# Electron and Phonon Transport in Multilayered Materials

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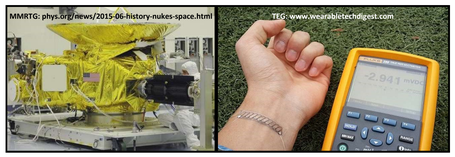
## Motivation

Thermoelectric Devices:

. Waste heat recovery
. Small size and weight
. Remote power
. Battery-free operation




*Efficiency* $\eta = \frac{\Delta T}{T_h}\frac{\sqrt{1+ZT}-1}{\sqrt{1+ZT}+\frac{T_c}{T_h}} \Leftarrow ZT = \frac{S^2\sigma}{\kappa_{el}+\kappa_{ph}}$

**Power Factor:** Electron transport

**Thermal Conductivity:** Phonon transport

Strategies to tune electron and phonon transport in multilayered Silicon/Germanium materials:

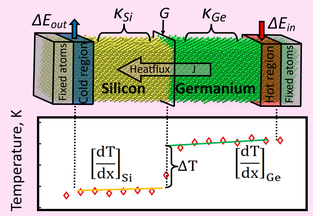
Vary layer thickness - length dependent power factor and thermal conductivity/conductance.

## Phonon Transport

### Methods

Non-Equilibrium Molecular Dynamics **(NEMD)**

. Thermal Conductivity, $\kappa$
. Interface Conductance, $G$




$$Heatflux\ [J] = \frac{1}{Area * t_{simulation}} \sum_{\#timesteps} \frac{\Delta E_{in} + \Delta E_{out}}{2}$$

$$Fourier's\ Law:\ G_{NEMD} = \frac{J}{\Delta T} \Longleftrightarrow \kappa = -\frac{J}{\left[\frac{dt}{dx}\right]}$$

Diffuse (DMM) & Acoustic Mismatch Models (DMM)

$$G^{DMM}_{Equilibrium} = \frac{3}{4} n_1 k_B \frac{c_2^2}{c_1^2+c_2^2}$$

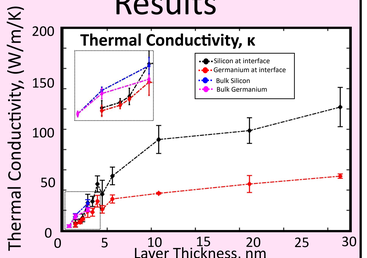
$$G^{DMM}_{Nonequilibrium} = \frac{3}{4} n_1 k_B \frac{c_2^3}{c_2^2+(c_1-c_2)^2}$$

$\mu$=cos$\theta$
$c$=speed of sound
$t_{12}$=transmission coeff.
$n$=number density

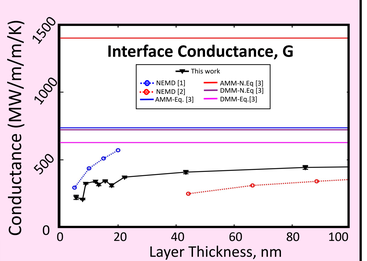
$$G^{AMM}_{Equilibrium} = \frac{3}{2} n_1 k_B c_1 \left(\frac{c_2}{c_1}\right)^3 \int_0^1 t_{12}(\mu_1)\mu_1 d\mu_1$$

$$G^{AMM}_{Nonequilibrium} = \frac{G^{AMM}_{Equilibrium}}{1-\frac{3}{2}\left(\frac{c_2}{c_1}\right)\left(\int_0^1 \mu_1^2 t_{12}(\mu_1)d\mu_1 + \frac{c_2}{c_1}\int_0^1 \mu_1\mu_2 t_{12}(\mu_1)d\mu_1\right)}$$

### Results




. Thermal conductivity increases with layer thickness until it approaches bulk value.

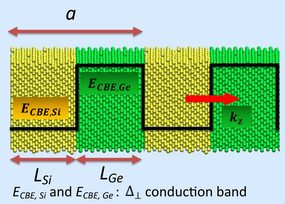



. Conductance increases with layer thickness.
. AMM and DMM overpredict conductance.

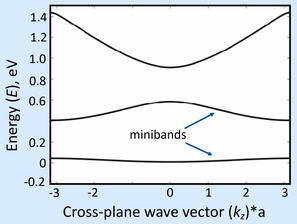
## Electron Transport

### Kronig-Penney (KP) Model for Si/Ge Superlattices

Superlattices are periodic multilayered materials and KP model can be used to predict their electronic dispersion relations/band structures.




$E_{CBE,\ Si}$ and $E_{CBE,\ Ge}$: $\Delta_\perp$ conduction band edges of Si and Ge, respectively.

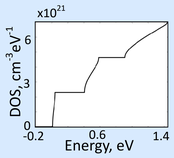



**KP band structure**

$E_{ni}$ : Energy of i$^{th}$ band at n$^{th}$ wave vector ($k_z$) point, $k_{zn}$ .

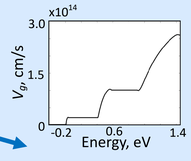
$V_{g,ni}$ : Group velocity of i$^{th}$ band at n$^{th}$ wave vector ($k_z$) point.

$$v_{g,ni} = \frac{1}{\hbar}\frac{\partial E_{ni}}{\partial k_{zn}}$$




KP Model

Electronic Band Structures




Density of States (DOS)

$$\rho_{DOS}(E) = \frac{m^*}{\pi^2\hbar^2} k_z, extendedzone$$

Group Velocities

$$v_g^2(E) = \frac{\sum_n \sum_i v_{g,ni}^2 u(E-E_{ni})}{\sum_n \sum_i u(E-E_{ni})}$$

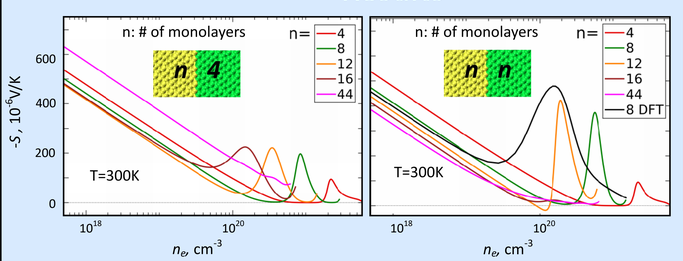
Boltzmann Transport Equation

Cross-plane Seebeck ($S$) coefficient computation

$$S = \frac{1}{eT}\frac{\int_0^\infty e^2\tau(E)v_g^2(E)\rho_{DOS}(E)\left(-\frac{\partial f_0}{\partial E}\right)(E-E_F)dE}{\int_0^\infty e^2(E)\tau(E)v_g^2(E)\rho_{DOS}(E)\left(-\frac{\partial f_0}{\partial E}\right)dE}$$

$\tau(E)$ is the relaxation time , $E_F$ is the Fermi level, and $F_0(E) = 1/(1+\exp((E-E_F)/k_BT))$ is the Fermi-Dirac distribution function.

### Results




. Seebeck coefficient peaks due to sharp increase in DOS and is oscillatory.

. Seebeck ($S$) computed with KP model compares in order of magnitude with DFT results.
. $S$ peak moves leftwards with increase in length and approaches bulk behavior at higher lengths.

## Electron-Phonon Coupling

### Methods

Quantum Espresso
. Electron calculations
. Phonon calculations

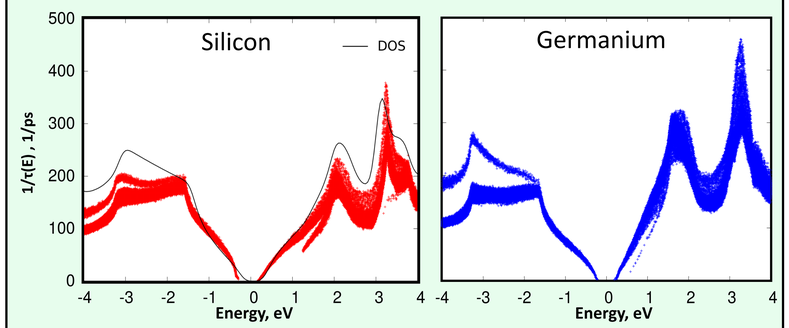
⇨ EPW
. Calculation of electron-phonon coupling

Electron-Phonon matrix elements

$$g^{\nu}_{mn}(\mathbf{k},\mathbf{q}) = \langle \psi_{m\mathbf{k}+\mathbf{q}} | \partial_{\mathbf{q}\nu} V | \psi_{n\mathbf{k}} \rangle$$

Bloch Representation (coarse grid) ⇔ Speed Up ⇔ Wannier Representation (truncation)

### Results




. Computationally expensive - calculations can only be done for small unit cells.
. Dense mesh is required for convergence.
. τ(E) is important for correct electron transport predictions.

## Conclusion

. Thermal conductivity and interface conductance increase with increasing layer thickness - MD improves prediction over AMM & DMM for nanostructures.
. The miniband formation in superlattices (SL) is responsible for sharp changes in DOS which give rise to the peaks in Seebeck coefficient ($S$).
. $S$ shows the highest peak at n=3 monolayers for SiGe superlattices studied and approaches bulk behavior with increase in # of layers.
. Prediction of τ is important for improving the level of approximation for electron transport calculations, and therefore, predicting thermoelectric efficiency.

[1] Samvedi, V. and Tomar, V., *Nanotechnology*, **20**, 365701 (2009), [2] Landry, E. S. and McGaughey, A. J. H., *Phys. Rev. B.*, **80**, 165304 (2009), [3] Merabia, S., *Phys. Rev. B.*, **86,** 094303 (2012), [4] Bahk, Je-Hyeong, et al. *Journal of electronic materials* ,**41.6,** 1498-1503,(2012).

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