Shiomi Lab

Multi-scale Phonon Simulation in Nanostructures and Modeling of Phonon Interface Properties

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Background: Progress in semi-conductor science

The Blue LED:
A Solid-State Lighting revolution

Artifcial lighting:
6.5% of the world's primary energy and 16% of the world's total generated electrical energy

Nano-scale and Multi-structured heat conduction

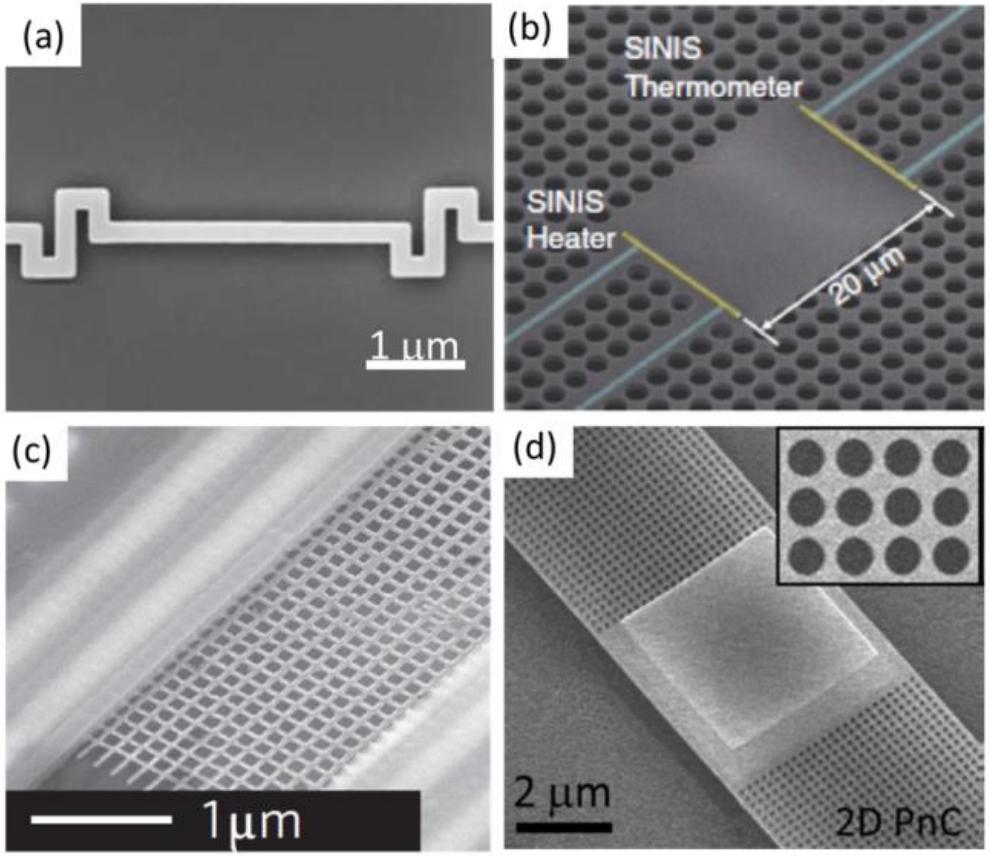


Fig: 8 SEM images of (a) Si serpentine nanowire, (b) SiN 2D PnC microstructure, (c) Si nanomesh structure, and (d) Si 2D PnC nanostructure

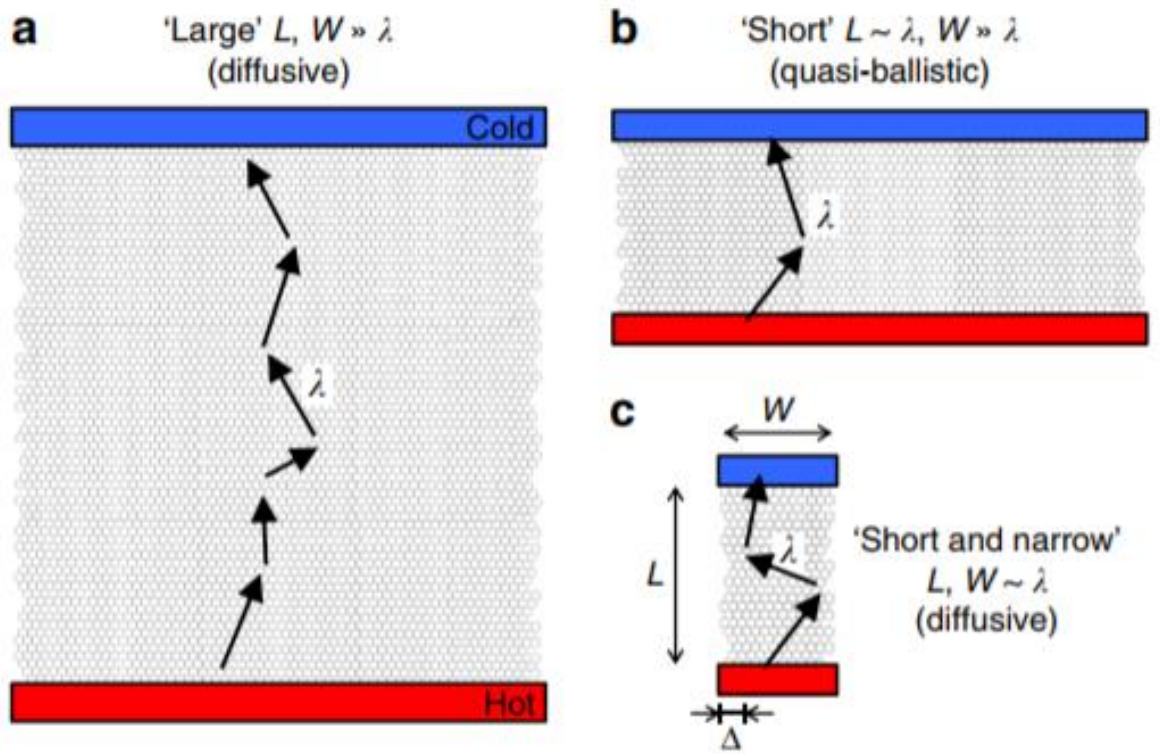


Fig: Schematic of size effects.
(a) Diffusive heat transport
(b) Quasi-ballistic heat flow
(c)) Return to a diffusive heat transport regime

Outline

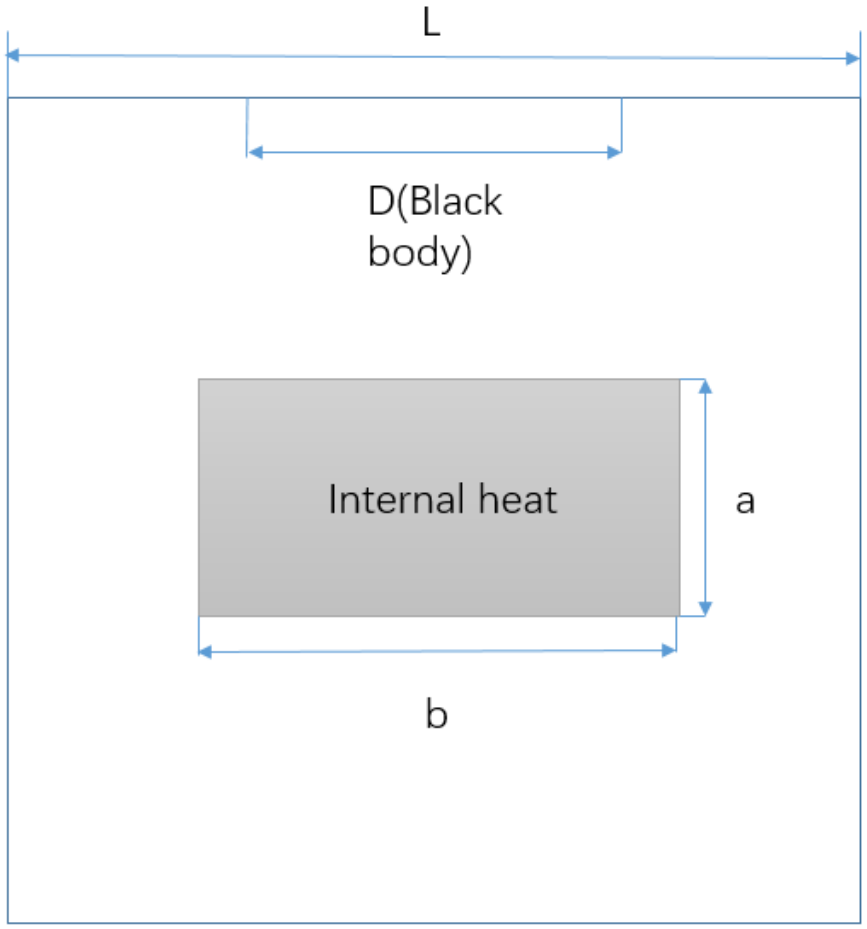
My work mainly consists of the following three parts:

1. Part one: MC method to simulate the temperature profile of nano-film with heat source
2. Part two: Phonon properties of interfaces across III-V semi-conductors using Atomistic Green's Function Method
3. Designing Nanostructures for Phonon Transport via Bayesian Optimization

Part One

Monte Carlo simulation for phonon transport within silicon structures at nanoscales with heat generation

The fundamental model



Two dimensional thermal transport in silicon films with internal heating

- BTE

$$\frac{\partial f}{\partial t} + v_g \nabla f = \frac{f_0 - f}{\tau} + \dot{S}_\Omega$$

- The gray approximation

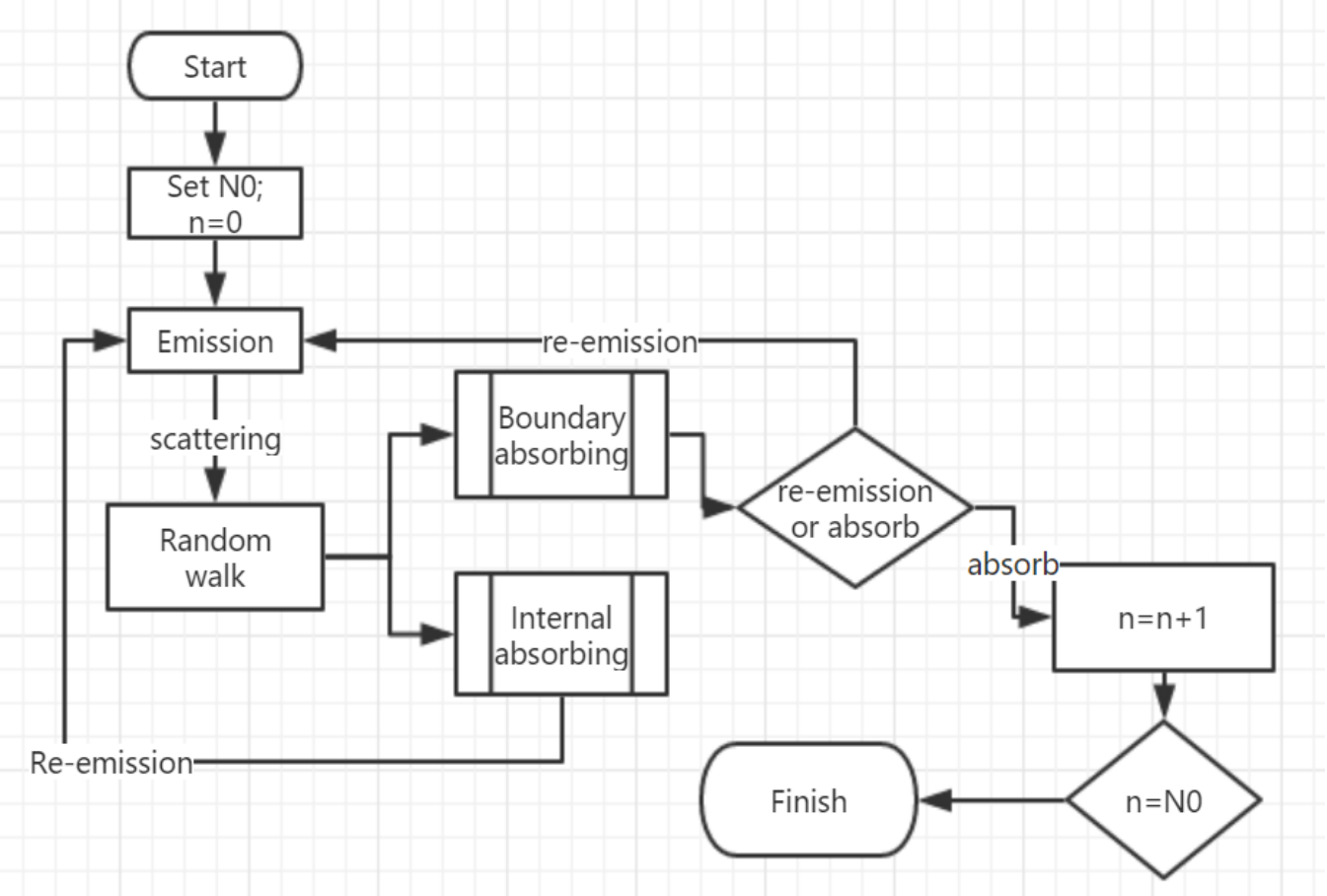
  Using a uniform MPF(Frequency)

- The similarity between phonon and photon

$$E = \sigma T^4$$

$$dQ_{em} = 4\epsilon\sigma T^4 dT$$

MC Method



Block diagram of the tracing algorithm

- Phonon bundle vector

$[sin(\theta)cos(\psi), sin(\theta)sin(\psi), cos(\psi)]$

- Emission angel
  - From the boundary

    $sin(\theta) = (R_{\theta b}^{1/2})$

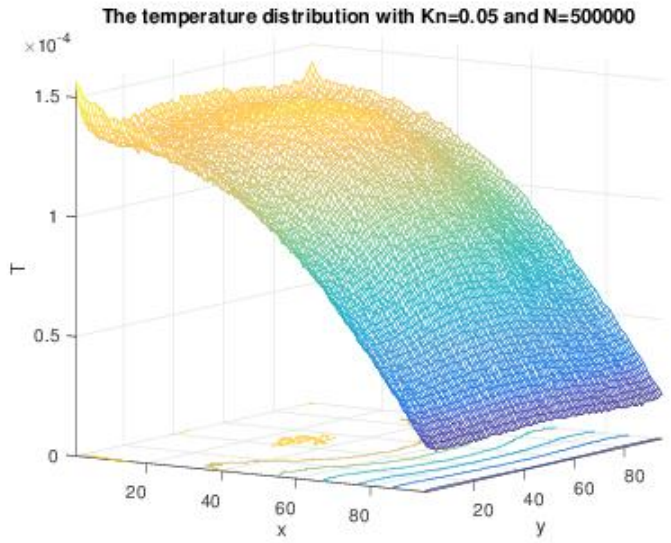
    $\psi = 2\pi(R_{\psi b}^{1/2})$
  - In the media

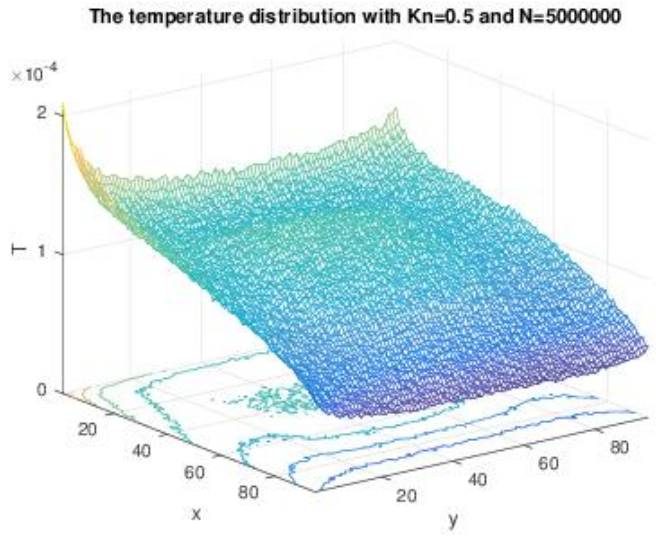
    $cos(\theta) = 1 - 2R_{\theta m}$

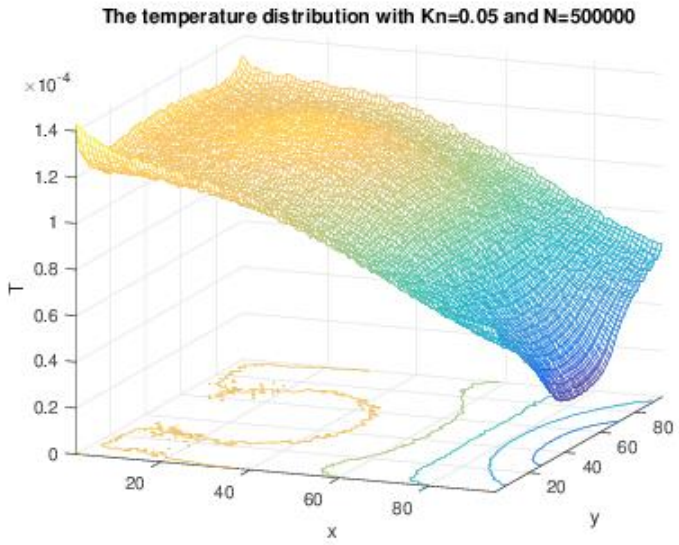
    $\psi = 2\pi(R_{\psi m}^{1/2})$
- The average travel distance

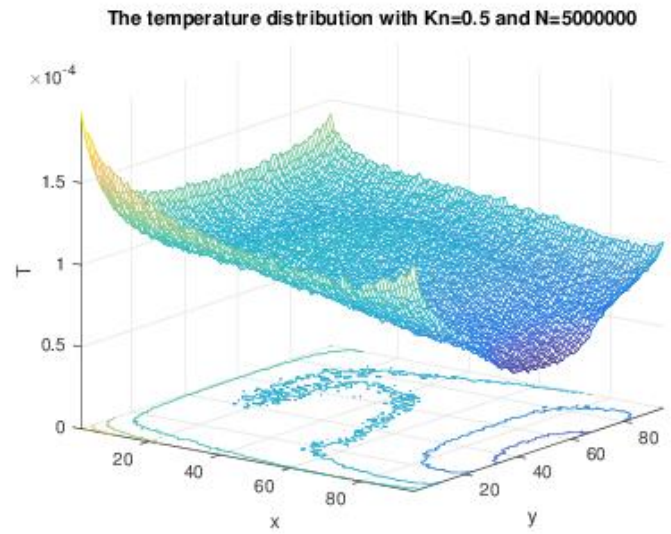
$$\Delta l = -LKnln(1 - R_s)$$

Results: Different boundary conditions









Discussion:

- Size effect

As Kn number becomes bigger, the ballistic effect begins governing the transport.

- Strongly Boundary-influenced

The great influence compared to in bulk materials was clearly shown

Kn=0.05 and 0.5 when L_out=1,0.5L

Summary

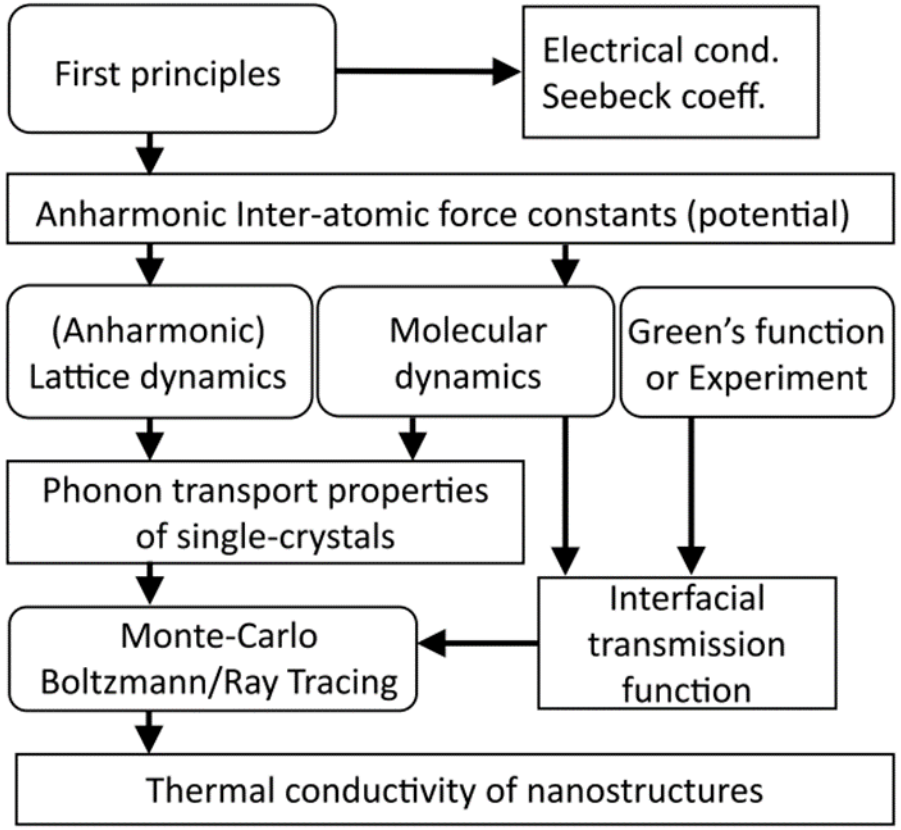
In our BTE-based MC work:

- We quantitatively study the phonon scattering effects.
- We include the internal heat source and study its effects.
- And we study the effects of different boundary conditions on heat conduction.

Part Two

Phonon properties of interfaces across III-V semi-conductors using Atomistic Green's Function Method

Status and Challenges: Multiscale phonon transport calculations



Multi phonon transport calculation(Junichiro Shiomi APL Materials 4, 104504 (2016))

MD:

- Computationally expensive
- Not strictly at low temperatures(Quantum Effects)
- Links to large scales when handling boundaries

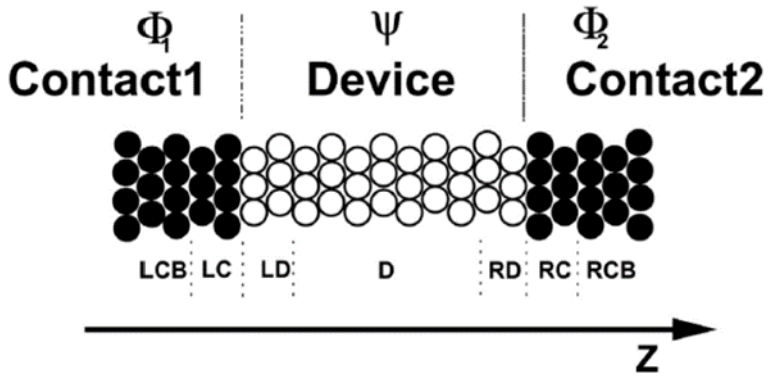
BTE:

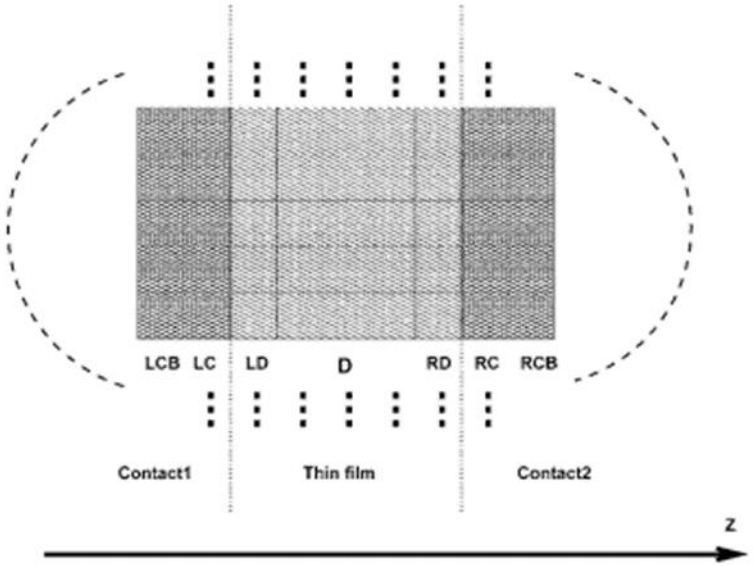
- Requires boundary scattering models
- Requires detailed understanding of phonon scattering and dispersion

The atomistic Green's function method (AGF) has emerged as a useful tool to study phonon transport across interfaces.
(Sadasivam, Sridhar, et al. Ann. Rev. Heat Transfer, 2014, 17: 89-145.)

Atomistic Green's Function

- Includes effect of bulk contacts
- Suitable for ballistic transport
  - Nanoscale devices at room temperature
  - Low-temperature conditions
  - Scattering dominated by boundaries and interfaces
- Required inputs
  - Equilibrium atomic positions
  - Inter-atomic potentials
  - Contact temperatures





AGF: The Methodology

Lattice Dynamics

$$[\omega^2 I - H]\mu = 0$$

$$H_{ij} = \frac{1}{\sqrt{M_i M_j}} k_{ij}$$

$$k_{ij} = -\frac{\partial^2 U^{harm}}{\partial u_i \partial u_j}$$

Green's Functions

$$L[u] = [\omega^2 I - H]u = 0$$

A perturbation

$$L[g] = \delta$$

$$g = [(\omega^2 + \delta i)I - H]^{-1}$$

Uncoupled Green Functions for contacts

$$g_1 = \lim_{\delta \to 0} [(\omega^2 + \delta i)I - H_1]^{-1}$$

$$g_2 = \lim_{\delta \to 0} [(\omega^2 + \delta i)I - H_2]^{-1}$$

AGF: The Methodology

The Device Green's Function

$$G = [\omega^2 I - H_d - \tau_1 g_1 \tau_1^T - \tau_2 g_2 \tau_2^T]$$

Overall matrix equation:

$$\begin{bmatrix} \omega^2\mathbf{I} - H_1 & -\tau_1^\dagger & 0 \\ -\tau_1 & \omega^2\mathbf{I} - H_d & -\tau_2 \\ 0 & -\tau_2^\dagger & \omega^2\mathbf{I} - H_2 \end{bmatrix} \begin{pmatrix} \phi_1^R + \chi_1 \\ \psi \\ \phi_2^R + \chi_2 \end{pmatrix} = 0$$

Transmission

- Definitions of convenience

$$A_j = i[g_j - g_j^T]$$

$$\Gamma_j = \tau_j A_j \tau_j^T$$

- The Transmission function

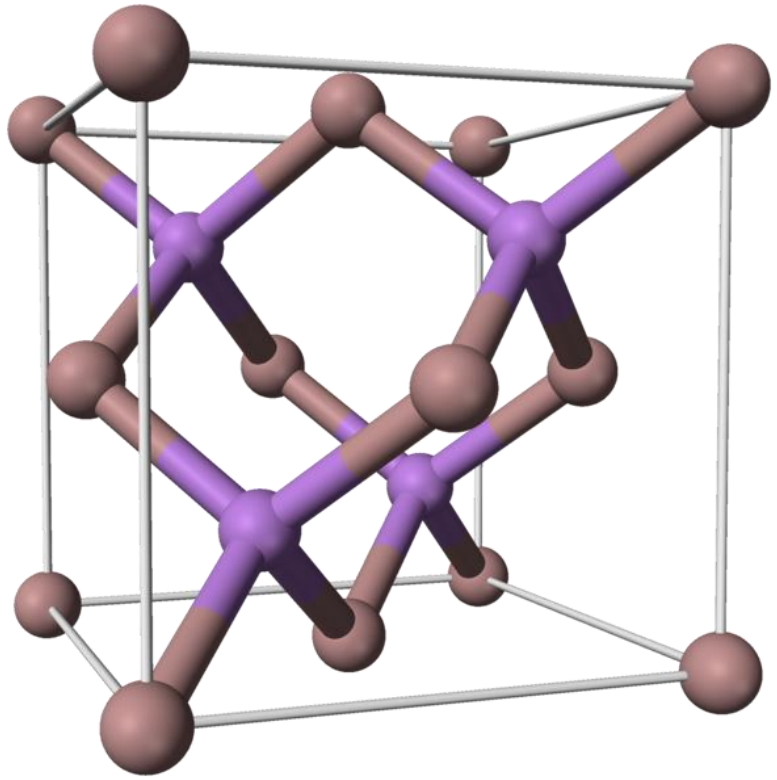
$$\Xi(\omega) = Trace[\Gamma_1 G \Gamma_2 G^T]$$

Simulation: Roadmap

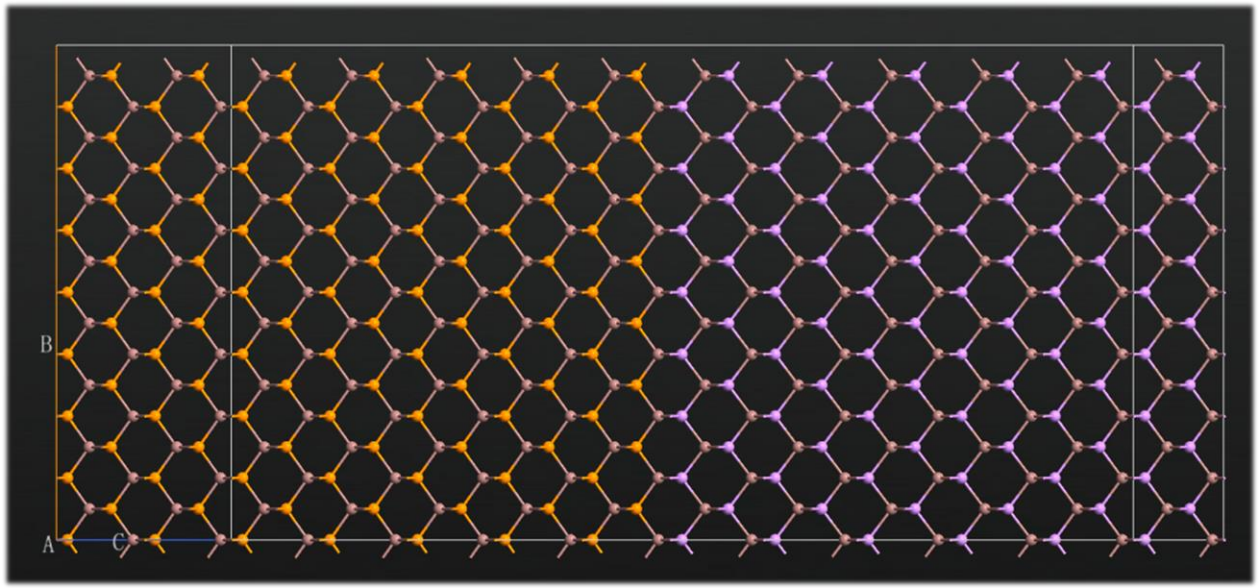
Two Inputs

1. The configuration 2. The interaction

Device: III-V semi-conductors



Zinc blende



Interface Device
(*AlP*,*AlAs*,*AlSb*,*GaP*,*GaAs*,*GaSb*,*InP*,
InAs,*InSb*)

Interaction: Tersoff-type Potential

PHYSICAL REVIEW B **75**, 115202 (2007)

Optimized Tersoff potential parameters for tetrahedrally bonded III-V semiconductors

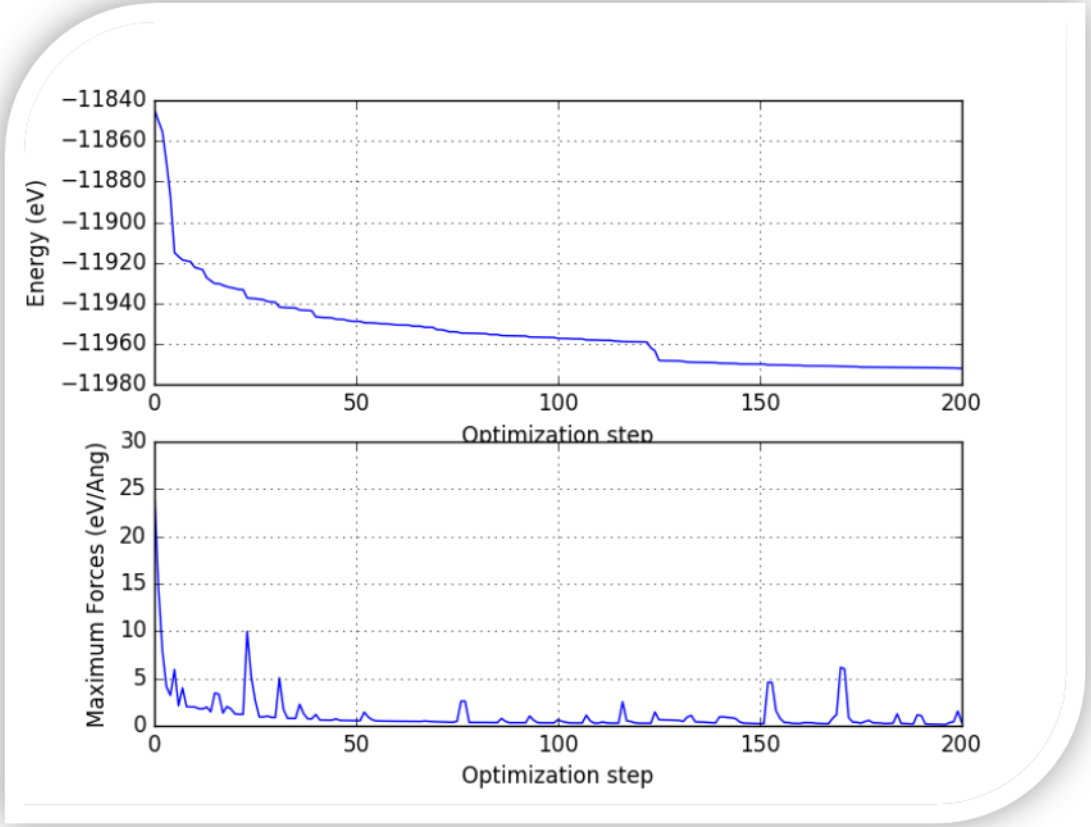
D. Powell, M. A. Migliorato, and A. G. Cullis
Department of Electronic and Electrical Engineering, University of Sheffield, Mappin Street, Sheffield, S1 3JD United Kingdom
(Received 21 November 2006; revised manuscript received 3 January 2007; published 9 March 2007)

We address the issue of accurate parametrization for the Abell-Tersoff empirical potential applied to tetrahedrally bonded semiconductor materials. Empirical potential methods for structural relaxation are widely used for group IV semiconductors while, with few notable exceptions, work on III-V materials has not been extensive. In the case of the Abell-Tersoff potential parametrizations exist only for III-As and III-N, and are designed to correctly predict only a limited number of cohesive and elastic properties. In this work we show how by fitting to a larger set of cohesive and elastic properties calculated from density functional theory, we are able to obtain parameters for III-As, III-N, III-P, and III-Sb zinc blende semiconductors, which can also correctly predict important nonlinear effects in the strain.

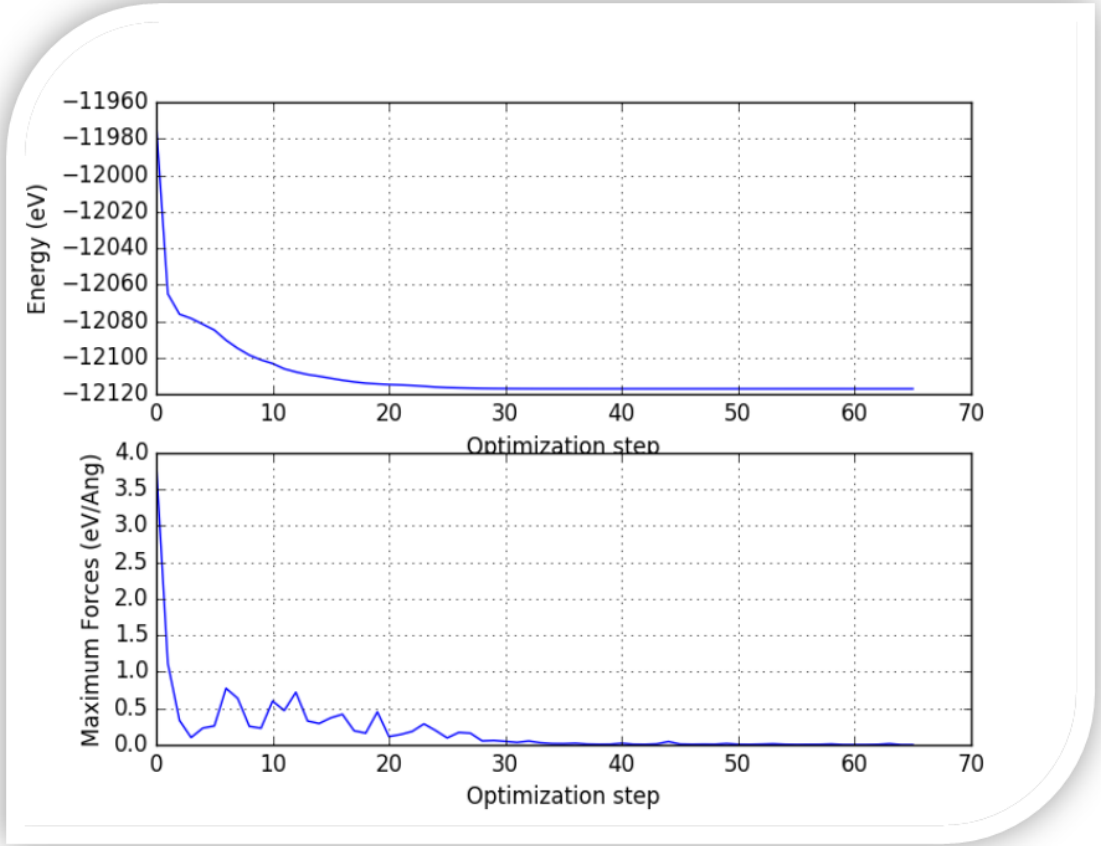
DOI: 10.1103/PhysRevB.75.115202 PACS number(s): 61.43.Bn, 61.50.Lt, 61.82.Fk, 62.40.+i

- First principle based calculation is quite costly
- This Tersoff type potential has been proved effective in many later works:
  - Phys. Rev. B 77, 235303(Quantum dots
  - Sci.Rep. 2014; 4: 7150.(Thermoelectric)
  - J. Phys.: Condens. Matter 25 425801(vibrational properties

Stress Relaxation: Two-step way

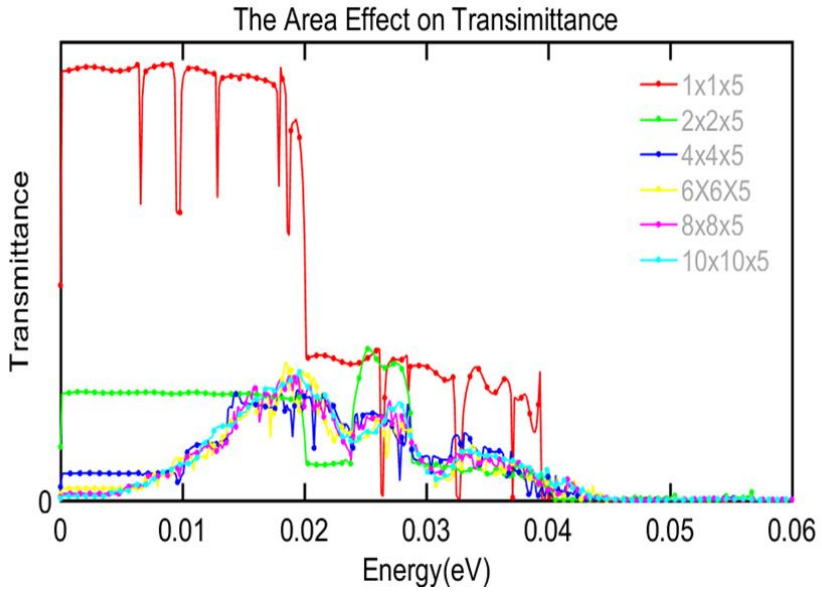


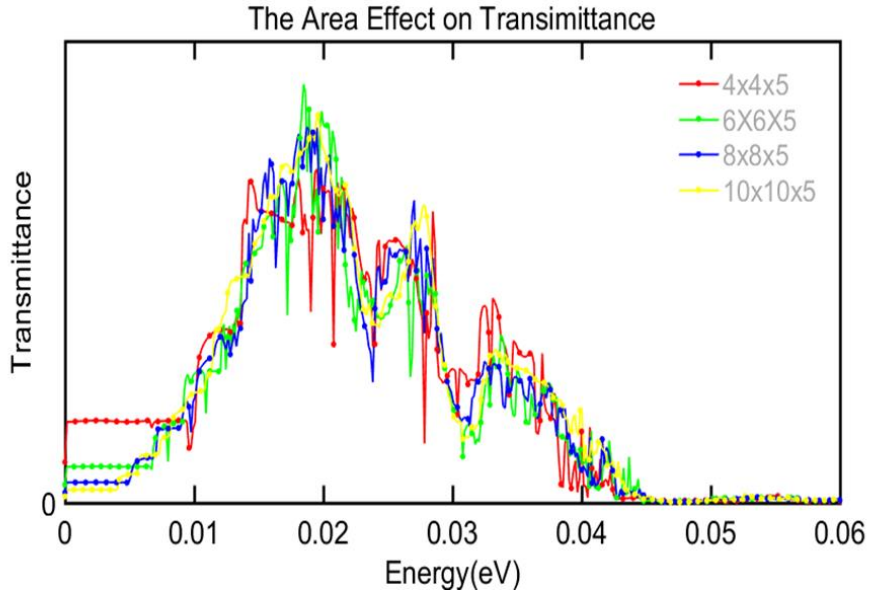
Central optimization with rigid constraints



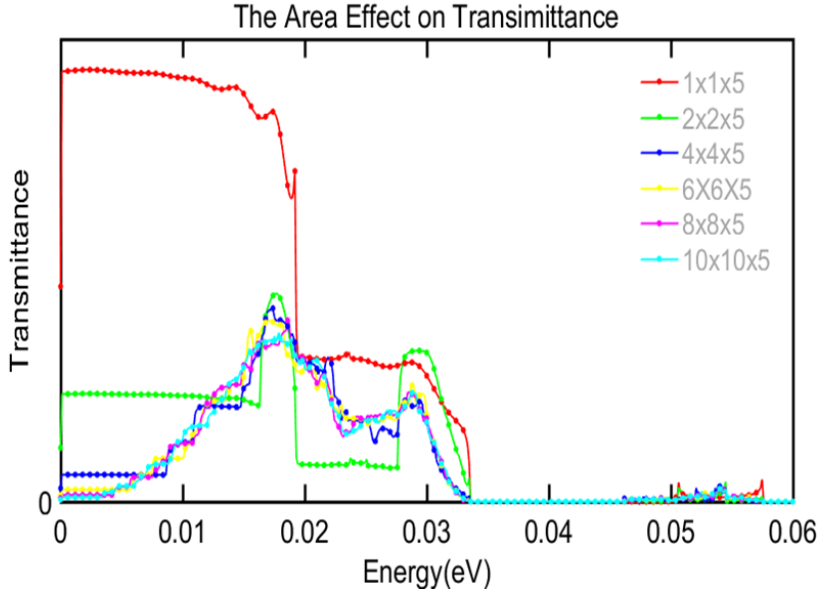
Whole device optimization

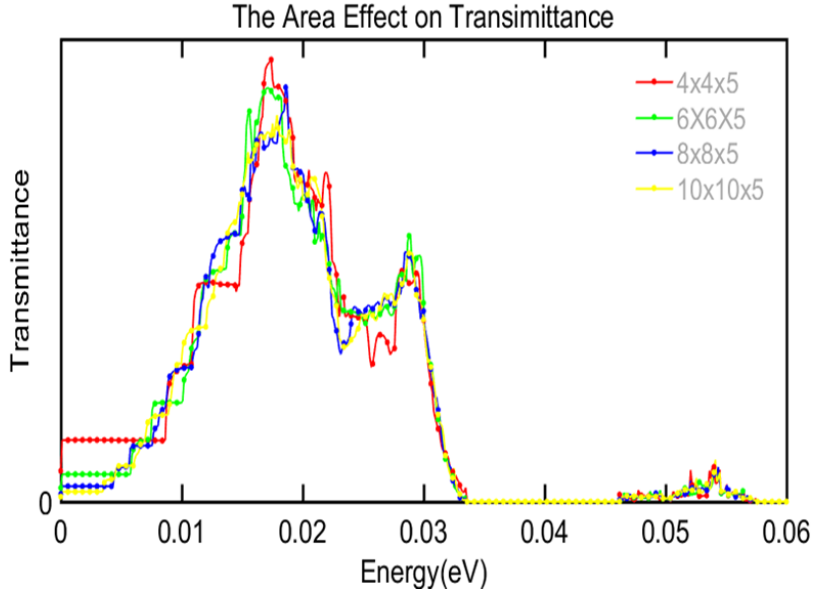
Convergence: The Area Effect





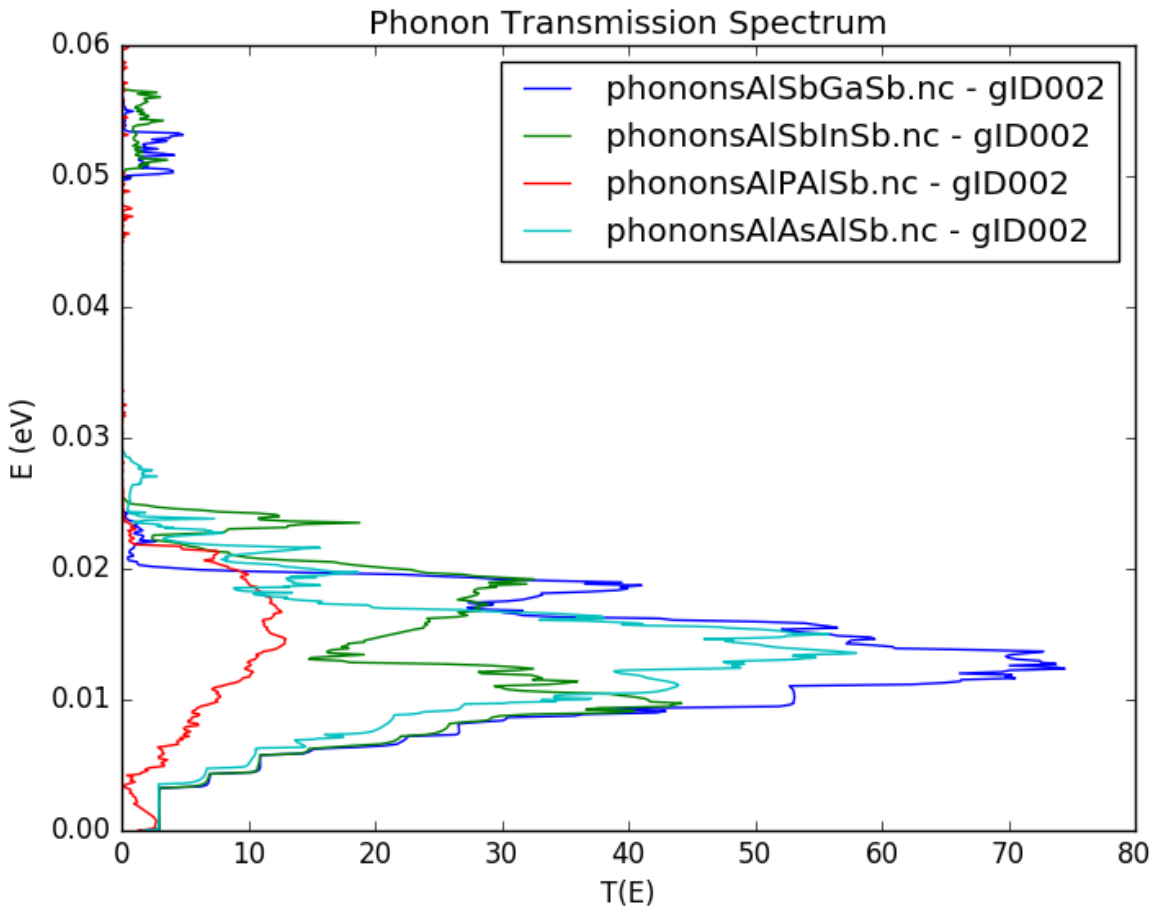
Si/Ge Interface



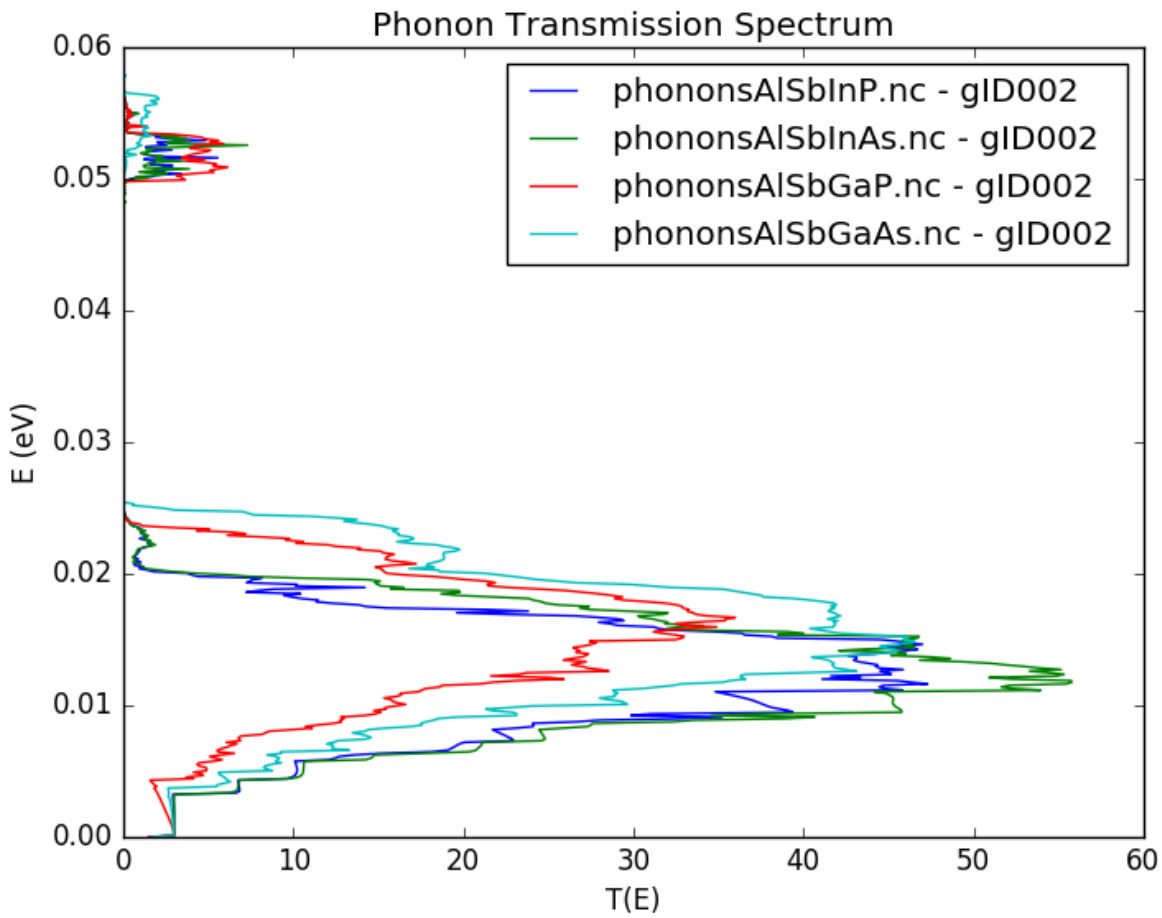


GaP/GaAs Interface

Results: Transmittance



AlSb(with one same ion)



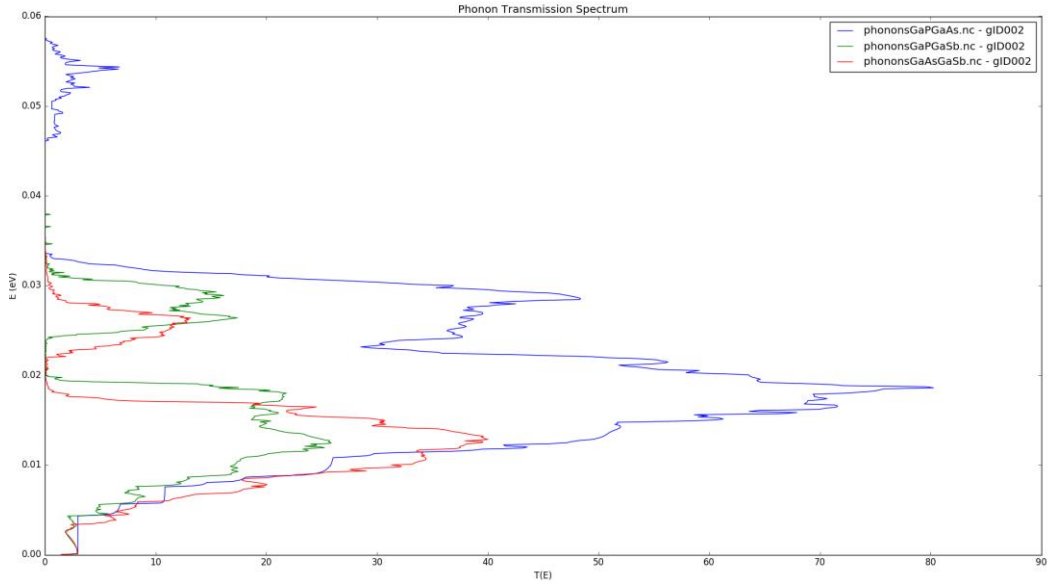
AlSb(with no same ion)

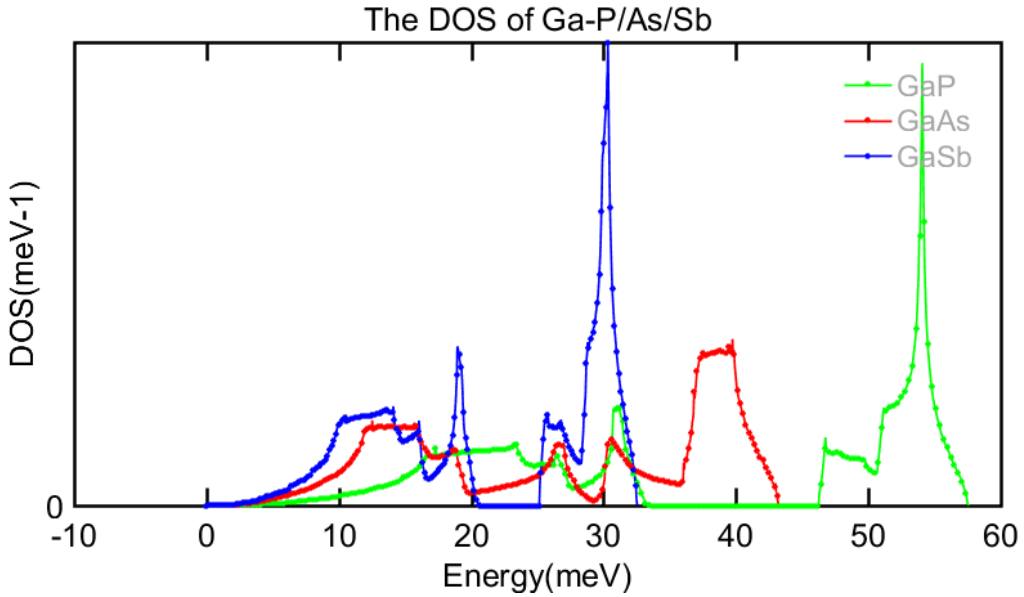
Thermal Conductance

MW/m^2k	AlAs	AlSb	GaP	GaAs	GaSb	InP	InAs	InSb
AlP	20.31	78.09	18.43	59.73	12.86	13.72	71.35	15.35
AlAs		25.43	38.05	59.65	22.34	34.55	59.65	19.31
AlSb			19.02	27.82	34.05	23.24	27.31	23.71
GaP				55.73	16.81	28.53	20.29	15.01
GaAs					19.62	42.64	30.50	21.94
GaSb						40.09	45.37	27.76
InP							43.47	18.97
InAs								28.49

Repetition: 8x8x5

Discussion: Thinking from the DOS





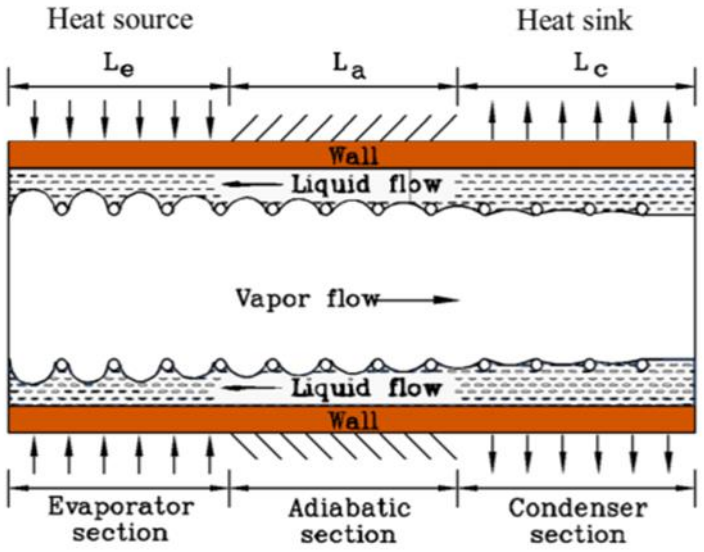
Phonon transmission across GaP/GaAs, GaP/GaSb and GaAs/GaSb

In the low frequency region, there are more similarity with GaP and GaAs in DOS, so the transmittance is large while in the high frequency region, the bigger difference in DOS caused a low transmittance.

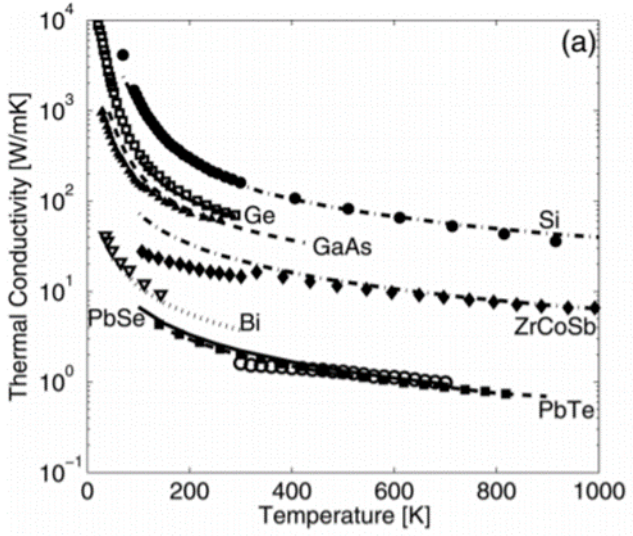
Part Three

Designing Nanostructures for Phonon Transport via Bayesian Optimization

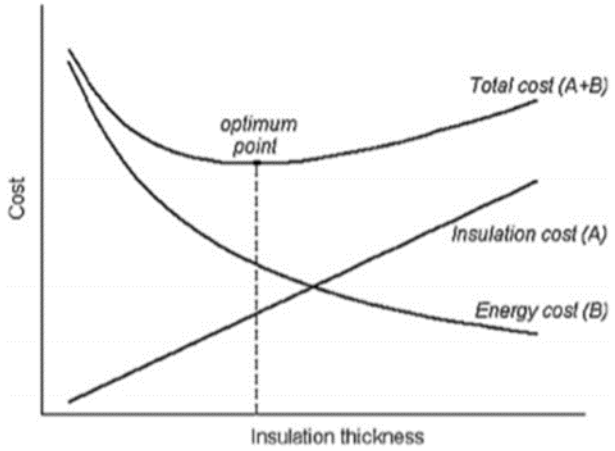
Motivation: Design the thermal properties



Heat Pipe (J.Heat Transfer 134(12), 123001)



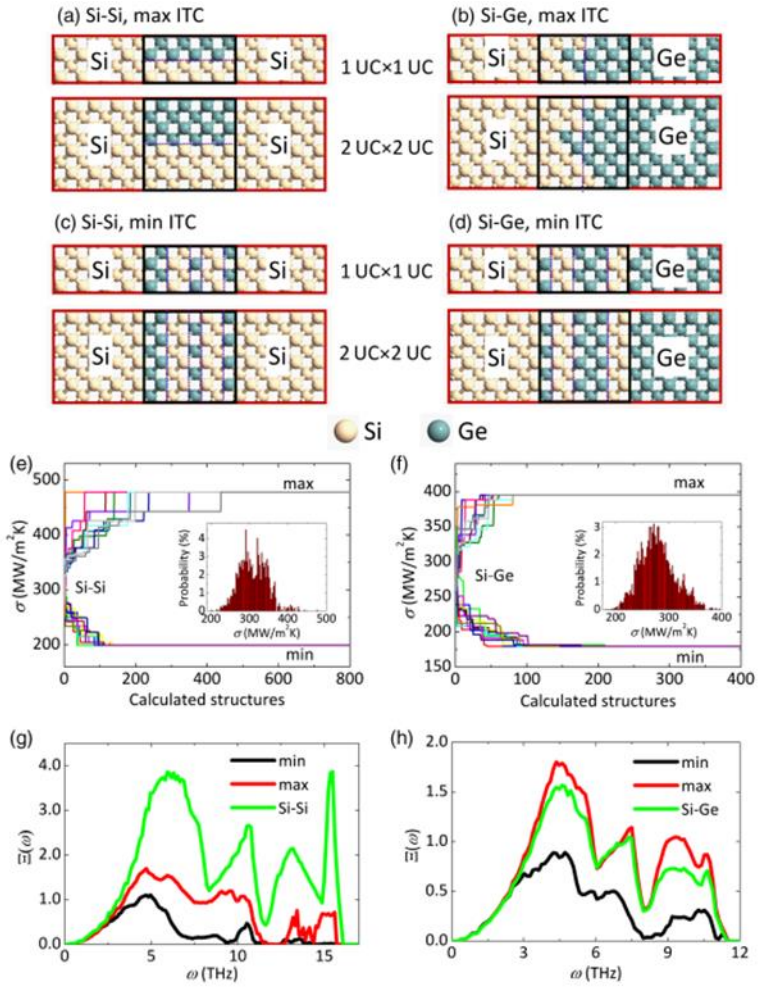
Thermoelectric Materials (J. Heat Transfer 135(6), 061605)



Thermal Insulation (Renewable and Sustainable Energy Reviews, 16(1), 415-425.)

Previous Work: Tuning the ITC

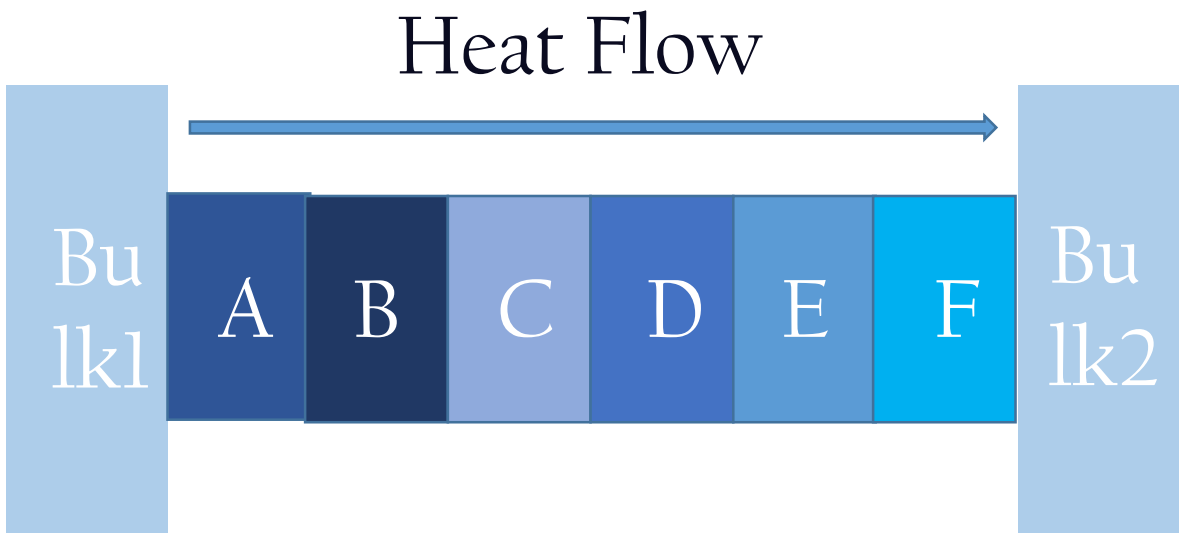
- Roughness (Phys. Rev. B 86, 235304 (2012), Phys. Rev. B 89, 054309 (2014))
- Vacancy defects (J. Chem. Phys. 142, 244703 (2015))
- Lattice orientation (J. Appl. Phys. 95, 6082 (2004), J. Appl. Phys. 113, 053513 (2013))
- Nanoinclusions (Nano Energy 13, 601 (2015))
- Interfacial adhesion or bonding (Appl. Phys. Lett. 106, 081603 (2015), ACS Appl. Mater. Interfaces 7, 23644 (2015))



Shenghong Ju(Phys. Rev. X 7, 021024)

The interfacial structure consists of either Si or Ge, and the optimization problem is how to arrange the Si and Ge atoms to obtain the largest and smallest ITC.

Material informatics: Minimum or Maximum ITC

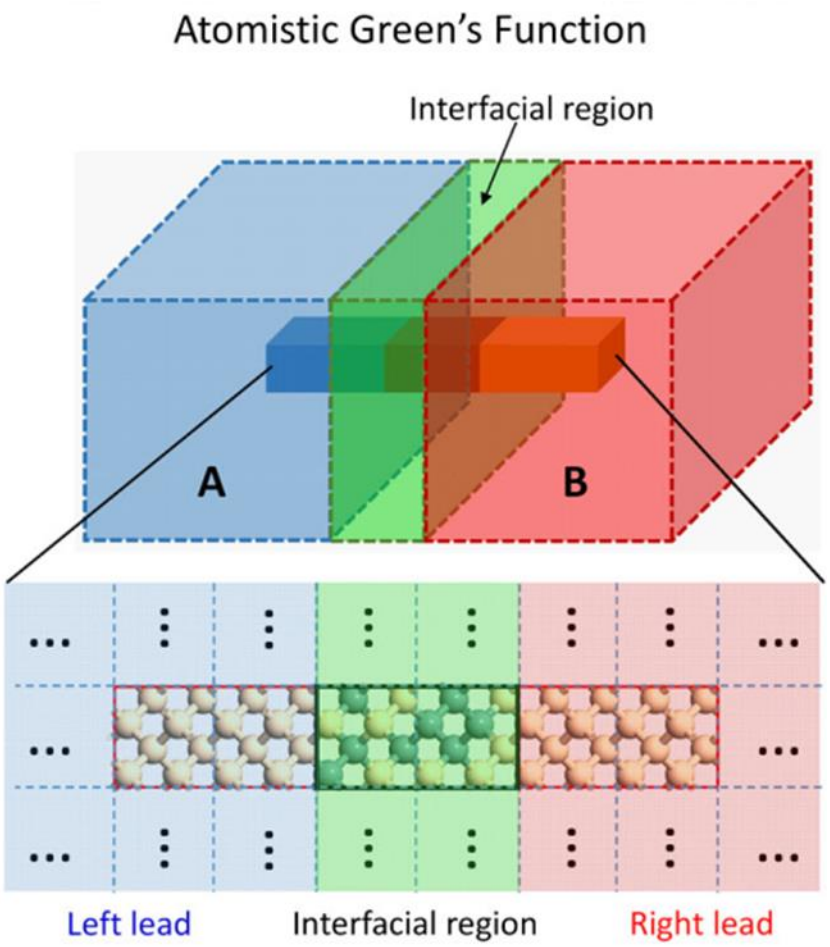


We choose four types of III-V semi-conductors:
AlP,AlAs,GaP,GaAs

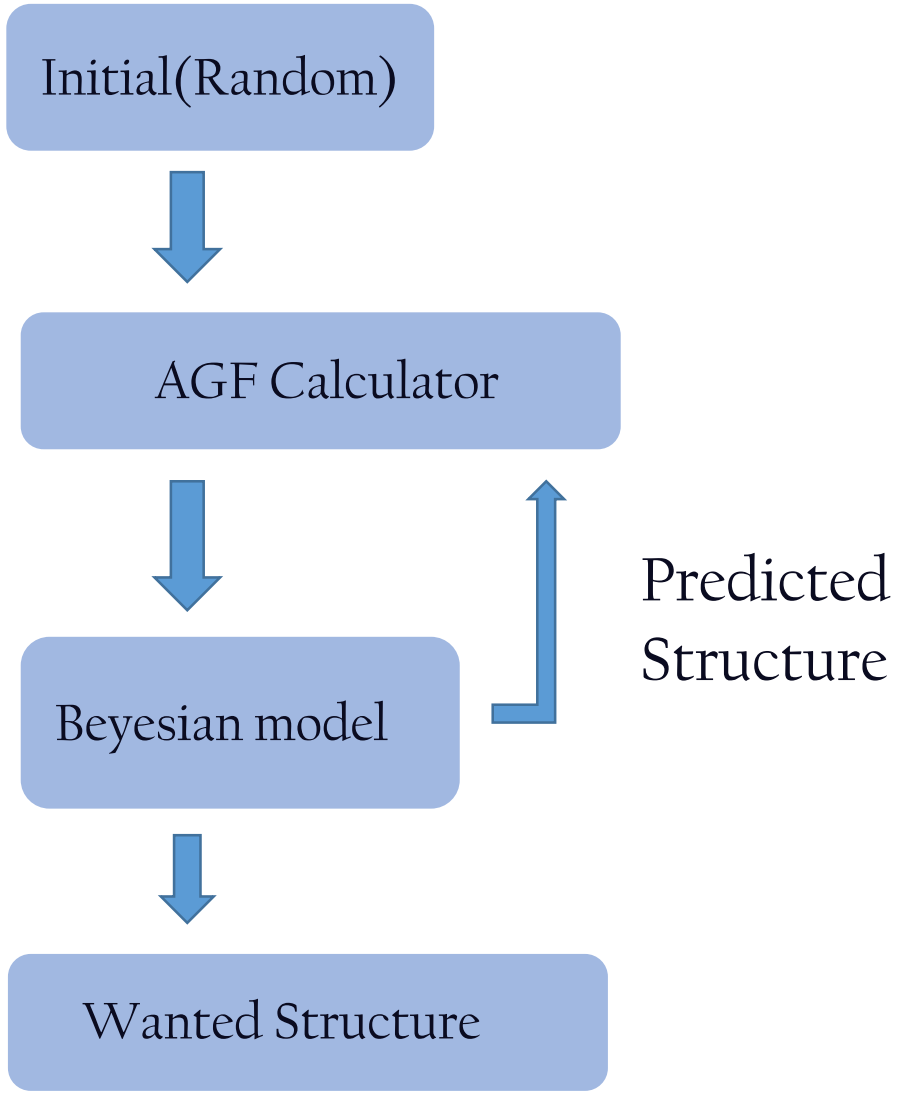
So, possible structures can be:
4^6=4096

If we calculate all the combinations, the time can be as long as 682 days!(one for about 4h with 12 cores)

Bayesian Optimization based on AGF method



Jusheng Hong Phys. Rev. X 7, 021024



Bayesian Intro: problem statement

We are interested in solving

$$x^* = argmin_x f(x)$$

Under the constraints that

- f is a black box for which no closed form is know(nor its gradients)
- f is expensive to evaluate
- And evaluations of $y = f(x)$ may be noisy

Bayesian Intro: Bayesian optimization loop

For $t = 1 : T$:

1. Given observations $(x_i, y_i = f(x_i))$ for $i = 1 : t$, build a probabilistic model for the objective f .Integrate out all possible true functions, using Gaussian process regression.
2. Optimize a cheap acquisition/utility function μ based on the posterior distribution for sampling the next point.

$$x_{t+1} = argmin_x \mu(x)$$

   Exploit uncertainty to balance exploration against exploitation.
3. Sample the next observation y_{t+1} at x_{t+1}

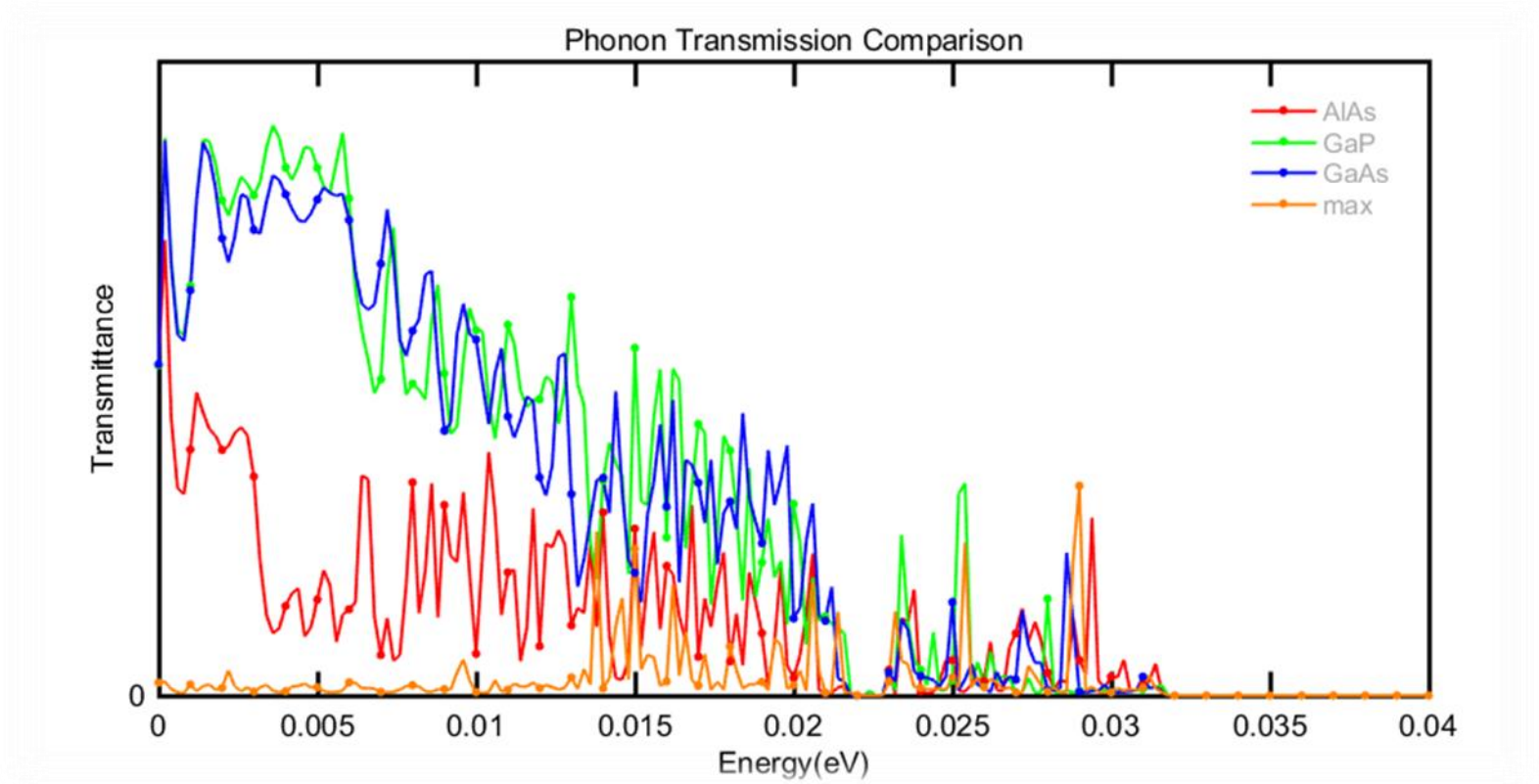
Bayesian Intro: Acquisition functions

Acquisition functions $\mu(x)$ specify which sample x should be tried next

- Expected improvement(default): $-EI(x) = -\mathcal{E}[f(x) - f(x_t^+)]$
- Lower confidence bound: $LCB(x) = \mu_{GB}(x) + \kappa\sigma_{GP}(x)$
- Probability of improvement: $-PI(x) = -P(f(x) \geq f(x_t^+) + \kappa)$

where x_t^+ is the best point observed so far.

Result: Maximum ITC



The Maximum ITC structure has an obvious lower transmittance in almost every frequency

The Maximum ITC structure we get is not Intuitive:
412314(1-AlP,2-AlAs,3-GaP,4-GaAs)

Part Four

The Conclusion and Prospects

Conclusion

In our work,

- We use the MC method to investigate the temperature profile of nano-films with internal source.
- We employ the AGF method to calculate the phonon interface transmission between III-V semi-conductors, which leaves enough data for analysis of physics.
- We combine the Beyesian Method(Machine Learning) with AGF calculation to help predict the design of structures with maximum or minimum ITC.
- Later work will focus on discovering the factors and mechanism affecting the phonon property at interface, maybe using tools like regression.

Prospect: Find out the mechanism of transmittance

Prediction of thermal boundary resistance by the machine learning method

Tianzhuo Zhan, Lei Fang & Yibin Xu

Thermal boundary resistance (TBR) is a key property for the thermal management of high power micro- and opto-electronic devices and for the development of high efficiency thermal barrier coatings and thermoelectric materials. Prediction of TBR is important for guiding the discovery of interfaces with very low or very high TBR. In this study, we report the prediction of TBR by the machine learning method. We trained machine learning models using the collected experimental TBR data as training data and materials properties that might affect TBR as descriptors. We found that the machine learning models have much better predictive accuracy than the commonly used acoustic mismatch model and diffuse mismatch model. Among the trained models, the Gaussian process regression and the support vector regression models have better predictive accuracy. Also, by comparing the prediction results using different descriptor sets, we found that the film thickness is an important descriptor in the prediction of TBR. These results indicate that machine learning is an accurate and cost-effective method for the prediction of TBR.

The descriptors used for the AMM and DMM predictions are temperature, density, speed of sound (longitudinal and transverse), and unit cell volume, which we define as "AMM and DMM descriptor.(Sci. Rep. 2017;7 ; 7109.)

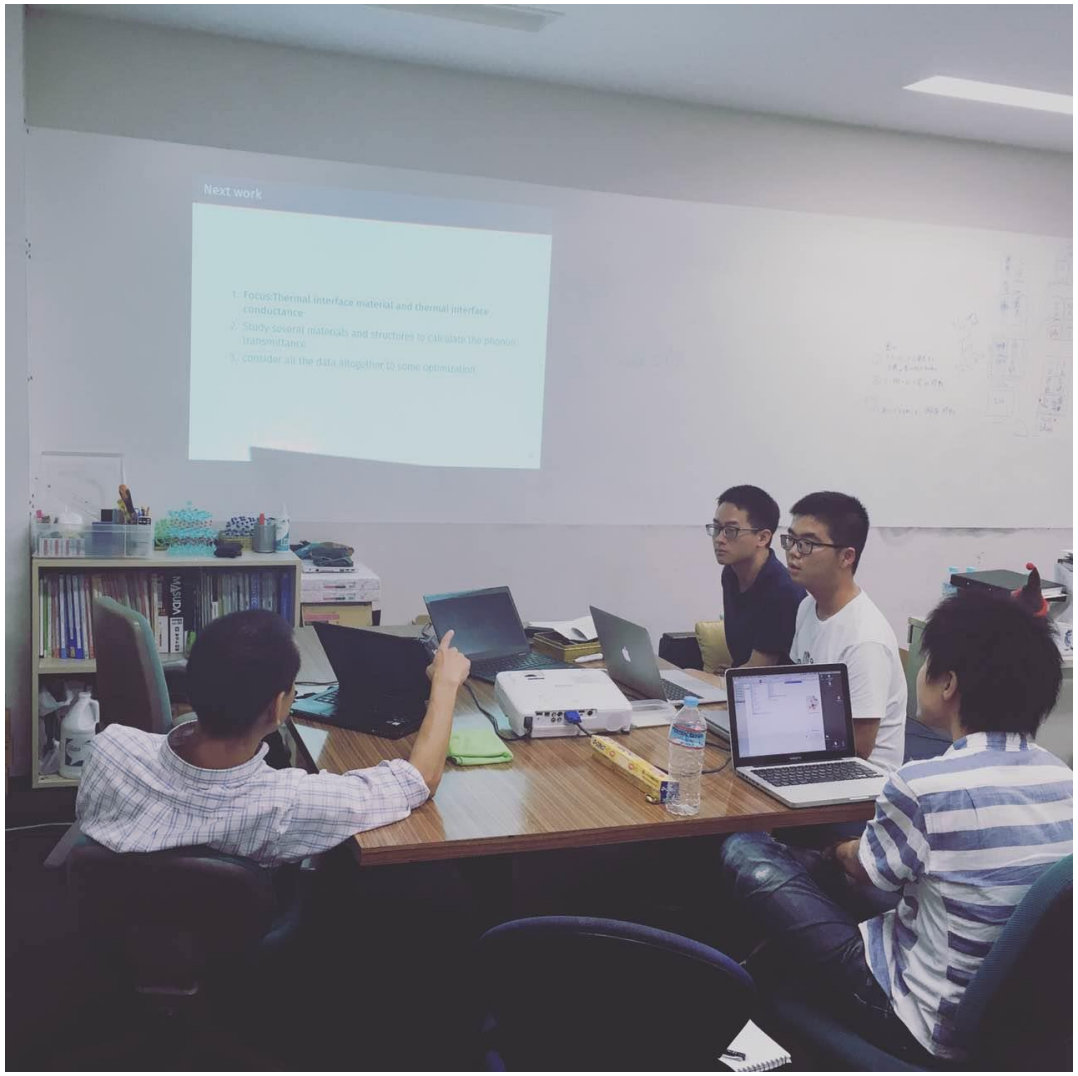
Our next step: include new factors and consider mechanism different from AMM and DMM, such as MFP.

Concluding remarks

I owe a lot to my engineering training because it [taught] me to tolerate approximations.
Previously to that I thought...one should just concentrate on exact equations all the time.
Then I got the idea that in the actual world all our equations are only approximate. We must just tend to greater and greater accuracy.
In spite of the equations being approximate, they can be beautiful.

——*Dirac*

A visit to NTNU



Summer research in University of Tokyo

Thank you!