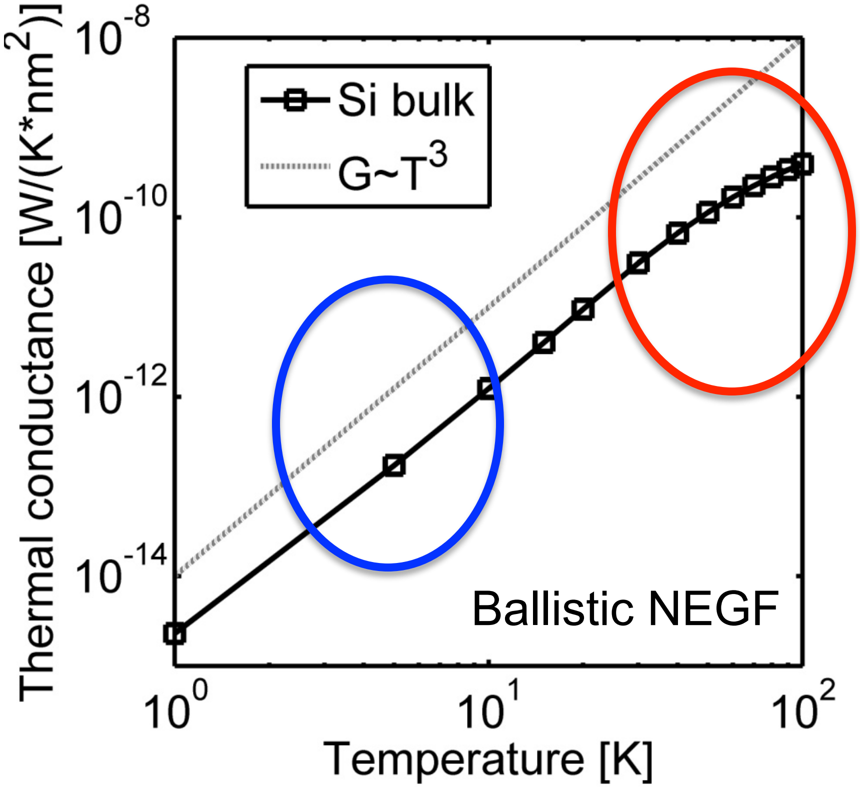
Anharmonic phonon-phonon scattering is described.
But there is one problem.

Ballistic thermal transport calculation deviating from the experimental result

Conventional phonon scattering theory predicts a ***T^3*** dependence for thermal conductance in low temperature



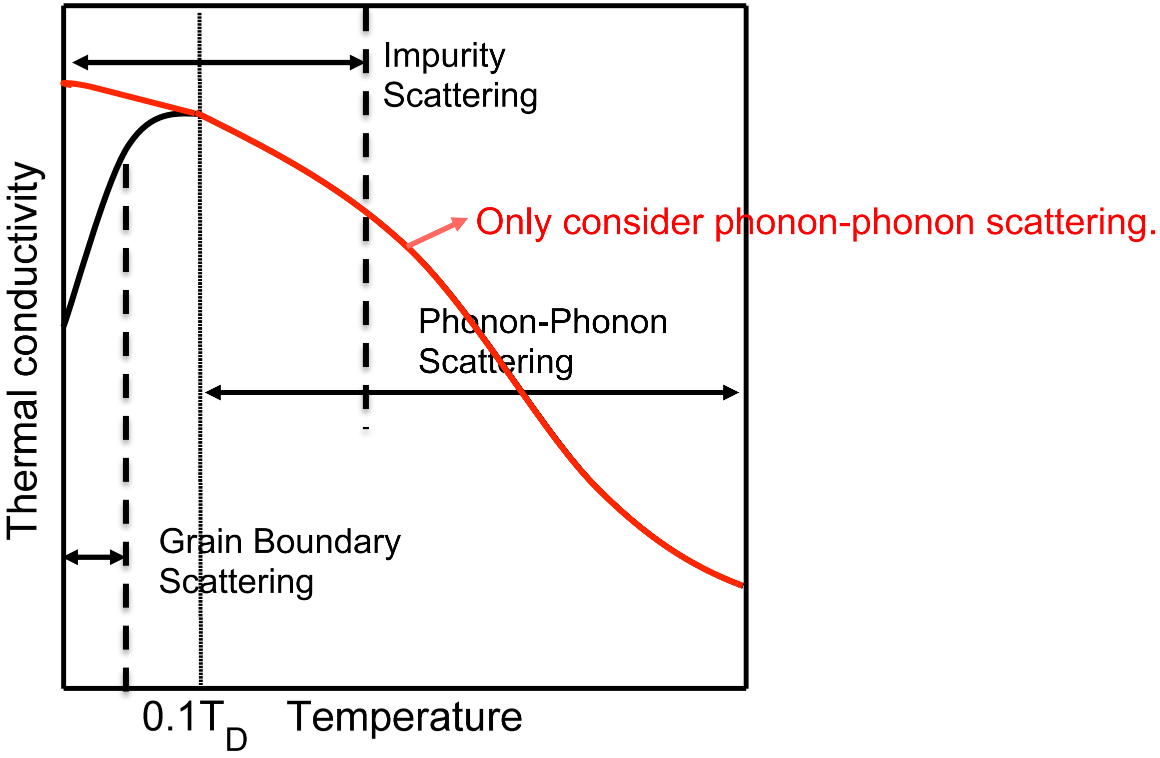
R.Berman, *Thermal conduction in Solids*, Clarendon, Oxford, 1974.



- ➢ Our calculation is consistent with the experimental result in the low temperature.
- ➢ The contradiction in the higher temperature needs scattering models.

Multiple phonon scattering mechanisms should be considered for correct physical meanings

Dominant scatterings profile



C.J. Glassbrenner, et. al[Phys. Rev.134,1508 (1964)
M.G. Holland, et. al, Proc. Int. Conf. Physics of Semiconductors, Exeter, England, 474 (1962)

Multiple phonon scattering mechanisms should be included.
Question: How to choose different phonon scattering?

Phonon scattering models: Relaxation time approximation model

$$I_Q = \frac{1}{h}\int_{-\infty}^{+\infty} dE\left(\Xi_{ph} M_{ph}\right) E\left(f_{BE}^{1} - f_{BE}^{2}\right)$$

$$\Xi_{ph} = \lambda_{ph}(E) / \left(L + \boxed{\lambda_{ph}(E)}\right)$$

Phonon mean free path $\lambda_{ph}(E)$ is given by

$$\lambda_{ph}(E) = \langle v_s \rangle \cdot \tau_p$$

C. Jeong, S. Datta, and M. Lundstrom, J. Appl. Phys. 111, 093708 (2012).

Phonon scattering mechanisms in BTE model:

1. Phonon grain boundary scattering: $\tau_b^{-1} = v_s / LF$
2. Phonon impurity scattering: (mass difference) $\tau_{IM}^{-1} = B\omega^4$
3. Phonon-phonon scattering: (Umklapp process) $\tau_{p-p}^{-1} = C\omega^2 T^{\alpha}$

Matthiessen rule: $\tau_p^{-1} = \tau_b^{-1} + \tau_{IM}^{-1} + \tau_{p-p}^{-1}$

M. G. Holland, Phys. Rev. 132, 2461 (1963).

Different RTA models can describe the scatterings in the phonon transport.

Connect RTA models, GF, with phonon Büttiker probe

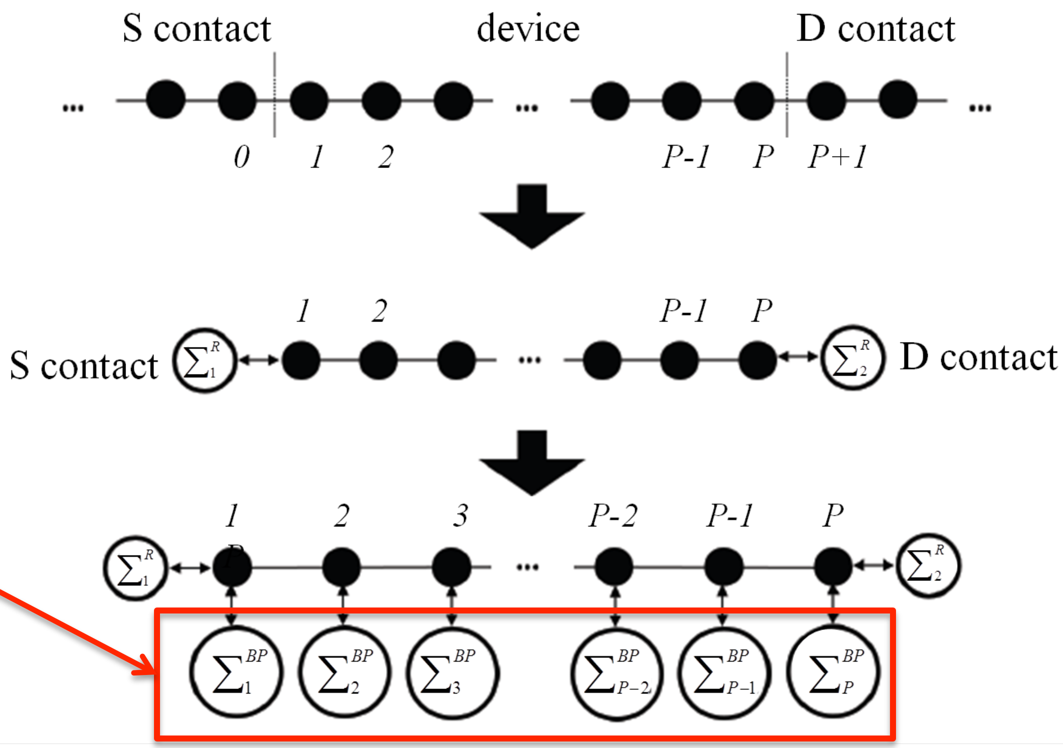
Retarded Green's function is:

$$G^r(E) = \frac{1}{E^2 - D - \Sigma^{BP}(E) - \Sigma^R_{contact}(E)}$$

Scattering self energy

$$\Sigma^{BP}(E) = -\frac{2i \cdot E}{\tau_p}$$

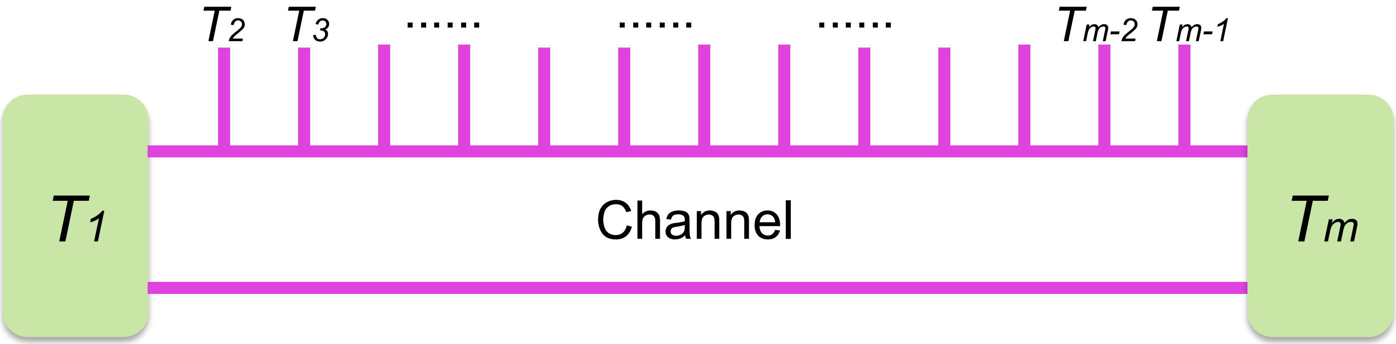
$$Here, \tau_p^{-1} = \tau_b^{-1} + \tau_{IM}^{-1} + \tau_{p-p}^{-1}$$

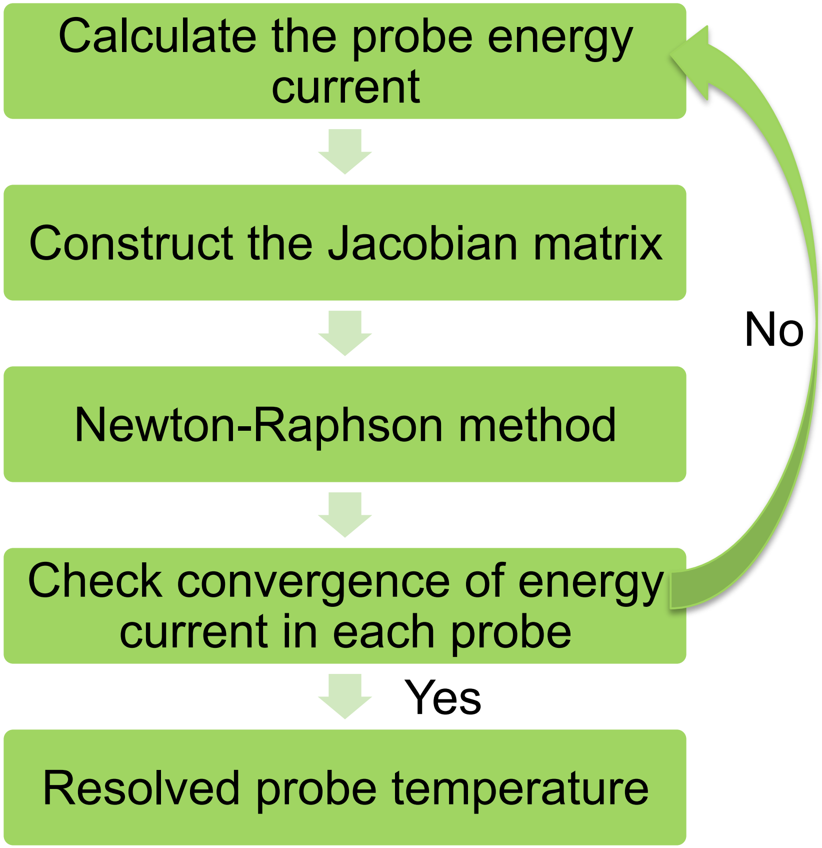


Virtual contact (Büttiker probe)

RTA models are connected with Green's function through the Virtual contact concept: Büttiker probe (BP).

Methodology of phonon Büttiker probe: Energy relaxed model





Calculate the probe energy current

Construct the Jacobian matrix

Newton-Raphson method

Check convergence of energy current in each probe

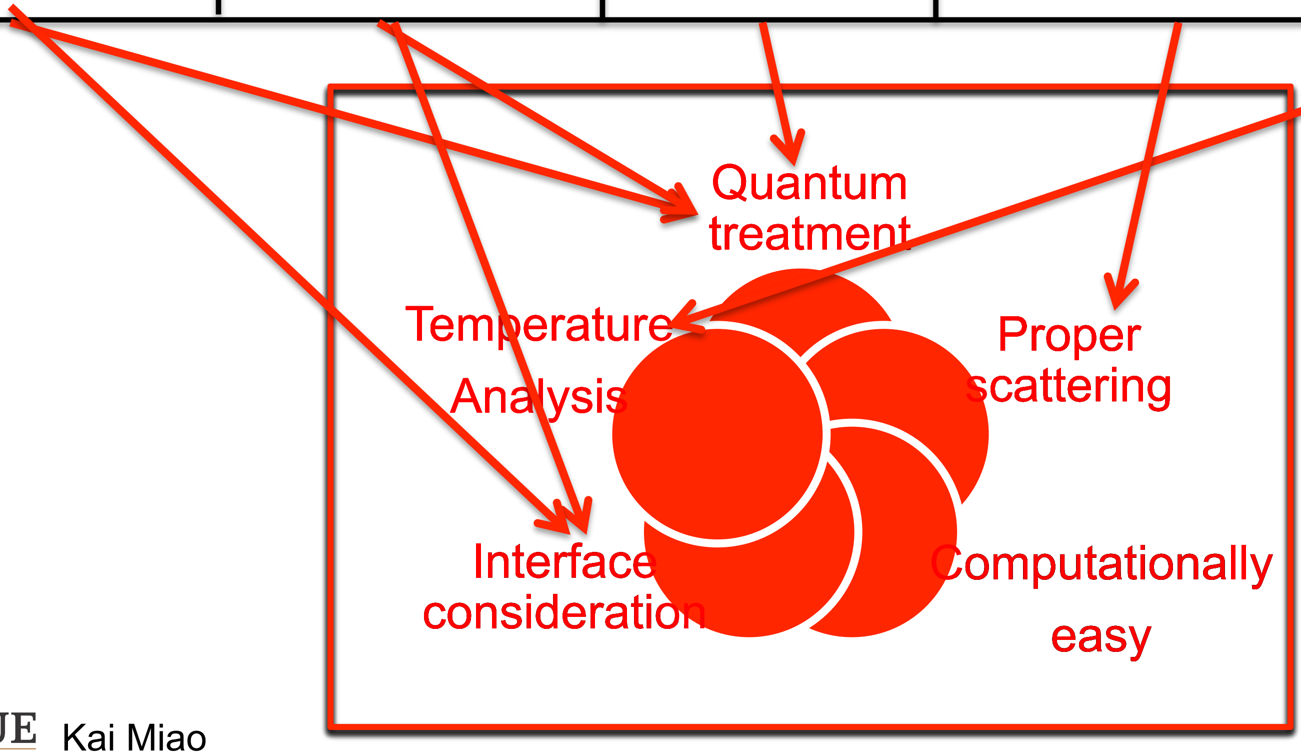
No

Yes

Resolved probe temperature

Successfully covering all 5 key ingredients

DFT/VFF	VFF	NEGF	RTA	BP
Geometry relaxation	1. Reproduce the phonon dispersion 2. Prepare the dynamical matrix	Ballistic phonon transport	1.Phonon grain boundary scattering 2.Phonon impurity scattering 3.Phonon-Phonon scattering	Diffusive phonon transport



Quantum treatment

Temperature Analysis

Proper scattering

Interface consideration

Computationally easy

Outline

Thermal Transport Study in Homogeneous Structure

Successful benchmark of thermal conductivity for Si and Ge

Phonon scattering mechanism in BTE transport:

1. Phonon grain boundary scattering

   τ_b^{-1} is from ref. 1.

2. Phonon impurity scattering (mass difference)

$$\tau_{IM}^{-1} = B\omega^4$$

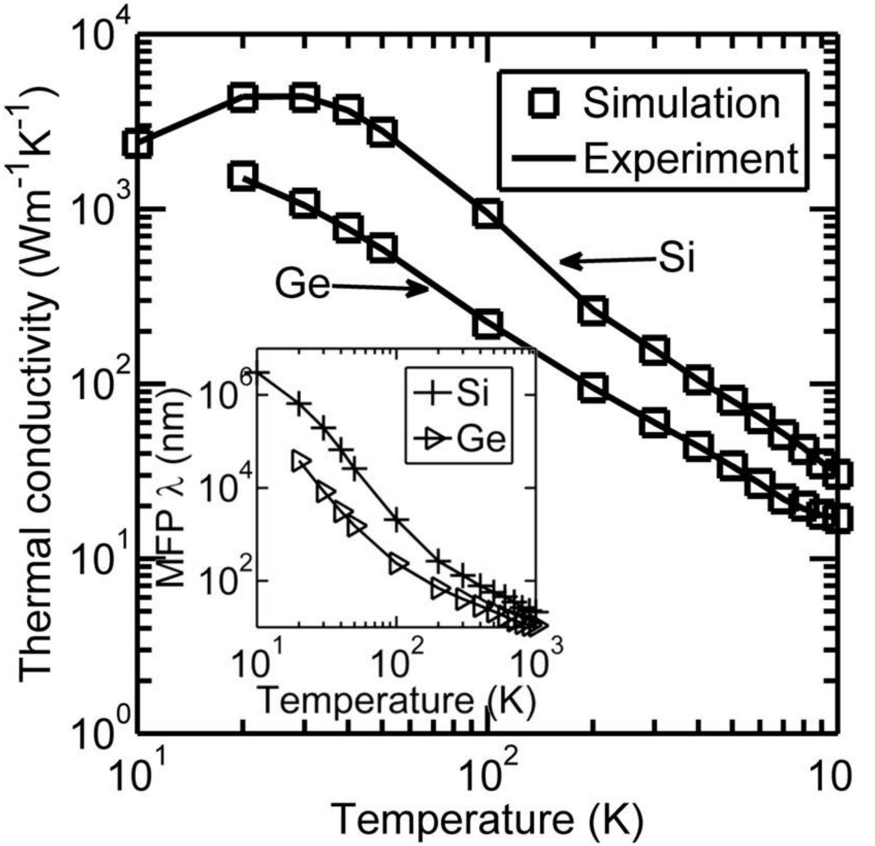
3. Phonon-phonon scattering (Umklapp process)

$$\tau_{p-p}^{-1} = C\omega^2 T^{\alpha}$$

Matthiessen rule:

$$\tau_p^{-1} = \tau_b^{-1} + \tau_{IM}^{-1} + \tau_{p-p}^{-1}$$

Material	$B(s^3)$	$C(sK^{-\alpha})$	α
Si	0.71×10^{-45}	1.74×10^{-21}	1.64
Ge	3.2×10^{-45}	1.12×10^{-20}	1.48



1. M. G. Holland, Phys. Rev. 132, 2461 (1963).
2. C. J. Glassbrenner, G. A. Slack, Phys. Rev. 134, 1058 (1964).

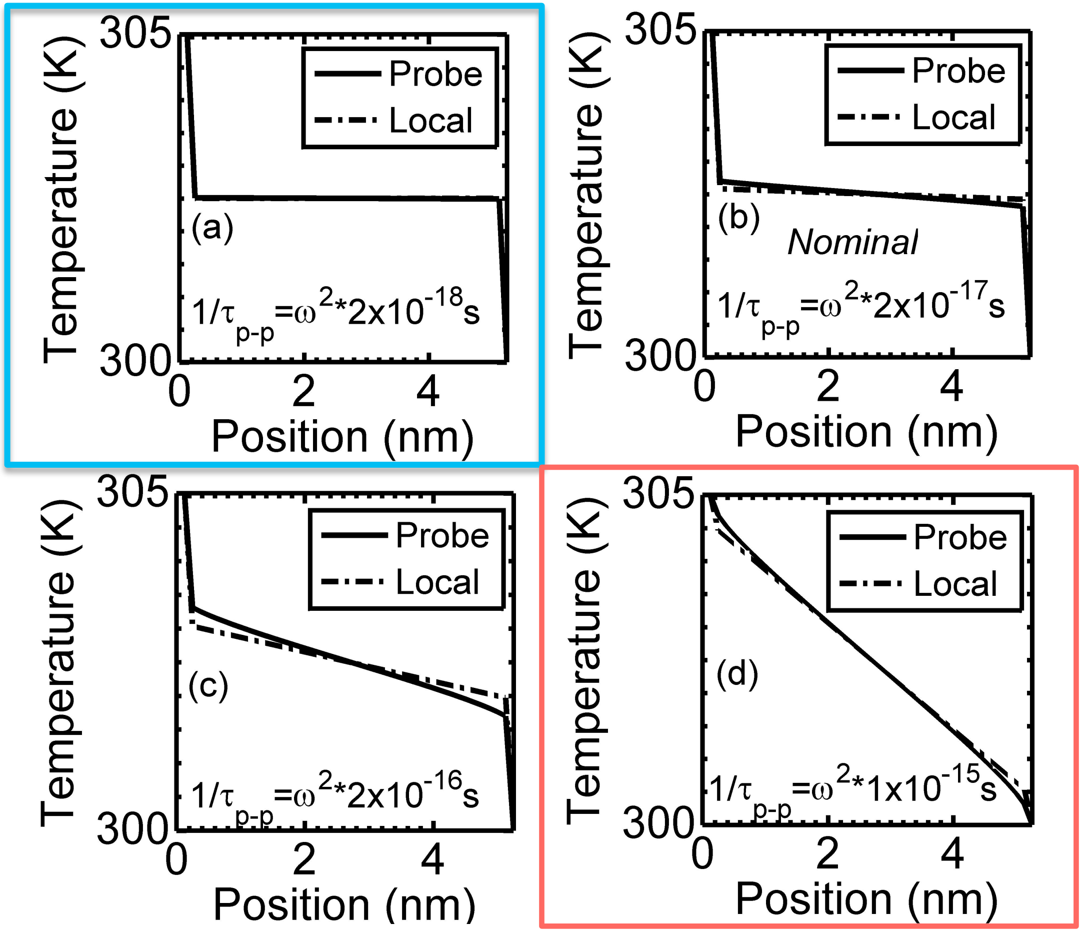
Thermal properties are matched well with experimental results.

Extraction of local temperature

Average phonon gas energy

E↑2 G↑< (E)dE ≈∫↑▒E↑2 A/e↑E/k↓B T↓local −1 dE.

Ballistic limit



Diffusive limit

Phonon scattering models: Relaxation time approximation(RTA) model

Phonon scattering mechanisms in BTE model:

1. Bulk

1. Phonon boundary scattering: $\tau_b^{-1} = v_s / LF$
2. Phonon impurity scattering: (mass difference) $\tau_{IM}^{-1} = B\omega^4$
3. Phonon-phonon scattering: (Umklapp process) $\tau_{p-p}^{-1} = C\omega^2 T^{\alpha}$

Matthiessen rule: $\tau_p^{-1} = \tau_b^{-1} + \tau_{IM}^{-1} + \tau_{p-p}^{-1}$

K. Miao, Appl. Phys. Lett. **108**, 113107 (2016);

2. UTB

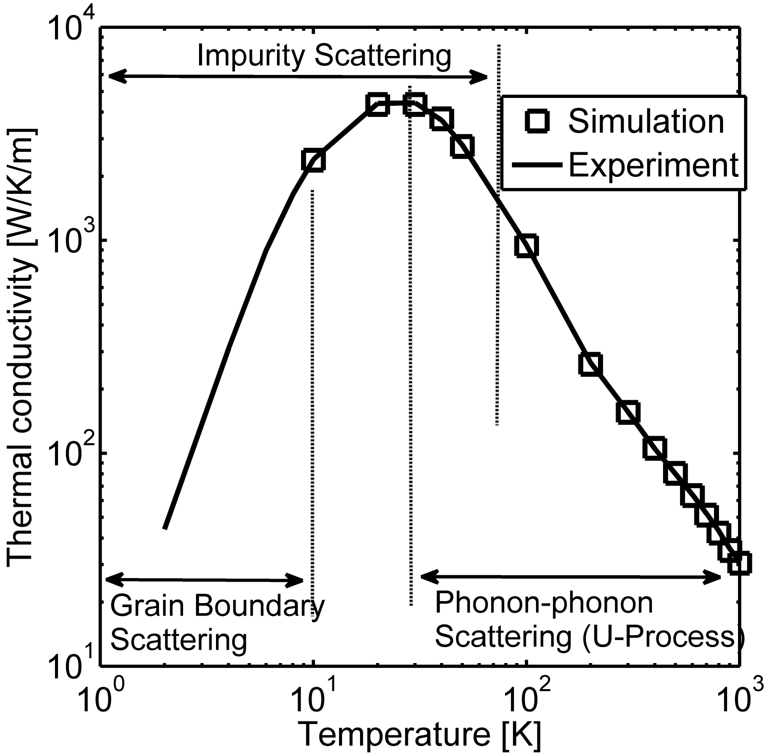
Phonon boundary scattering: $\tau_b^{-1} = v_s / d$

R. Cheaito et al,PRL 109, 195901 (2012)

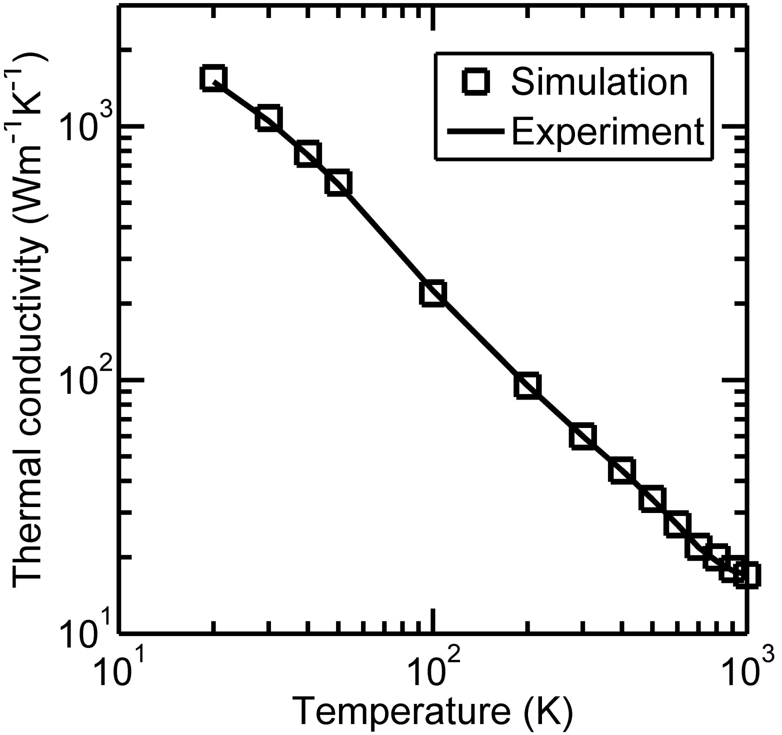
Different RTA models can describe the scatterings in the phonon transport.

Thermal conductivity for bulk Ge

Scattering dominant profile



Thermal conductivity for Ge

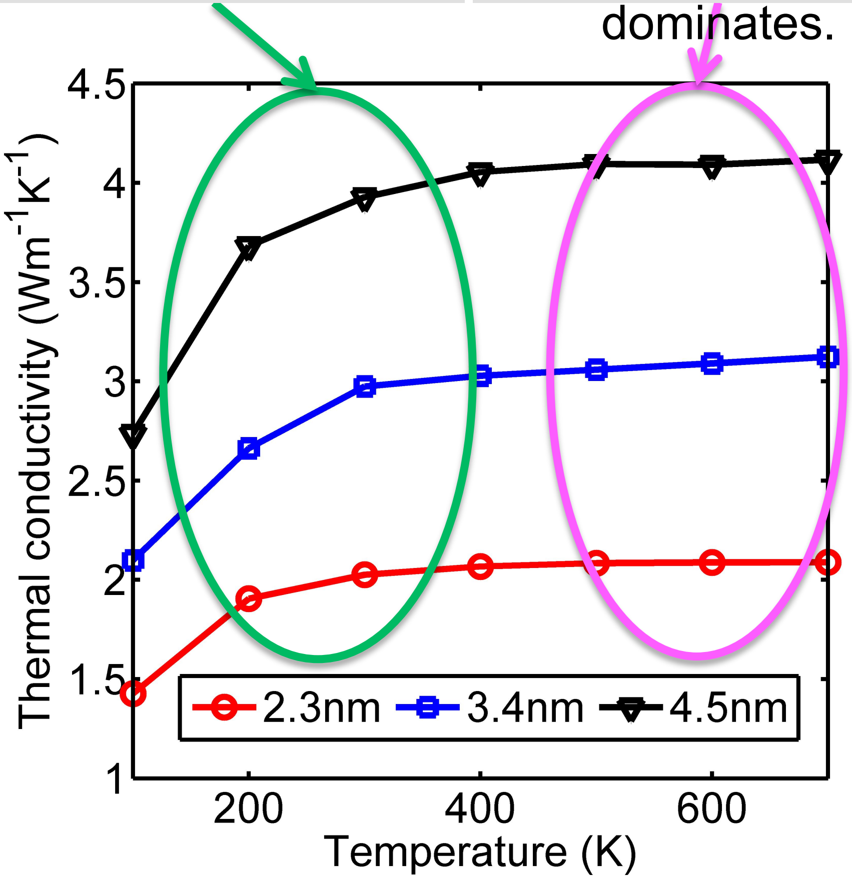


For Ge bulk structure, phonon-phonon scattering is the dominant scattering mechanism when K>20K.

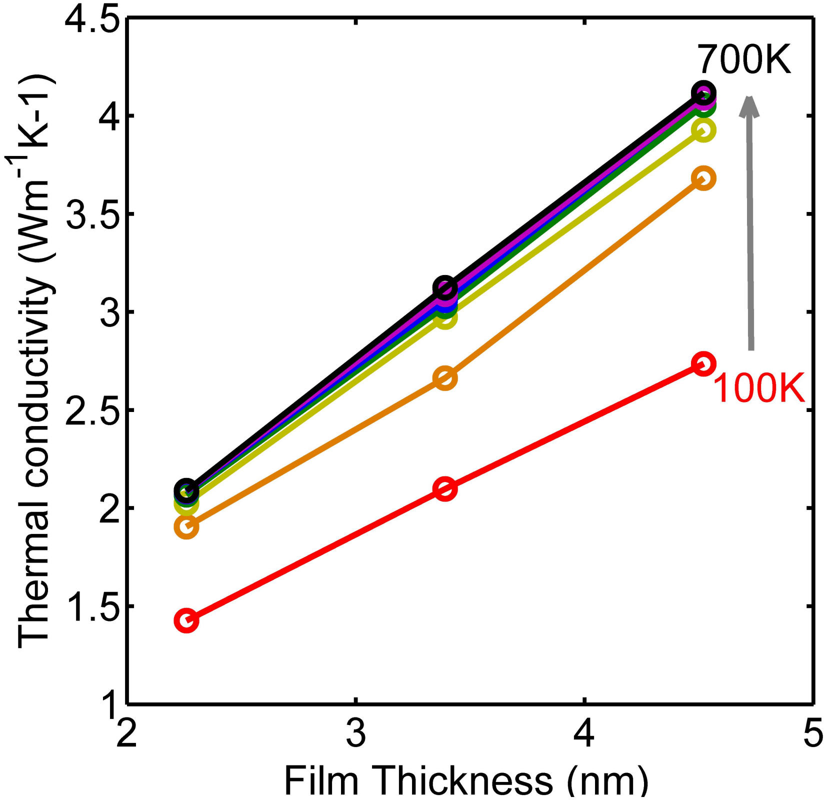
Thermal conductivity for Ge UTB

Boundary scattering dominates.

Boundary and p-p scattering dominates.



κ is linearly dependent on the film thickness.



Boundary scattering mechanism dominates in thin UTB structure.

Kai Miao

Conclusions

1. First apply the NEGF+Buettiker probe model to solve the phonon transport.

2. Thermal conductivity and mean free path are calculated and benchmarked with experimental data.

3. Show the method to extract the local temperature in the device. Understand the relation between scattering and temperature drop.

4. Show the scattering-dominating picture in the whole temperature range.

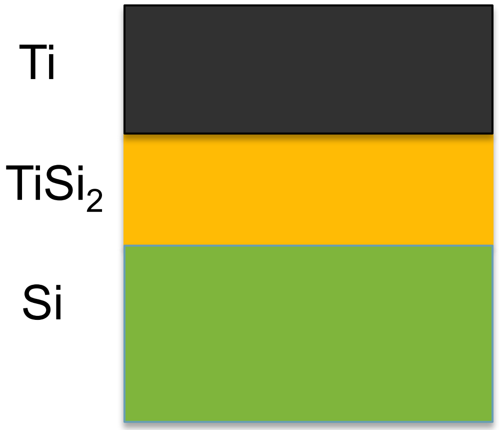
5. Compare the difference of thermal transport between bulk and UTB.

Thermal Transport Study in Heterostructure

Introduction of silicide materials

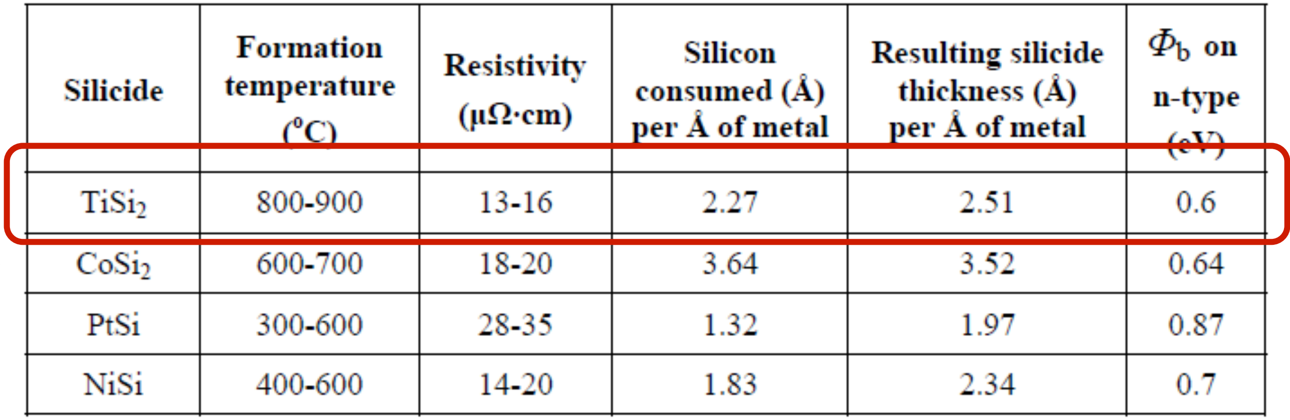
Ideal contact

Realistic contact



*Nano Lett., Vol. 7, No. 4, **2007***

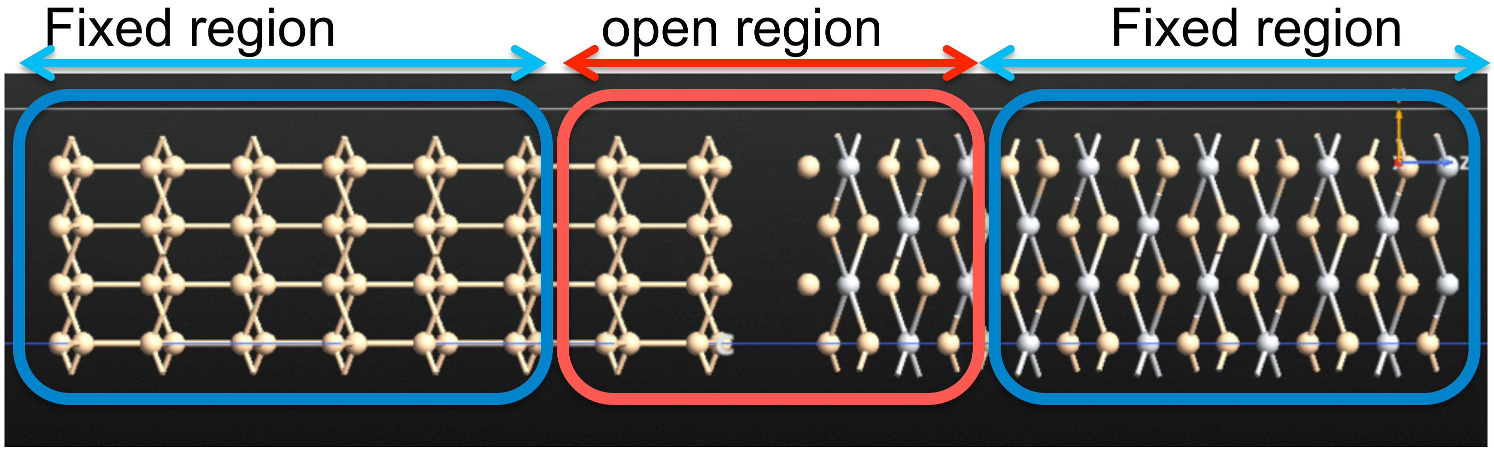
Preferred silicides for applications are PtSi2,TiSi2, NiSi and CoSi2 due to their overall excellent properties.



Silicide	Formation temperature (°C)	Resistivity (μΩ·cm)	Silicon consumed (Å) per Å of metal	Resulting silicide thickness (Å) per Å of metal	Φ_b on n-type (eV)
$TiSi_2$	800-900	13-16	2.27	2.51	0.6
$CoSi_2$	600-700	18-20	3.64	3.52	0.64
PtSi	300-600	28-35	1.32	1.97	0.87
NiSi	400-600	14-20	1.83	2.34	0.7

S. P. Murarka, *Silicides for VLSI Applications*, London: Academic press, 1983.

Relaxation process and read-in method



DFT (GGA basis) method is used to relax this heterostructure

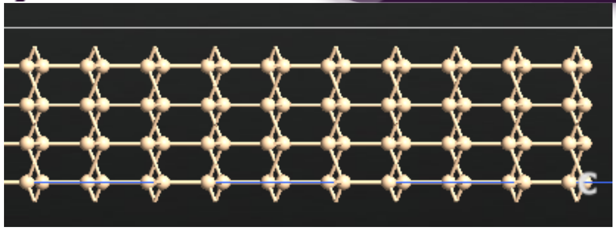
1
- New lattice structure is read into NEMO5.

2
- Strain solver constructs the dynamical matrix.

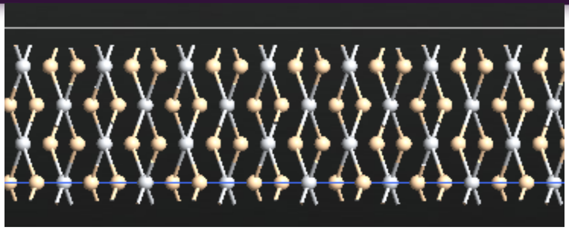
3
- RGF and NEGF are both available to do the transport calculation.

Thermal conductance in Quasi1D system

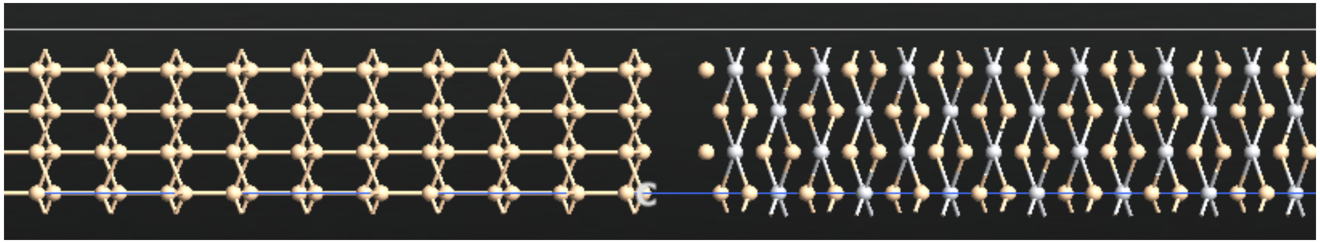
Case 1:
Si[111] bulk

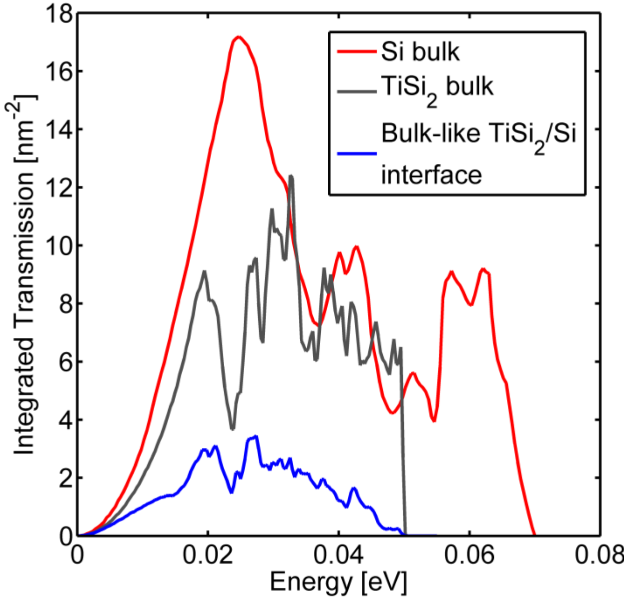


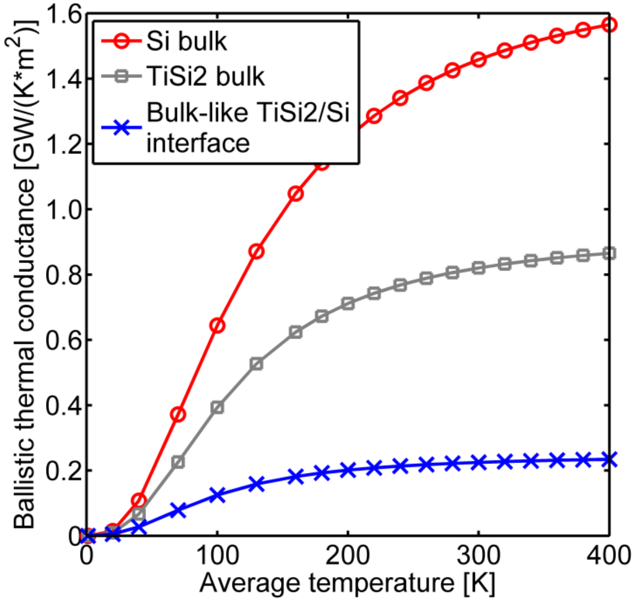
Case 2:
$TiSi_2$[100] bulk



Case 3:
Si[111]/ $TiSi_2$[100]



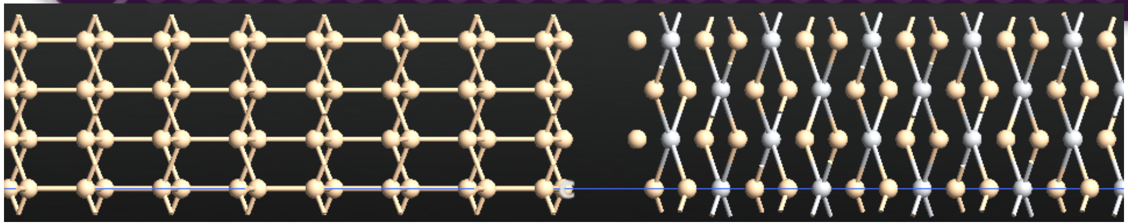




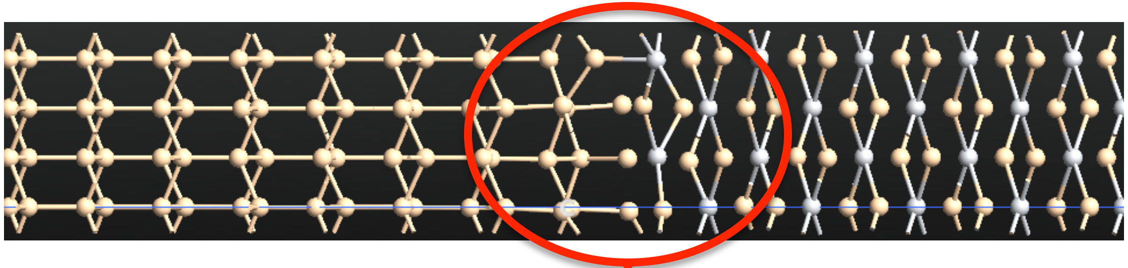
Thermal conductance drop is mainly caused by the interface phonon mismatch.

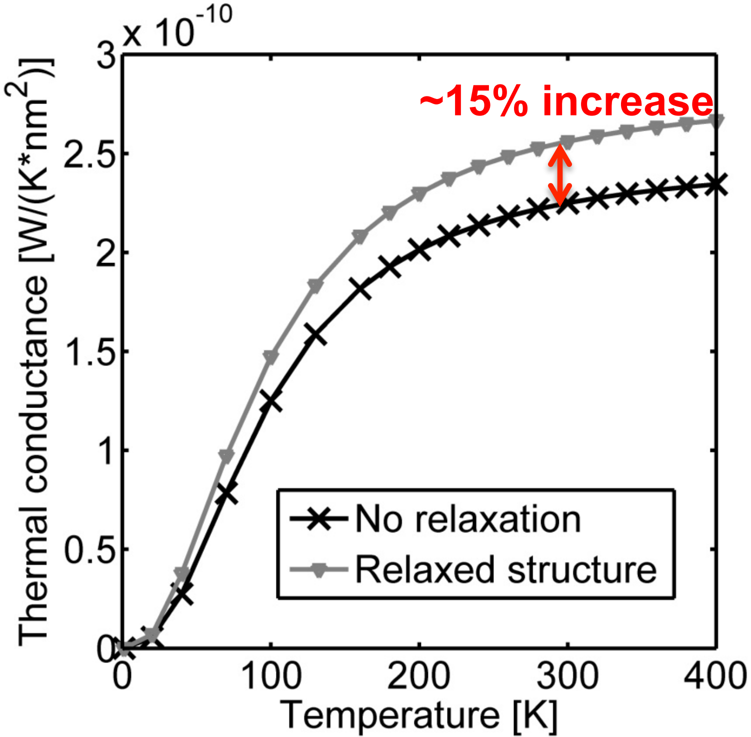
Thermal conductance increasing due to the relaxation

Case 1:
No geometry relaxation



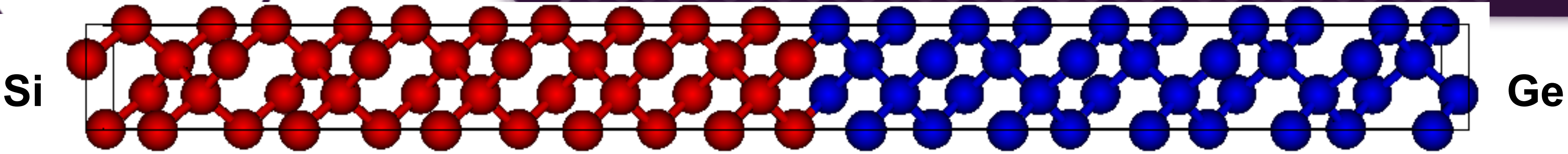
Case 2:
Considering relaxation

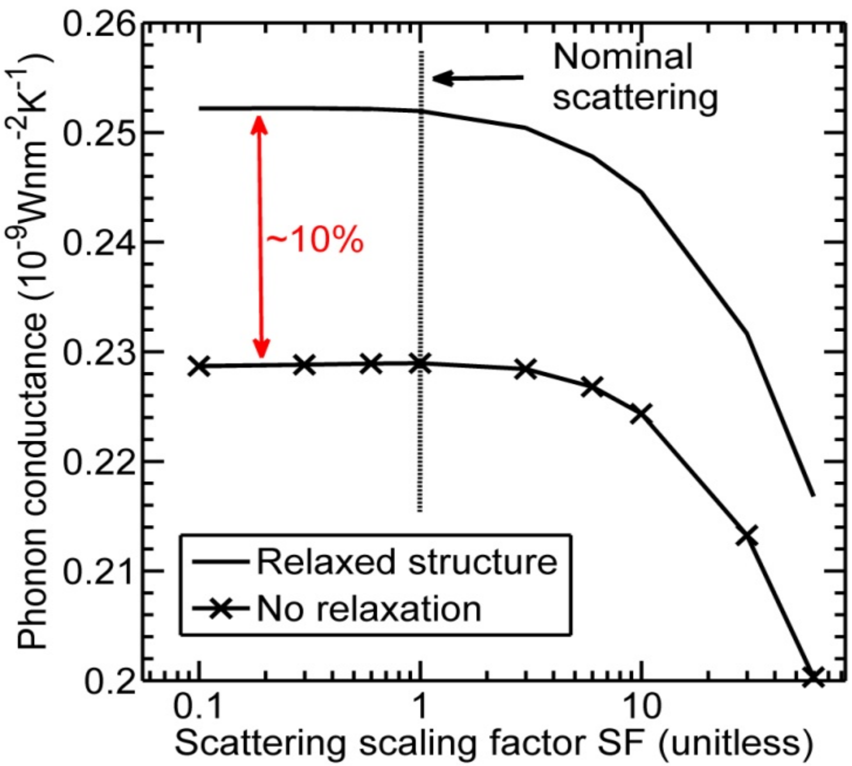




Relaxation process make the structure transition from Si to TiSi2 more smooth → Lattice mismatch is reduced → Thermal conductance is increased.

Relaxation with VFF model

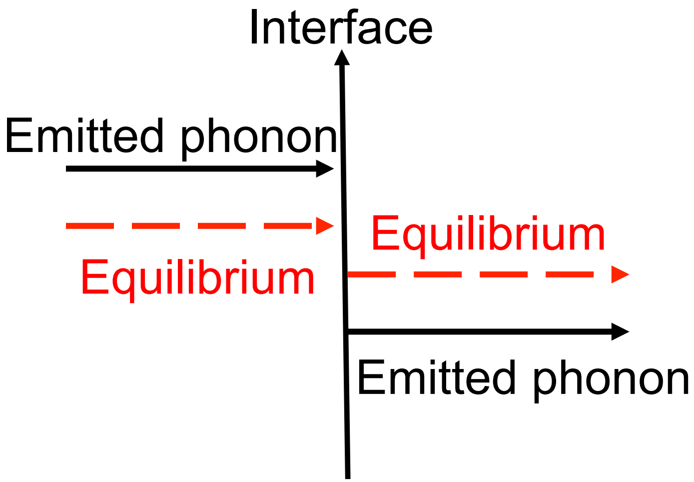




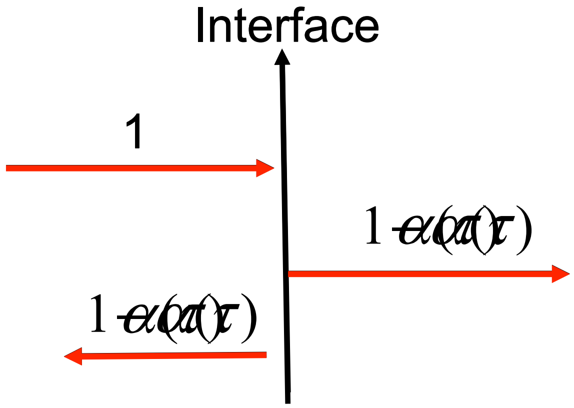
Relaxation increases the thermal conductance → Using VFF model gives a same conductance enhancement as by using DFT model.

Limitations of the classical Landauer treatment

Physics picture



Theoretical interpolation



C. Gang, et al. Microscale Thermophysical Engineering, 5:71–88, 2001

$$Q=\frac{1}{(2\pi)^3}\int\sum_{v}\hbar\omega u_z\alpha_{L\rightarrow R}\left[f_{BE}(\omega,T_L)-f_{BE}(\omega,T_R)\right]d(\hbar\omega)$$

1. Emitted phonon at the interface is out of equilibrium.
2. Local equivalent equilibrium temperatures are redefined.
3. Incorrect result of a nonzero thermal interface resistance is predicted in homogeneous structure.

Landauer formula with NEGF

Landauer formula with NEGF:

$$I_{left}=\int_{-\infty}^{+\infty}\sum_{j=1,j\neq i}^{N_A}\sum_{n=1,n\neq m}^{3}\frac{1}{h}E\left[\mathcal{T}_{left,right}(E)\left(\frac{1}{e^{E/k_B T_{right}}-1}-\frac{1}{e^{E/k_B T_{left}}-1}\right)+\mathcal{T}_{(i,m)left}(E)\left(\frac{1}{e^{E/k_B T_{i.m}}-1}-\frac{1}{e^{E/k_B T_{left}}-1}\right)\right]dE$$

$I_{right} = -I_{left}$

If there is no scattering, $\mathcal{T}_{(i,m)left}$ is 0, which gives:

$$I_{left}=\int_{-\infty}^{+\infty}\sum_{j=1,j\neq i}^{N_A}\sum_{n=1,n\neq m}^{3}\frac{1}{h}E\left[\mathcal{T}_{left,right}(E)\left(\frac{1}{e^{E/k_B T_{right}}-1}-\frac{1}{e^{E/k_B T_{left}}-1}\right)\right]dE$$

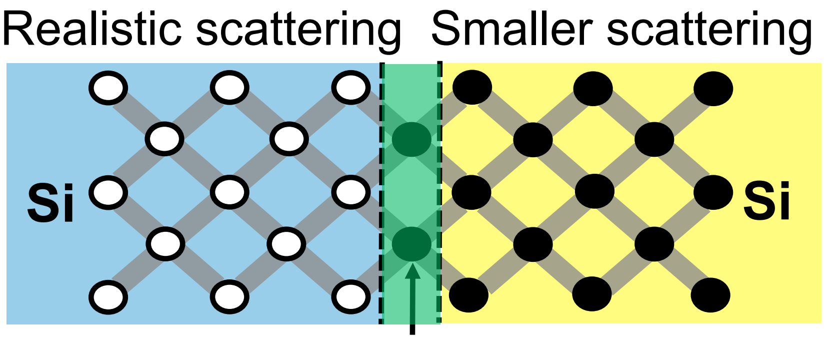
‖

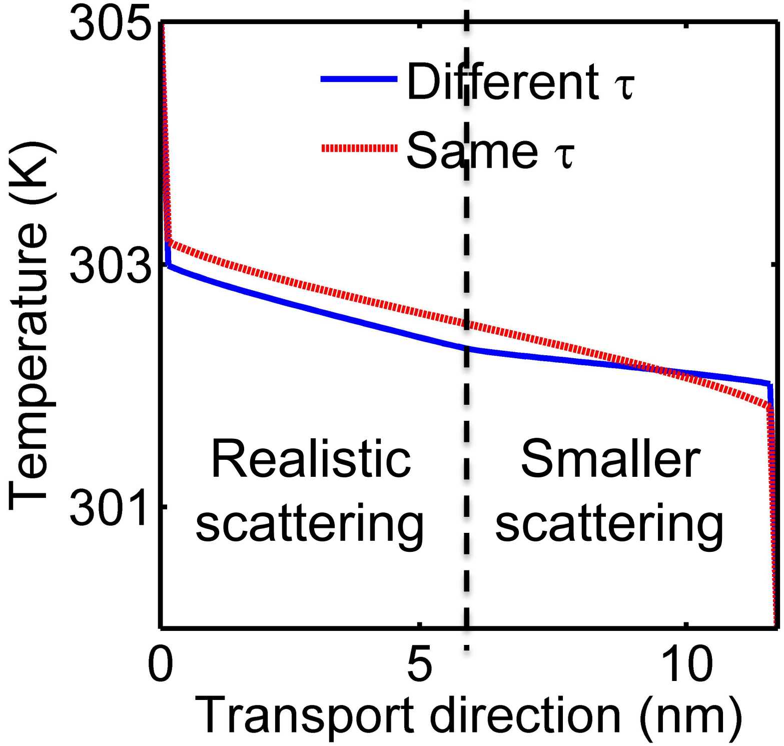
Landauer formula with traditional treatment:

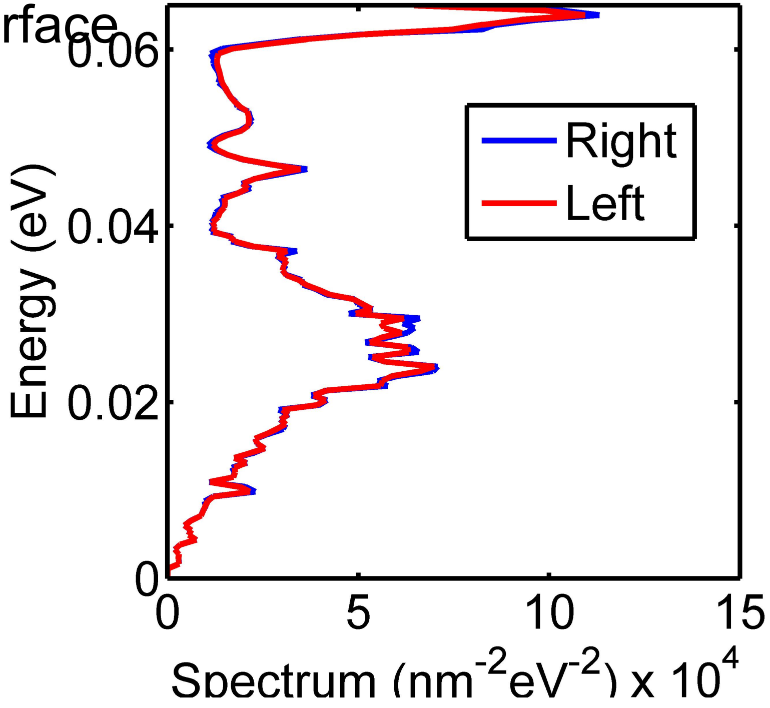
$$Q=\frac{1}{(2\pi)^3}\int\sum_{v}\text{h}\omega u_z a_{L\rightarrow R}\left[f_{BE}(\omega,T_L)-f_{BE}(\omega,T_R)\right]d(\text{h}\omega)$$

C. Gang, et al. Microscale Thermophysical Engineering, 5:71–88, 2001

Landauer formula with quantum NEGF and scattering

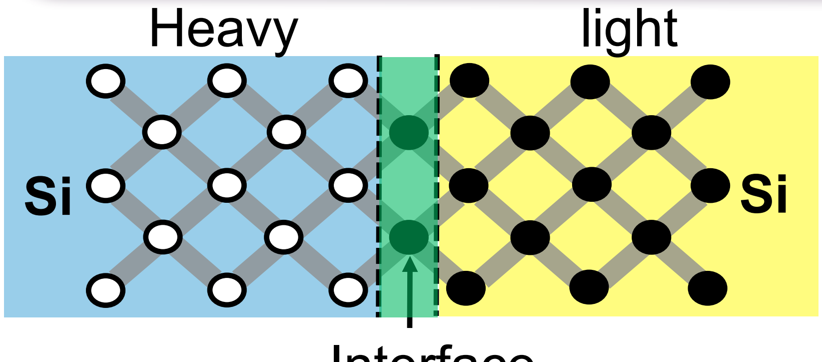


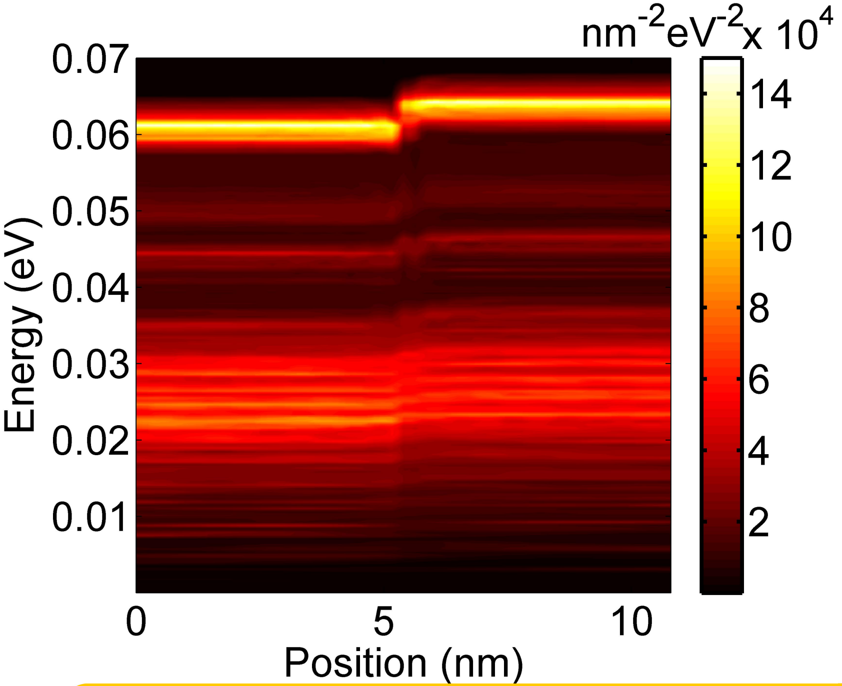


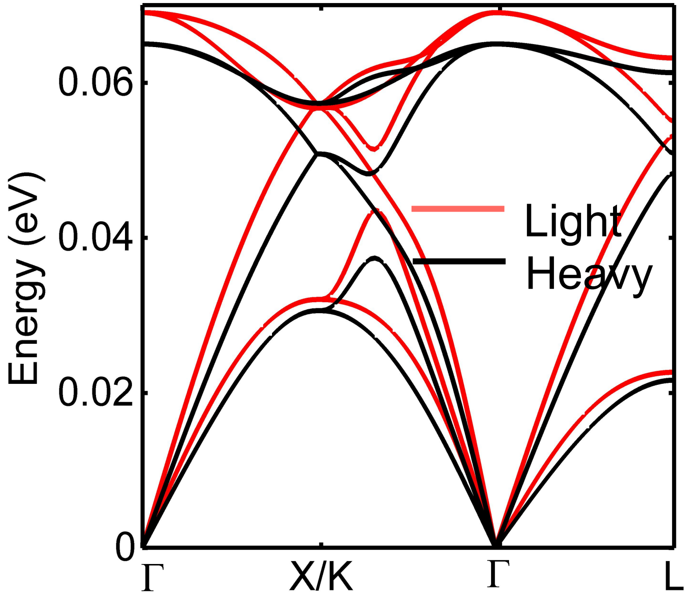


The different scattering rate will give a different temperature drop in device
Interface resistance can be neglected.

DOS at Si(30)/Si(28) interface

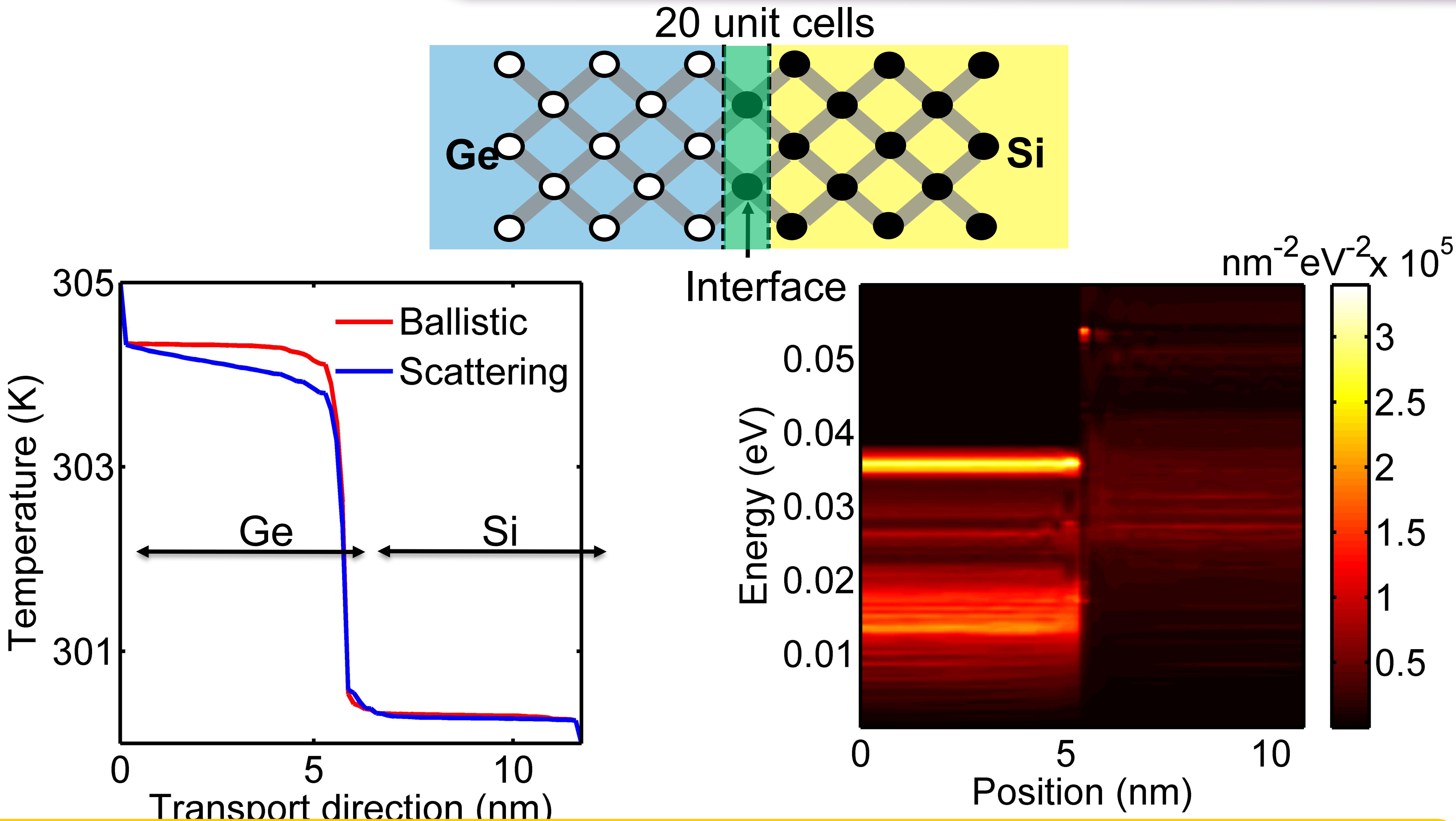






Mass difference will affect the phonon dispersion dramatically, hence the interface interference DOS appears.

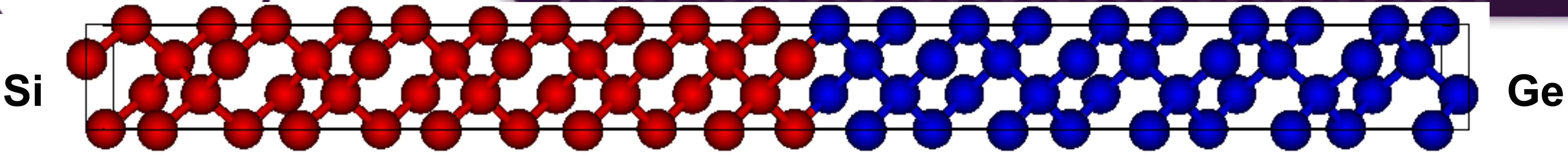
Temperature profile inside the device



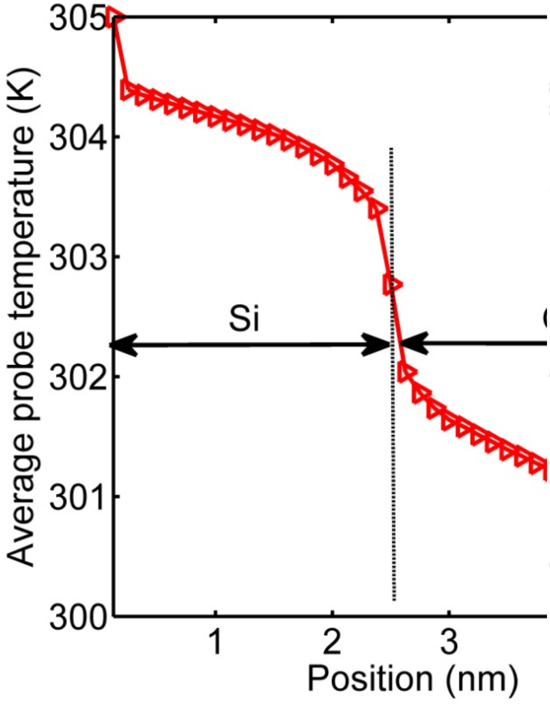
Temperature drop inside the Si/Ge heterostructure is due to:

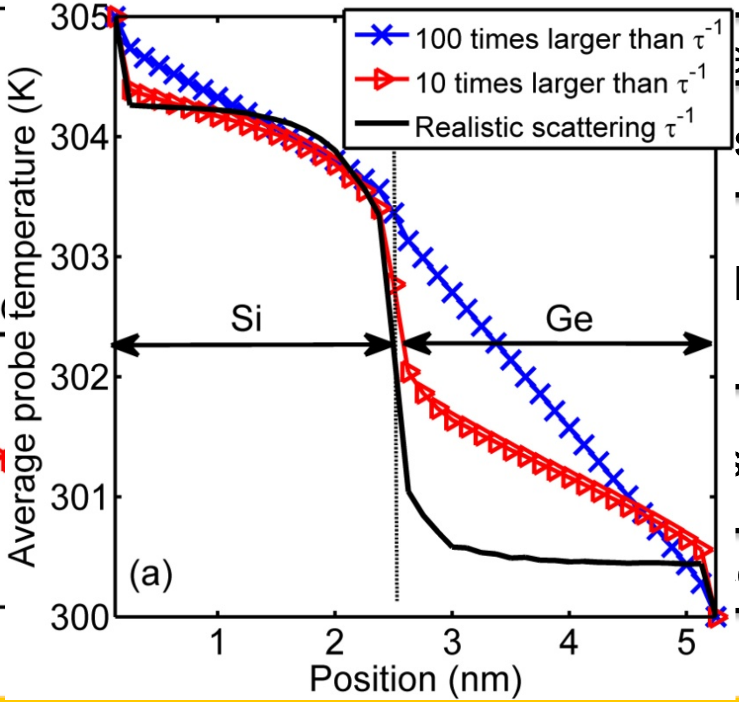
1. Scattering in material;
2. Interface reflection→ dispersion mismatch.

Influence of interfacial thermal resistance to the temperature profile across Si/Ge interface



Si/Ge bulk: 5nm;Hot spot (Si): 305K.;Cold spot (Ge): 300K.Transport direction: [100]





e resistance

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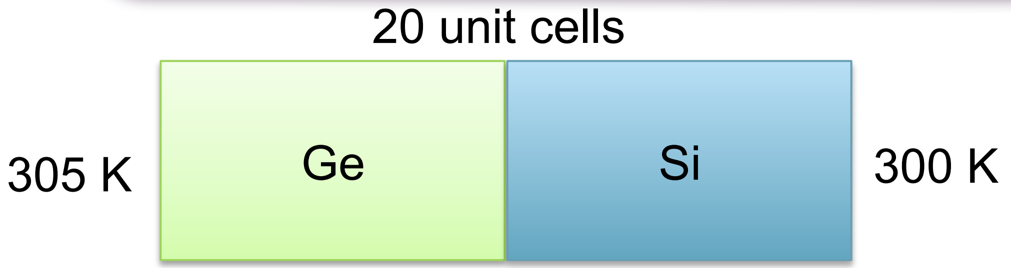
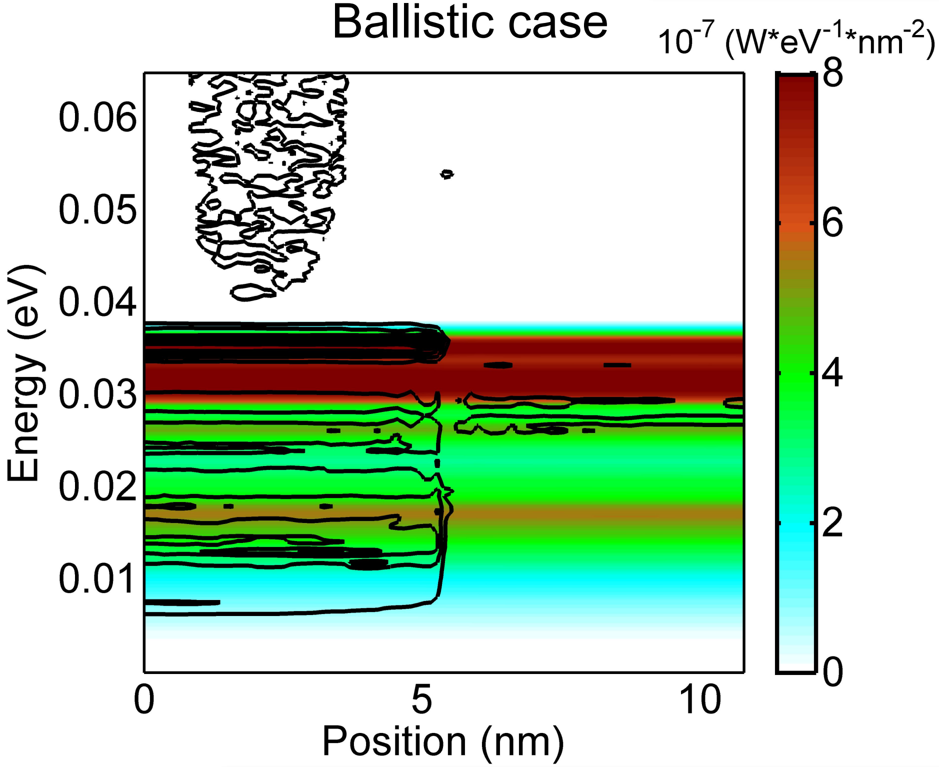
e resistance

1. Different scattering rate will cause different temperature drops inside the device.
2. With the small scattering, dispersion mismatch causes the temperature drop at the interface. This effect decays with larger scattering rate.

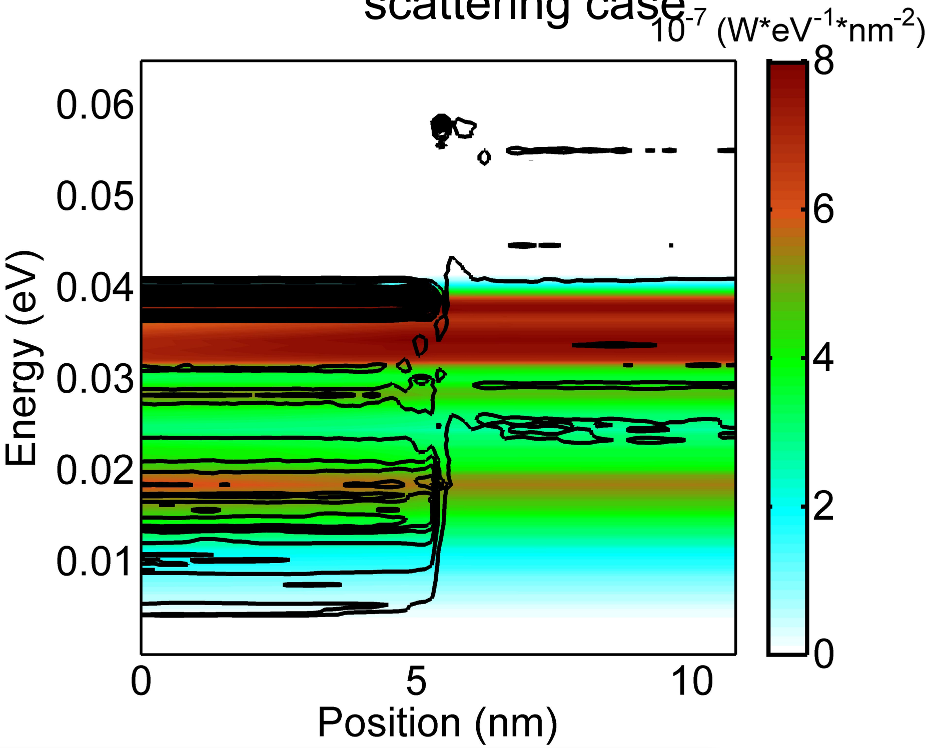
Energy resolved current and DOS



Ballistic case



scattering case

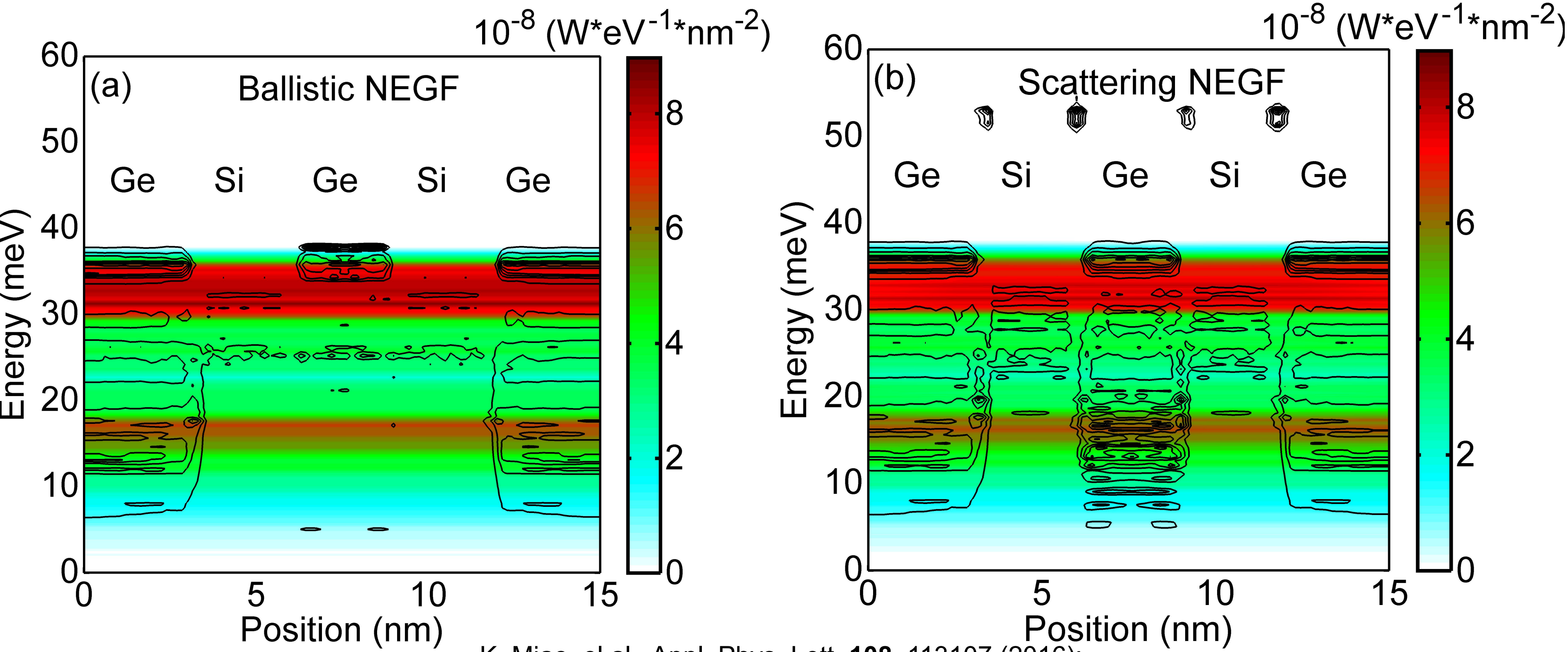


Scattering case will change the resonant state pattern
→ Tunneling of High energy phonons.

Kai Miao

Energy resolved phonon current & Phonon density of states

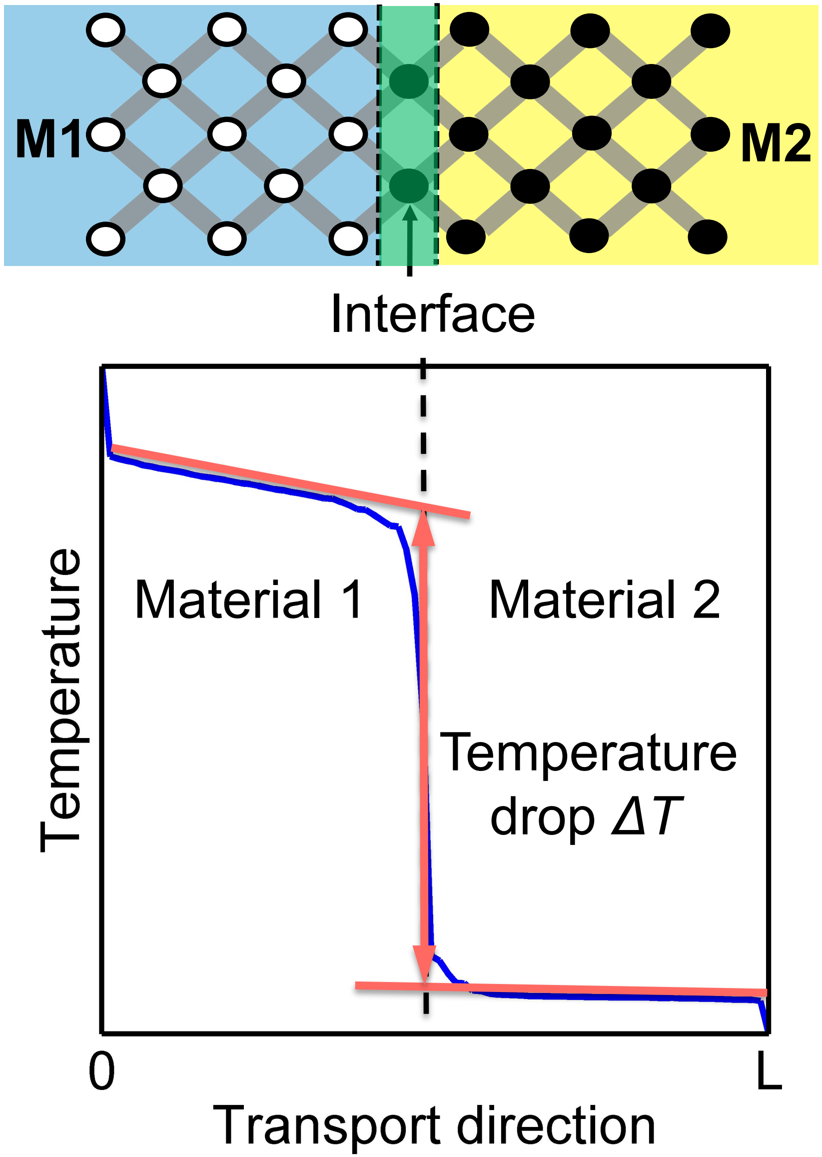
Colorful contour plot is the energy resolved phonon current in Si/Ge heterostructure. Contour line is the phonon density of states inside the device.



K. Miao, el al., Appl. Phys. Lett. **108**, 113107 (2016);

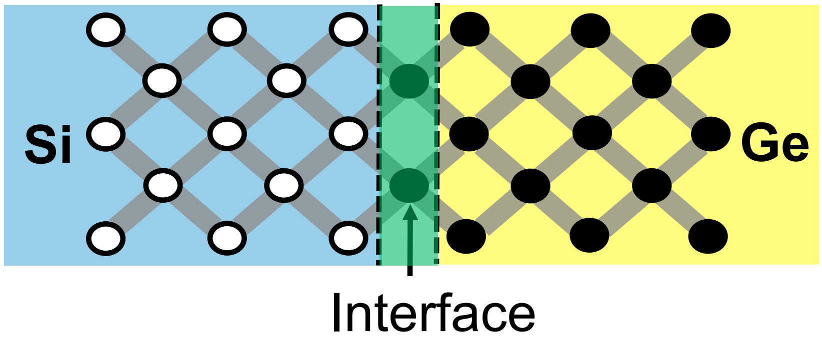
1. Quantum mechanism is considered with the application of NEGF+Büttiker probe.
2. NEMO5 is capable to understand the phonon transport more straightforward.

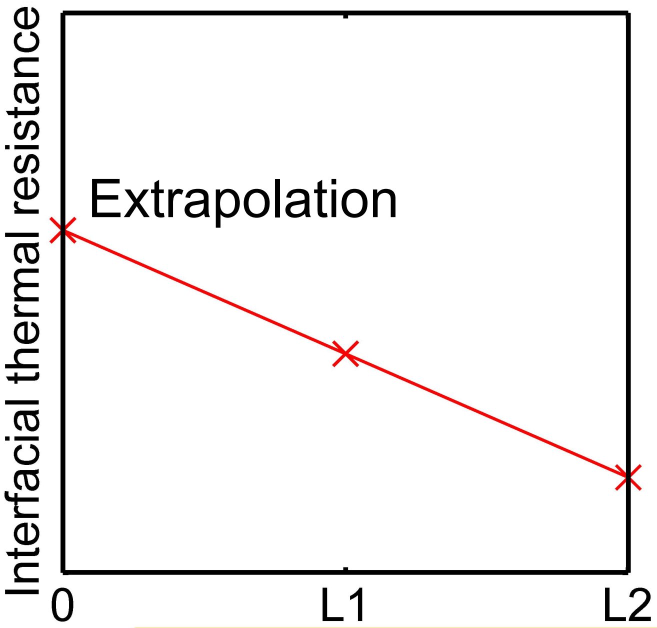
Interface resistance extraction



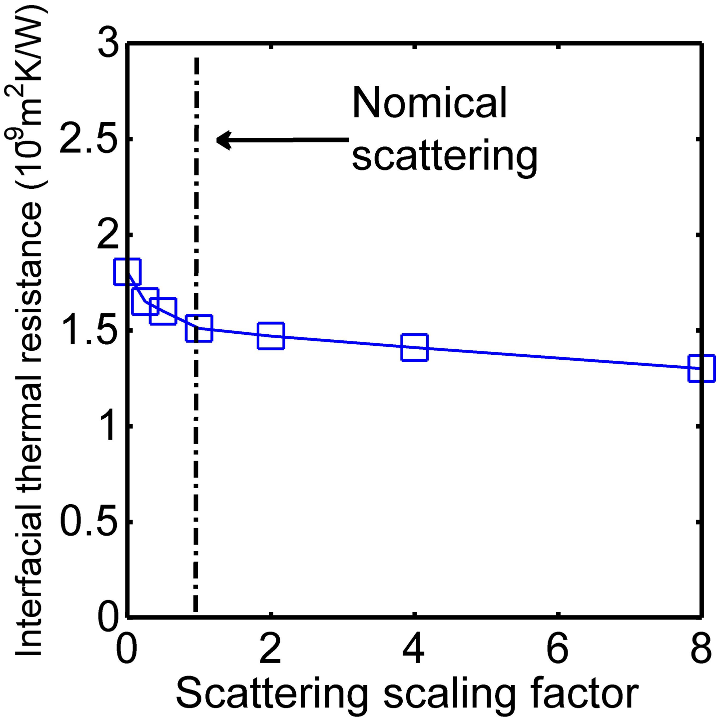
Extraction of interfacial thermal resistance

Method



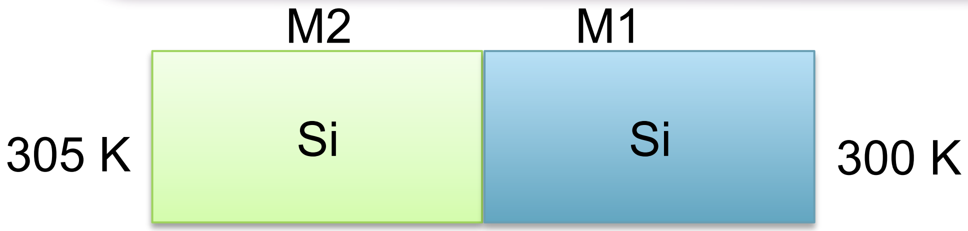


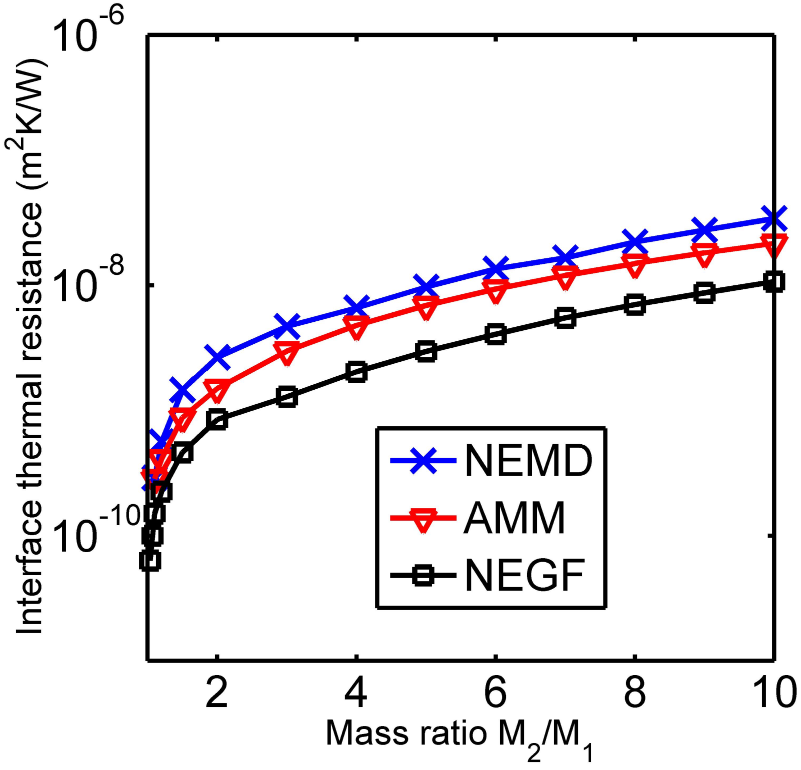
Resistance



Interfacial resistance is largely independent on the scattering strength.

Comparison of interface thermal resistance with MD

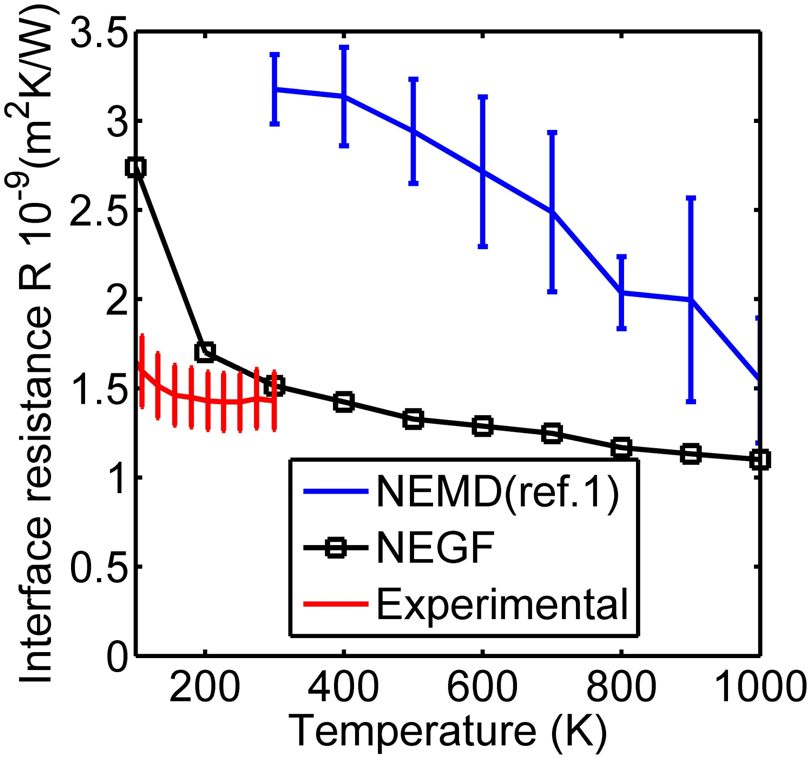




A significant difference between NEMD and NEGF is noticed.

1. NEMD needs a large structure to predict the thermal transport in bulk.
2. NEMD needs a large time steps to achieve conserved transport results.

Results



Ref.1: E. S. Landry and A. J. H. McGaughey
Phys. Rev. B **80**, 2009
Experimental: Superlattices and Microstructures,
Vol. 28, No. 3, 2000

Conclusions

1. Include the process of relaxation calculation in the heterostructure.

2. Show the capability of this work to solve phonon transport of interface problem.

3. Intrinsic scattering is not the main reason for the interface resistance.
The mismatch of phonon dispersion is!

4. Interfacial thermal resistance is largely independent on the intrinsic scatterings.

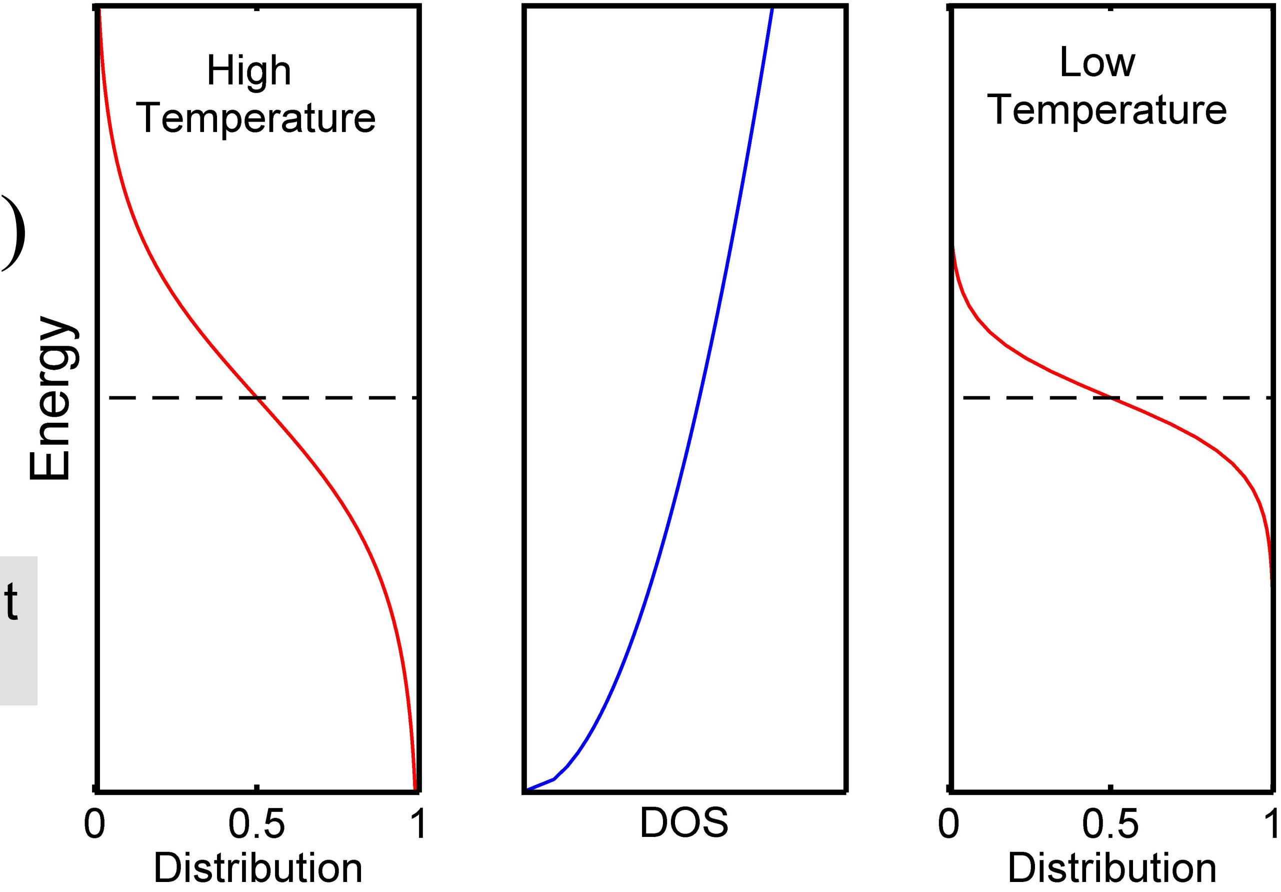
5. Variance between our model and other models are explored.

Transport Study with Electron-Phonon Coupling

Different temperatures in the device

Example in a n type device.

$$I \propto DOS \cdot (f_1 - f_2)$$

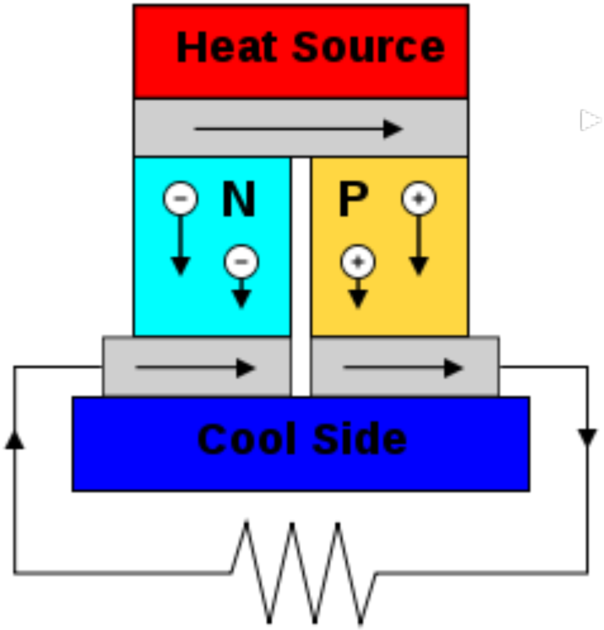


Why should we care about this mechanism?

Temperature will bring electron flow in the device.

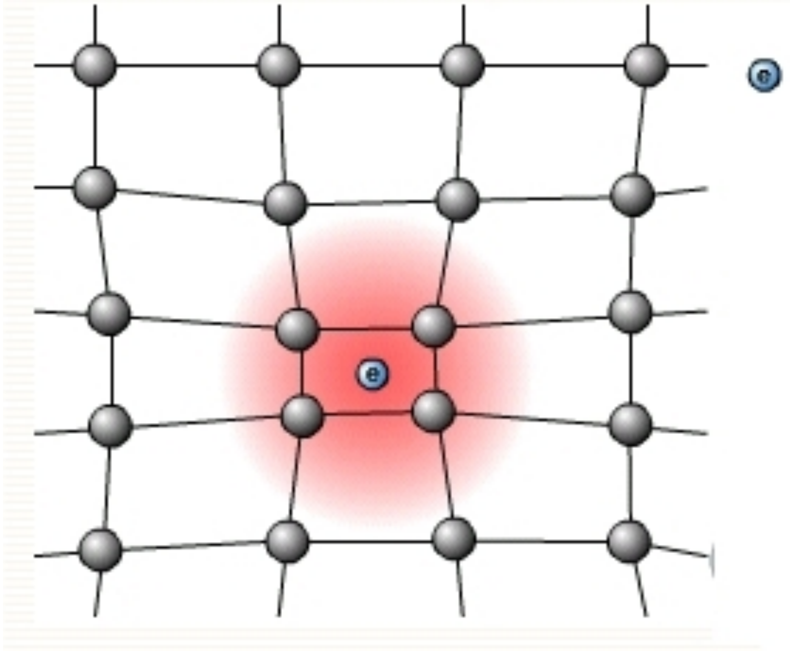
Temperature-driven electron flow

Thermoelectric generator



Seebeck effect: electron current is generated by temperature.

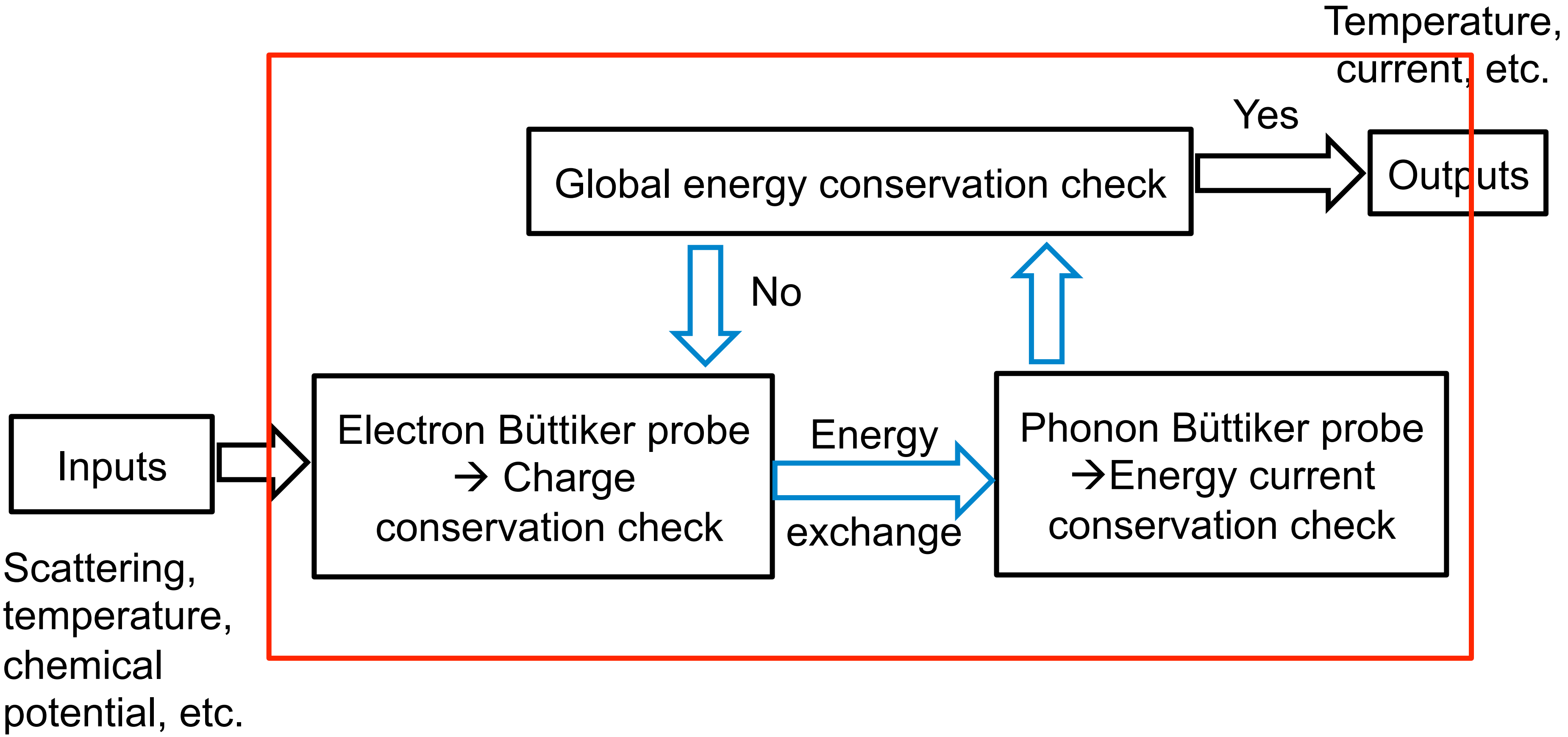
Electron-phonon coupling



Electron is coupled with phonon inside the device/materials.

Electron and phonon transport with coupling due to temperature difference should be understood.

Electron-phonon coupling model



Temperature, current, etc.

Yes

Outputs

Global energy conservation check

No

Inputs

Scattering, temperature, chemical potential, etc.

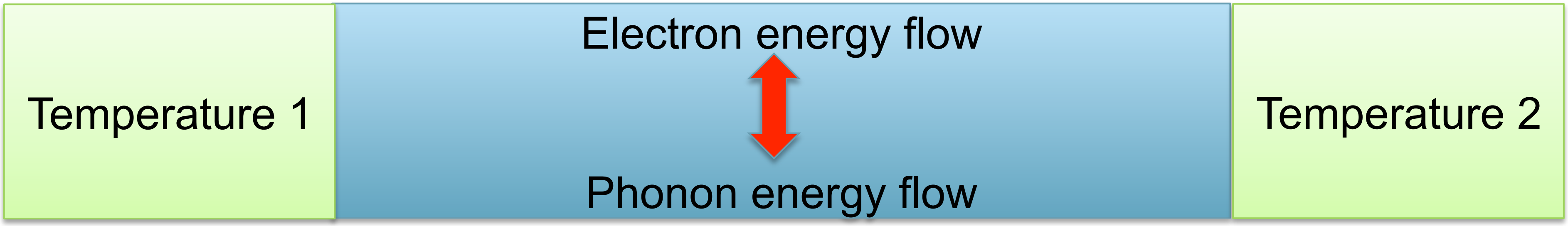
Electron Büttiker probe
→ Charge conservation check

Energy exchange

Phonon Büttiker probe
→Energy current conservation check

NEMO5 can couple electron and phonon transport inside the device to do the electronic and thermal analysis.

Electron-phonon coupling model



Electron transport:

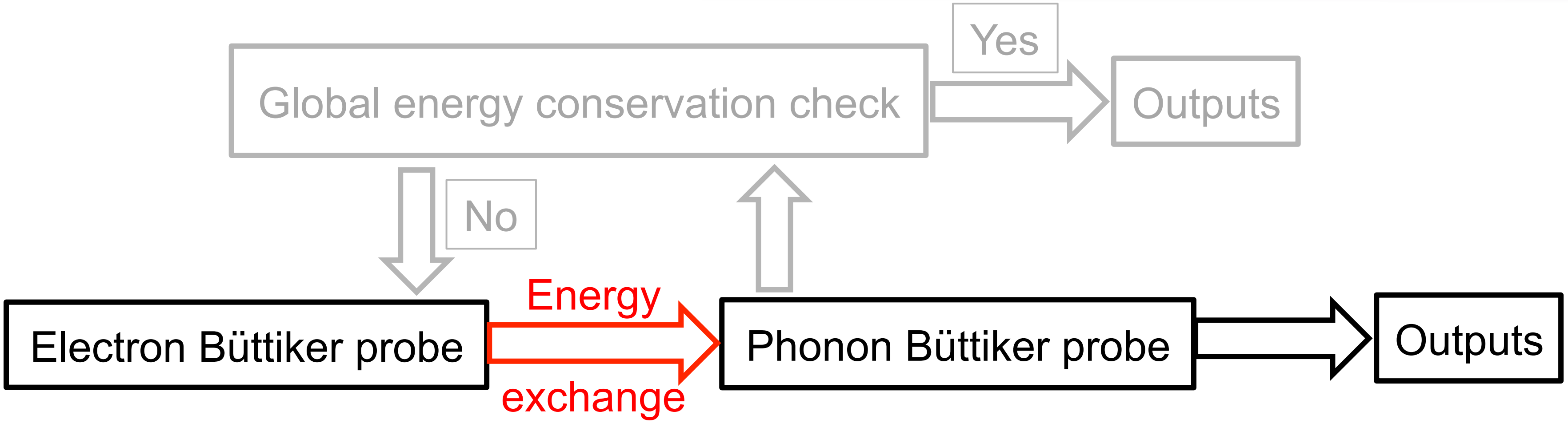
1. Tight-binding model (**10 bands** model)
2. NEGF+Büttiker probe

Phonon transport:

1. Valence force field model (**3 bands** model)
2. NEGF+Büttiker probe

One probe is attached for each atom for both electron and phonon case.

Effect of including e-p coupling



Global energy conservation check

Yes

Outputs

No

Electron Büttiker probe

Energy exchange

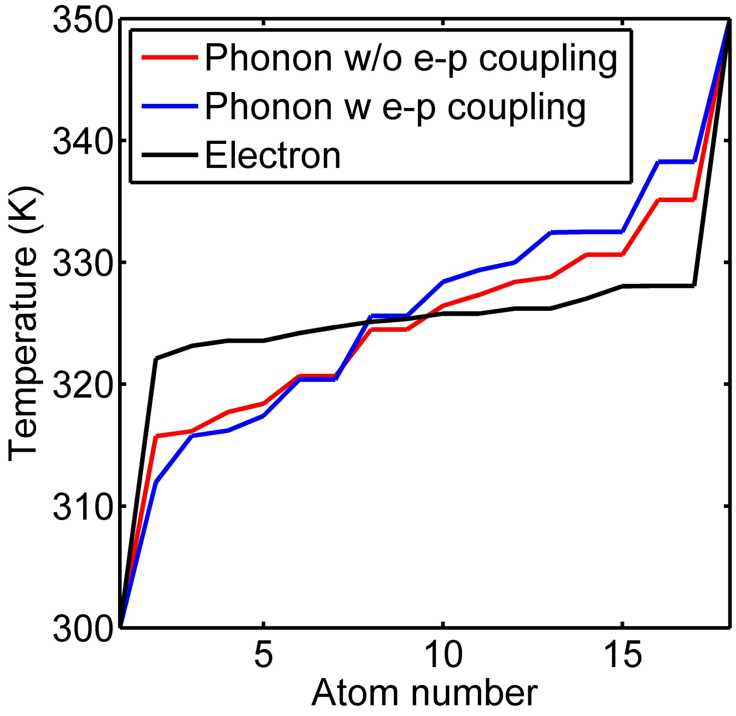
Phonon Büttiker probe

Outputs

Black: included in the simulation

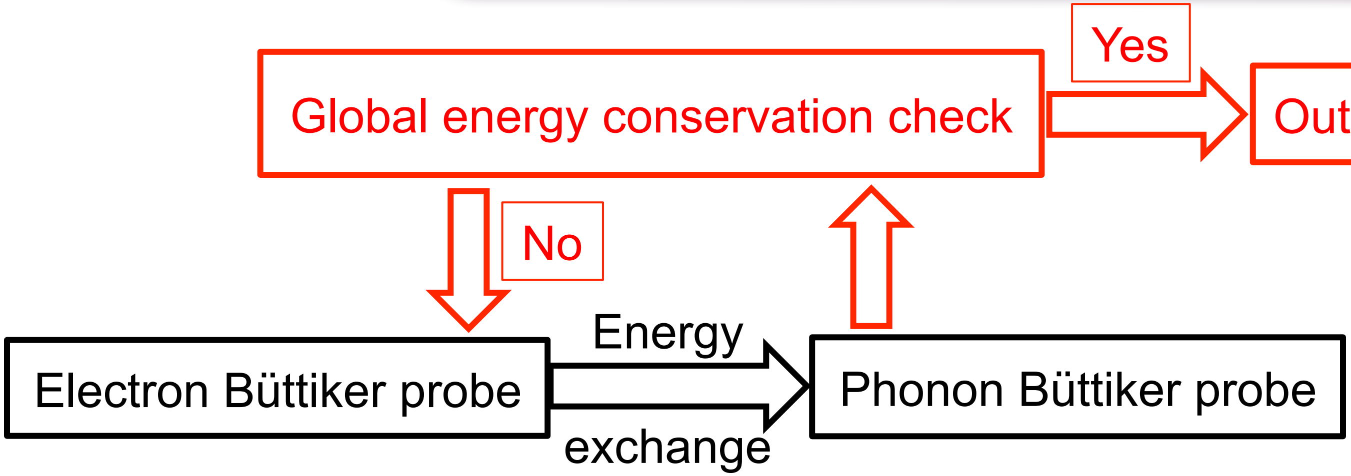
Gray: not included in the simulation

Red: Can be turned on or off



Phonon temperature drop is increased with e-p coupling.

Energy conservation check



Yes

Global energy conservation check

Outputs

No

Electron Büttiker probe

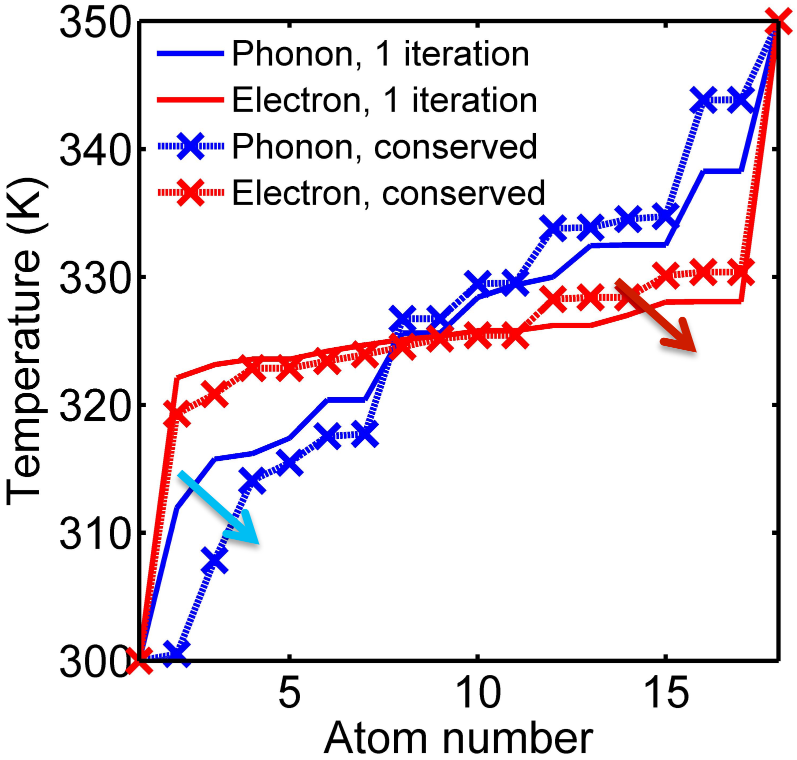
Energy exchange

Phonon Büttiker probe

Black: included in the simulation

Red: Can be turned on or off

Self-consistent iteration with e-p coupling results in a larger temperature drop for both electron and phonon.



NEMO5 implementation

Energy dependent models are added into NEMO5.

1. Scattering rates

Acoustic phonon scattering

$$\dot{\gamma}_{e\text{-}p,\mathrm{A}} = \frac{\pi \varphi_{d,\mathrm{A}}^2 k_\mathrm{B} T_p D_e[E_e(p_e)]}{\hbar \rho u_{p,\mathrm{A}}^2}$$

Optical phonon scattering

absorption

$$\tau_{e\text{-}p,\mathrm{O}}^{-1} = \frac{\varphi_{d,\mathrm{O}}^{\prime 2} f_p^{\circ}(\omega_{p,\mathrm{O}}) m_{e,e}^{3/2} [E_e(p) + \hbar\omega_{p,\mathrm{O}}]^{1/2}}{2^{1/2} \pi \hbar^3 \rho \omega_{p,\mathrm{O}}},$$

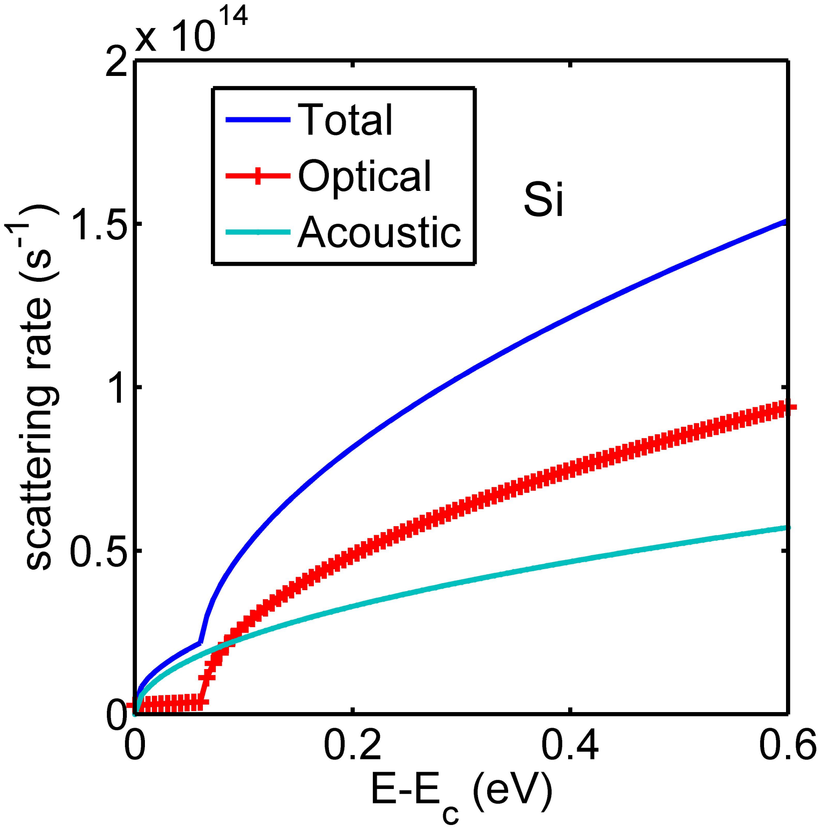
emission

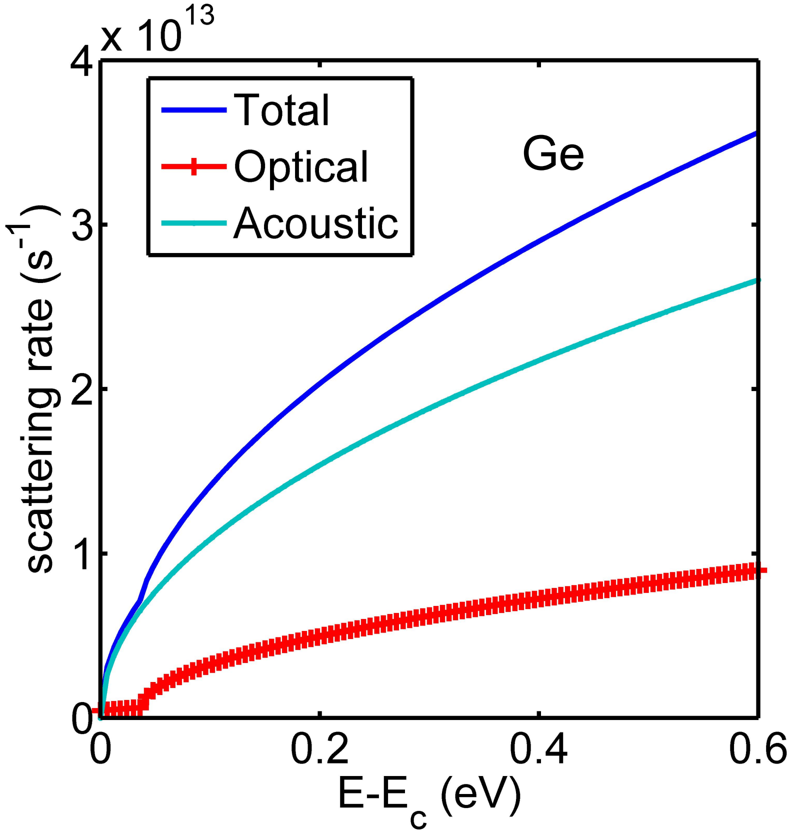
$$\tau_{e\text{-}p,\mathrm{O}}^{-1} = \frac{\varphi_{d,\mathrm{O}}^{\prime 2} [f_p^{\circ}(\omega_{p,\mathrm{O}}) + 1] m_{e,e}^{3/2} [E_e(p) - \hbar\omega_{p,\mathrm{O}}]^{1/2}}{2^{1/2} \pi \hbar^3 \rho \omega_{p,\mathrm{O}}},$$

2. Relation between scattering rate and self energy

$$\gamma(\vec{k}_\parallel, E) = -\frac{4}{\hbar} \mathrm{Im}\left[\left(\Sigma_{BP}^{R}(\vec{k}_\parallel, E)\right)\right]$$

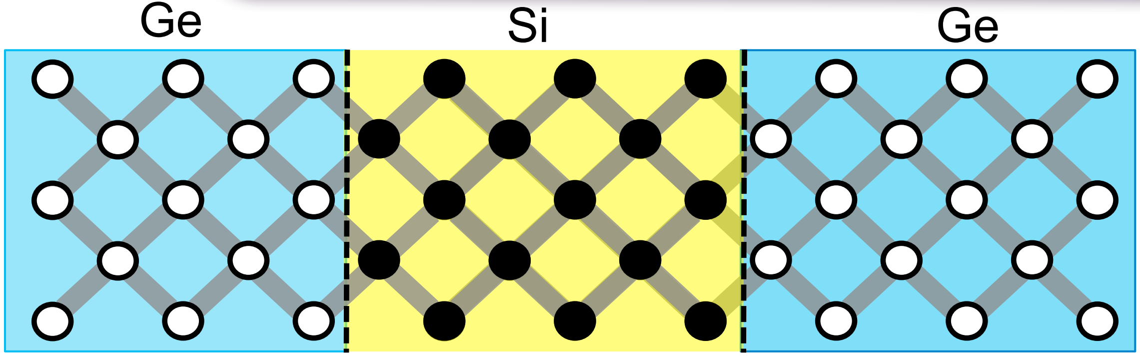
Scattering mechanisms

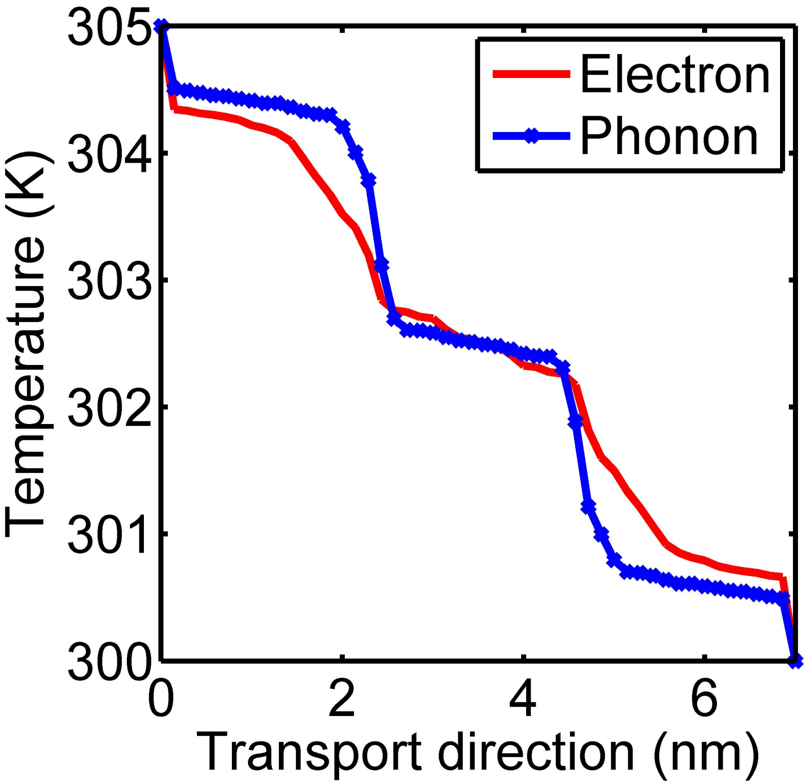




Here, the acoustic and optical phonon scattering are considered.

Results



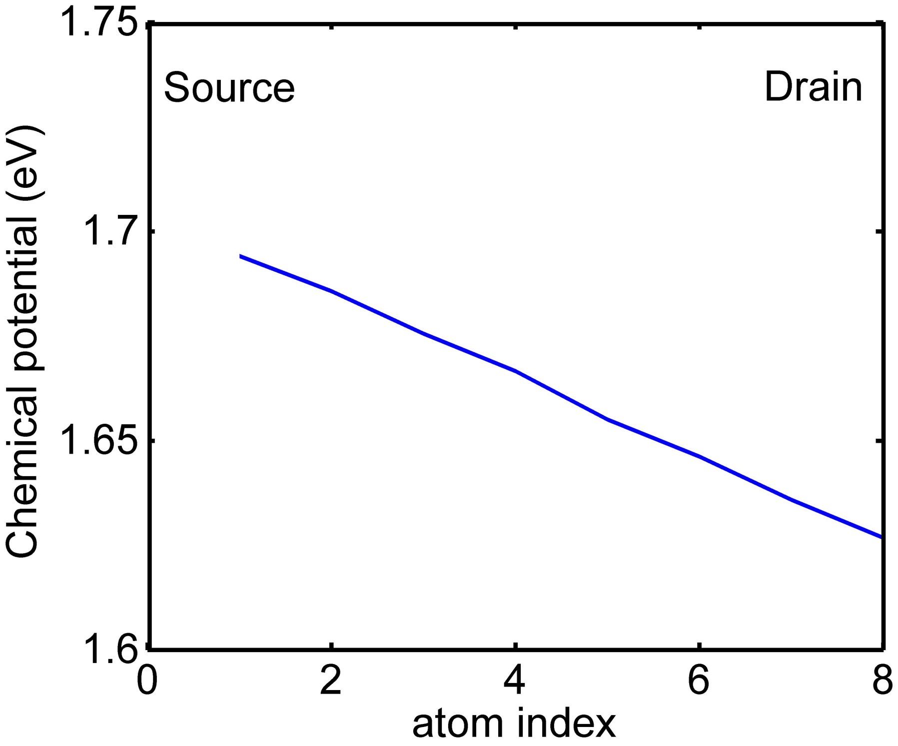


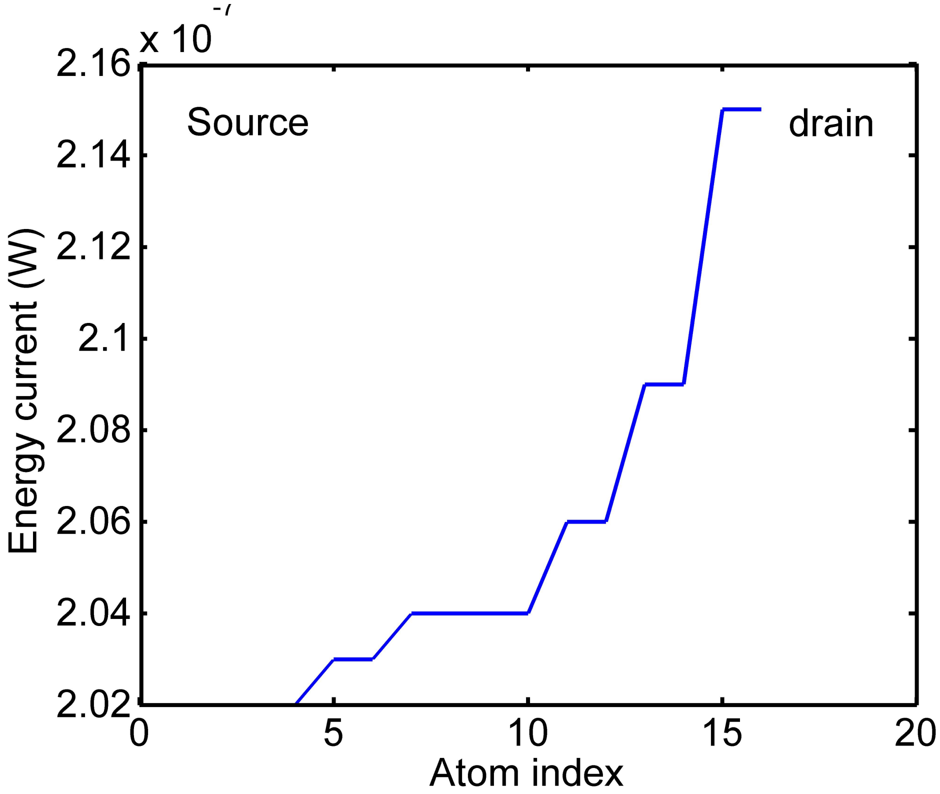
1.More electron temperature drops in Si and Ge region compared to phonon case.

2. More phonon temperature drops at the Si/Ge interface.

Future work

Preliminary result about the energy exchange inside the device:





Here is dissipated in the drain side. In future, we will apply our method in real large device to capture the self-heating effect.

Future work

Foundation

- Self-consistence electron phonon coupling model is implemented into NEMO5

Future improvement

- Enable more effeicient RGF.
- More applications in different devices.

FRAMEWORK

Electron-phonon coupling in NEMO5

- Electron transport with Tight-binding basis is verified.
- Phonon transport with VFF model is ready.
- The self consistence with e-p coupling is implemented.

Core

EFFICIENCY

- Implement Buettiker probe with RGF.

1

Superlattice

- Test the general lead model in both electron and phonon buettiker

2

Applications

- LED device simulation.
- Method-Semiconductor simulation.

3

Acknowledgement

Committee member:
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Prof. Lundstrom, Prof. Datta

Prof. Ruan, Prof. R. Rahman, Prof. Dr. J. Huang, Dr. J. Fonseca, Dr. B. Novakovic, Dr. C. Bowen, Dr. P. Sengupta, Dr. M. Salmani, Dr. M. Luisier, Dr. G. Hegde, Dr. S. Park, Dr. L. Zeng, Dr. A. Paul, Dr. S. Lee, Dr. H. Ryu, Dr. Y. Tan, Dr. Z. Jiang, Dr. Y. He., Dr. S. Sadasivam, Dr. X. Wang and Dr. Y. Gao.

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