A BEYOND FOURIER SEMI-ANALYTICAL THERMAL MODEL BASED ON TWO-FLUX APPROACH

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Non-Fourier heat transfer at the nanoscale

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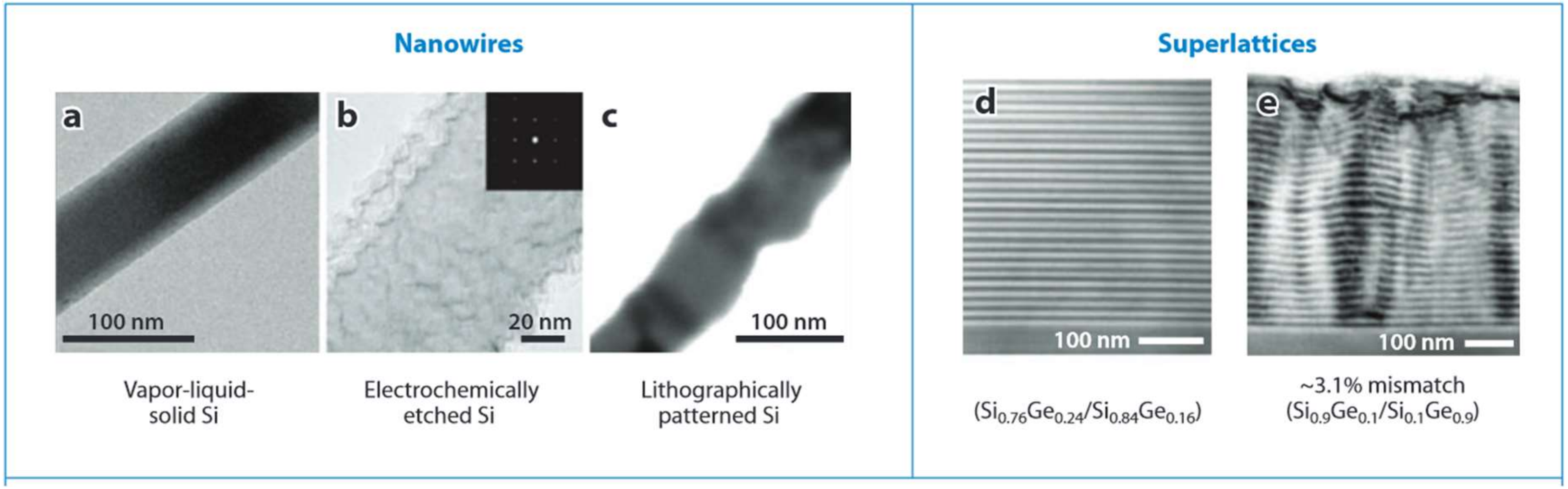
Heat transfer in nanostructures



Modeling heat transport at the nanoscale: L < mfp of phonon

→ **Interfaces and out of equilibrium transport**

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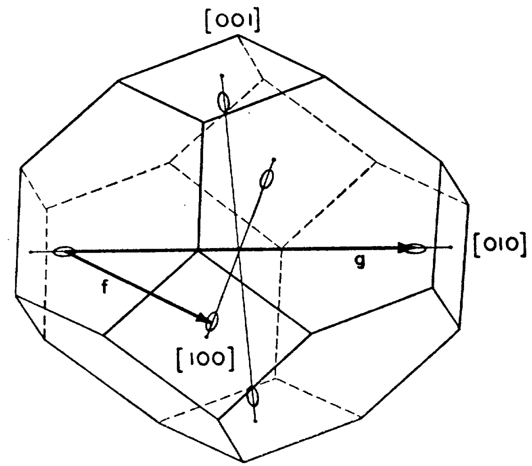
Home made DFT based ab-initio based Full-Band Monte Carlo simulator



- Full-band description of (30x30x30 3D k-space):
- Phonon dispersions:
  - From DFT
- Phonon-phonon scattering rates:
  - From DFT
- Advantages
  - Anisotropic properties captured
  - Scattering mechanisms describe at the particle level
  - Interface: reflection and transmission from atomistic approaches
  - Non equilibrium distribution
  - Complex geometry from nm to µm scale

(Davier, JPCM 2018)

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Particle scattering at semi-transparent interface

- Specular reflection/transmission

- **Diffusive reflection/transmission**

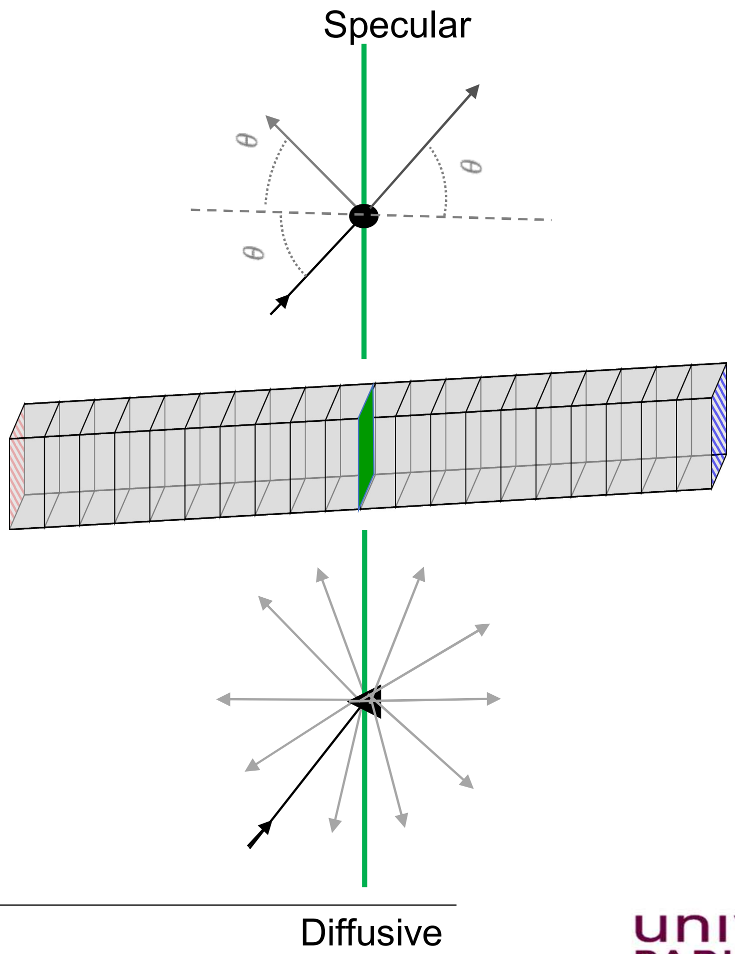
-Transmission probability via DMM

Cf. Larroque, JAP 123, 2 (2018): $t_{A\rightarrow B}(\omega) = \dfrac{I^B(\omega)}{I^A(\omega) + I^B(\omega)}$

- Final angle randomized

- **Conservations of**

- Phonon angular frequency
- Parallel heat flux



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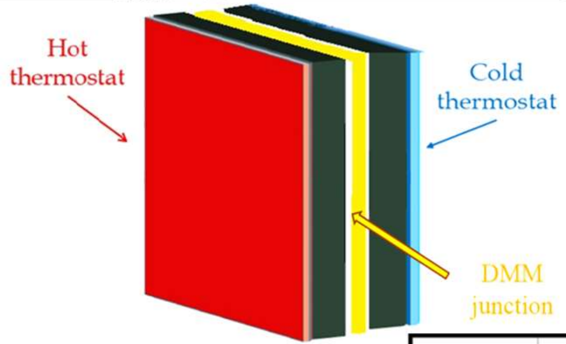
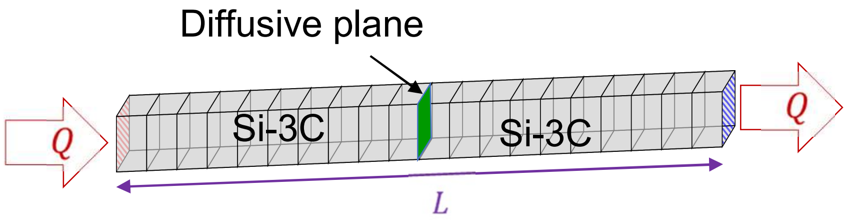
Thermal conductivity in short system??

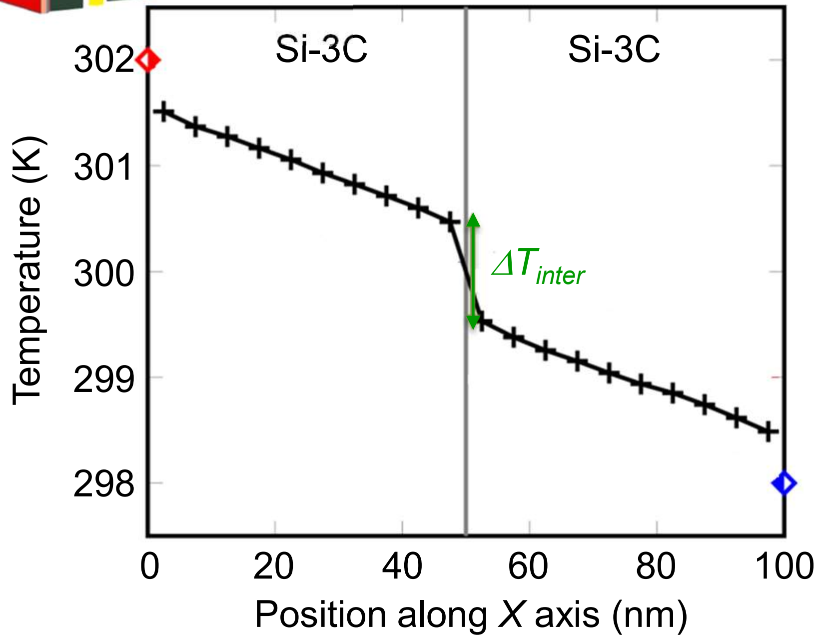




Semi-transparent interface: $t(\omega) = \frac{1}{2}$

→ Linear decrease of *T* along the distance

→ Drop of *T* at contacts and interface



Thermal conductivity of one side

$\kappa_{th} = Q/gradT$

Q = heat flux density

ΔT_{inter} = temperature offset at interface

In short device: $gradT \rightarrow 0$, $\kappa_{th} \rightarrow \infty > \kappa_{ballistic}$!!

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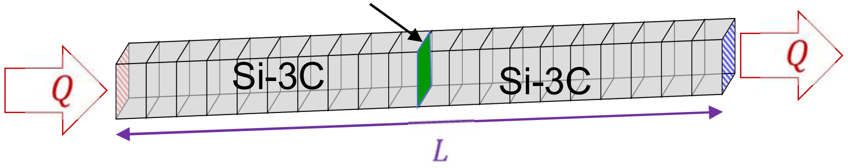
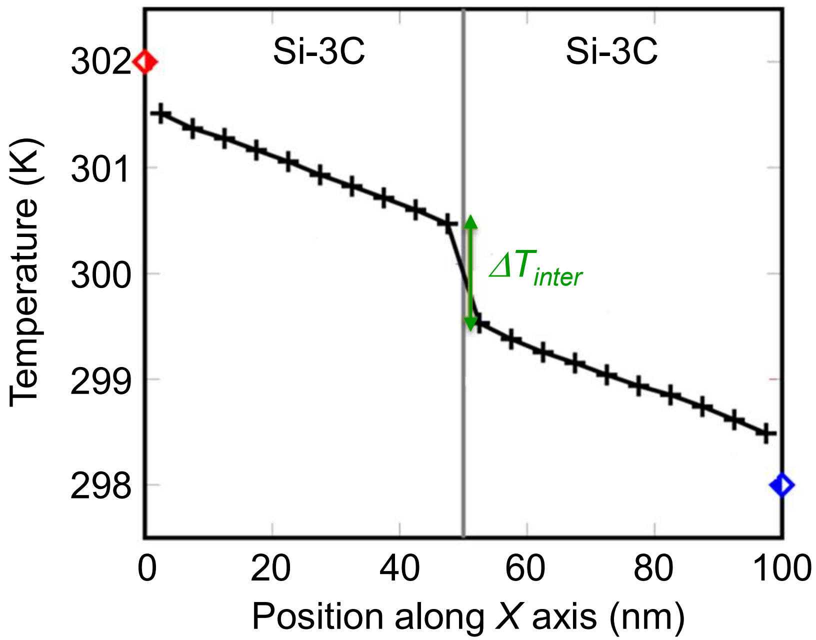
Interface conductance in a cross plane homo-junction





Semi-transparent interface: $t(\omega) = \frac{1}{2}$

→ Linear decrease of *T* along the distance

→ Drop of *T* at contacts and interface

Interface thermal conductance:

$$G = \frac{Q}{\Delta T_{inter}}$$

Q = heat flux

ΔT_{inter} = temperature offset at interface

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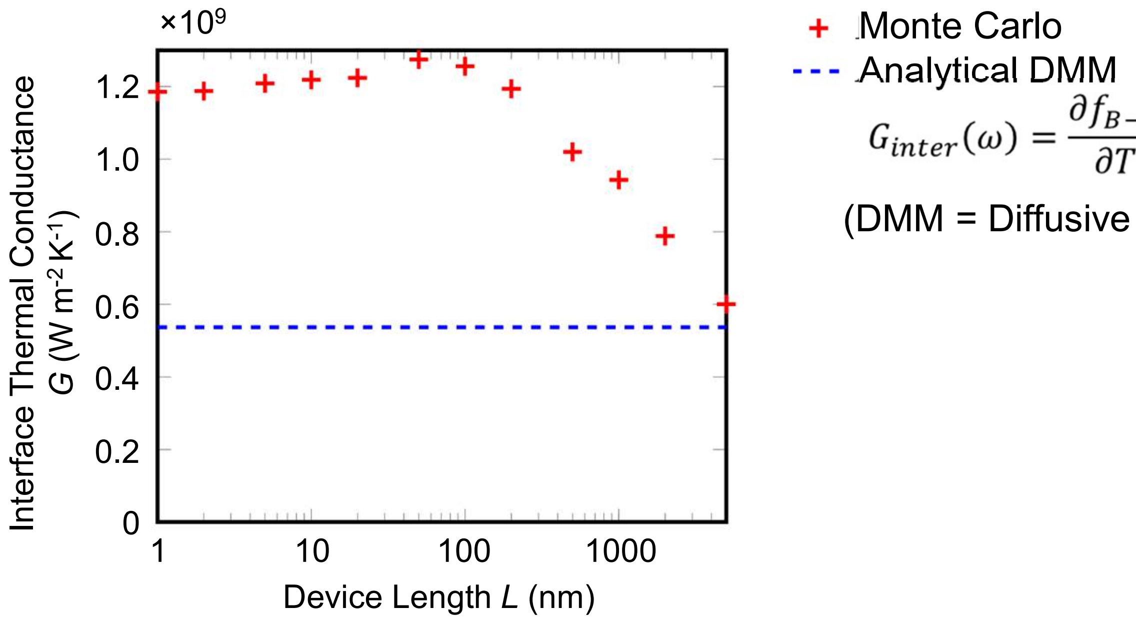
Temperature in a homo-junction – Interface conductance (2)



$$G_{inter}(\omega) = \frac{\partial f_{B-E}}{\partial T}(\omega, T_{eq}) I_A(\omega)\, t_{A\to B}(\omega)$$

(DMM = Diffusive Mismatch Model)

→ MC and analytical DMM results are different in ballistic and intermediate regimes

→ MC gives an unexpected length-dependence of *G*

➔ *Not consistent !!!*

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Short version of a long story: “Thermal Boundary Resistance”

Swartz, E. T., et R. O. Pohl. *Reviews of Modern Physics* 61, nº 3 (1989)

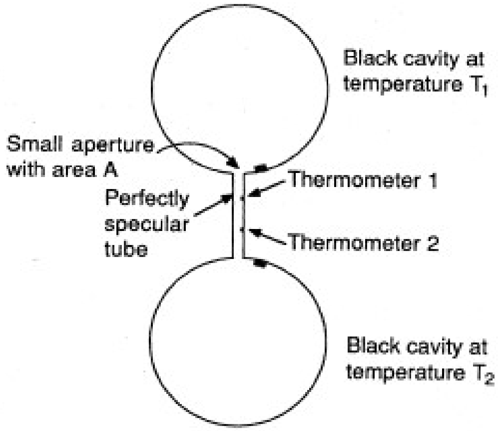


FIG. 8. Blackbody cavities separated by a perfectly specular tube. The placement of the thermometers shown is faulty; ideal thermometers would measure a zero ΔT. If the ideal thermom-

… The fundamental property of an interface is the thermal boundary conductivity, which is defined, as above, as the ratio of the heat flux across an interface per unit area to the temperature difference between the distributions of phonons *incident* on the two sides of an interface.

$$G = \frac{Q}{\Delta T_{inter}}$$

Q = heat flux density

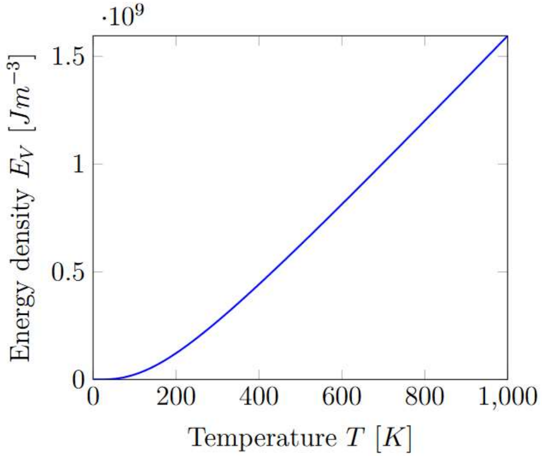
ΔT_{inter} = temperature offset at interface

While the problem of merely defining the temperature on either side of an interface is nontrivial, the problem of experimentally measuring that temperature without the thermometer's affecting that temperature is even more challenging. …

- Defining a temperature near an interface (out of equilibrium) is an (theoretical and experimental) issue
- Different models and pseudo local temperatures have been defined in the literature :

Little, W. A. *Can. J. Phys* 37, 49 (1959)
Simons, S. *Journal of Physics C: Solid State Physics* 7, 22 (1974)
Chen, G. *Physical Review B* 57, 23 (1998), …

Monte Carlo simulation and temperature of incident phonons



- Given the local energy density *E*,

the « standard » pseudo temperature *T* is defined by :

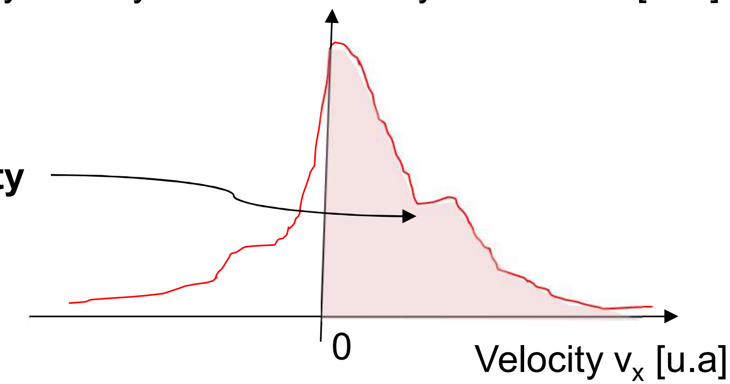
$$E(T) = \frac{V_s}{(2\pi)^3} \sum_s \hbar\omega_s f_{BE}(\omega_s, T)$$

- Considering heat flux density *Q* instead of energy density

$$Q(T) = \frac{V_s}{(2\pi)^3} \sum_s \hbar\omega_s \, |v_s| \, f_{BE}(\omega_s, T)$$

- Considering only **phonon with positive velocity**

$$Q^+(T^+) = \frac{V_s}{(2\pi)^3} \sum_{\substack{s \\ v_s > 0}} \hbar\omega_s \, |v_s| \, f_{BE}(\omega_s, T^+)$$



Definitions of pseudo T, T^+ and T^-

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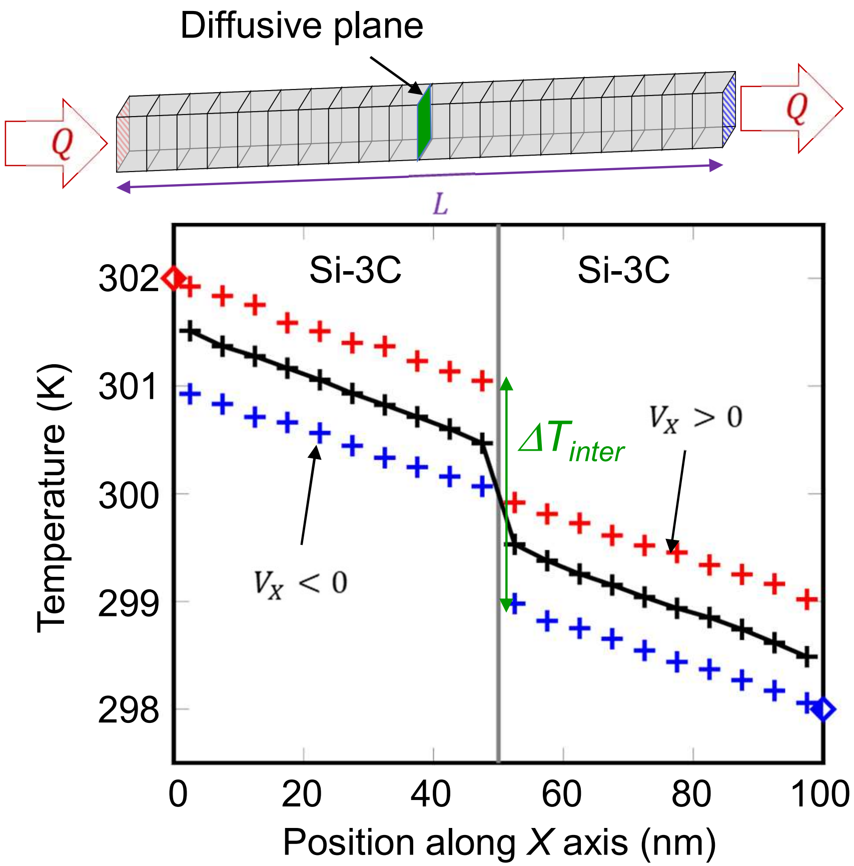
TemperatureS in a homo-junction



Semi-transparent interface: $t(\omega) = \frac{1}{2}$

☞ **We must consider the appropriate population of phonons to extract the temperature on both sides**

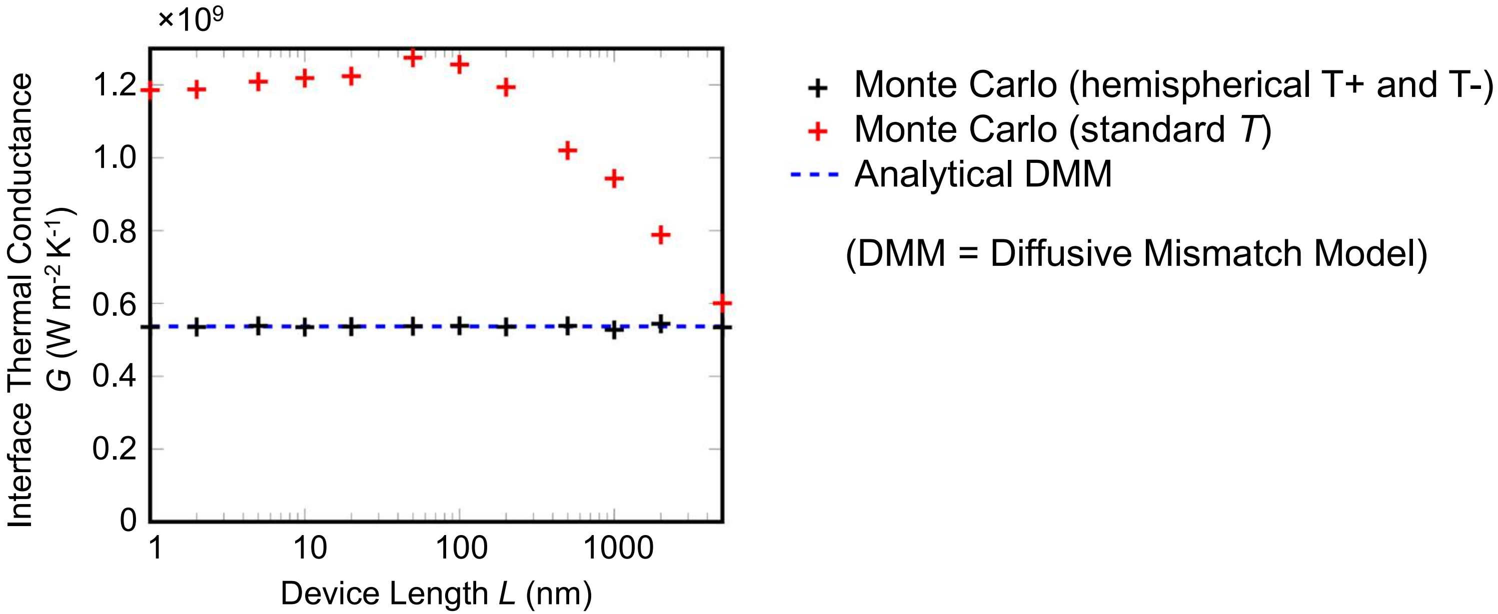
Interface thermal conductance:

$$G = \frac{Q}{\Delta T_{inter}}$$

Q = heat flux density

ΔT_{inter} = temperature offset at interface

Temperature in a homo-junction – Interface conductance



(DMM = Diffusive Mismatch Model)

→ Good agreement between MC and DMM results

→ Conductance independent of length

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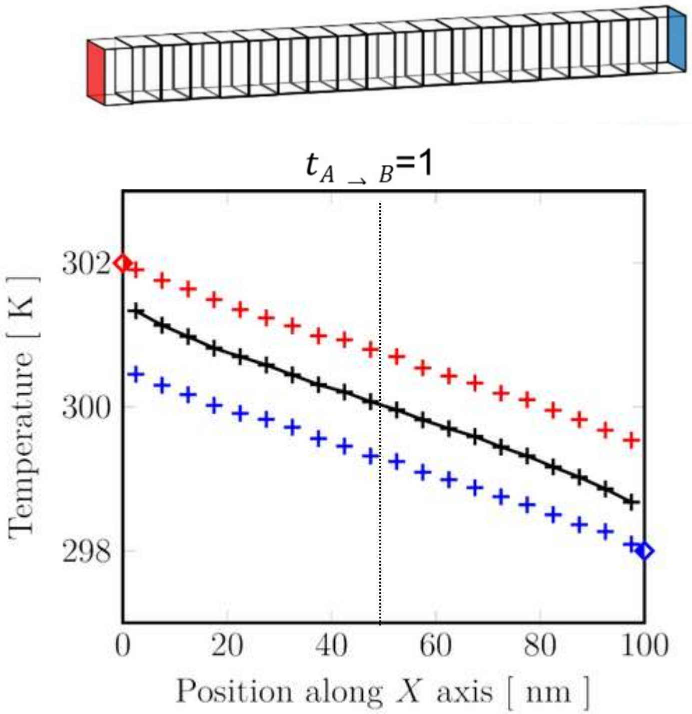
Extreme cases: **virtual interface**



- The **classical virtual interface paradox**
  → infinite ITC for an imaginary interface in the same material > ballistic case

→ No interface?

$Q=G_{inter}(T^+-T^-)$

$$Q = \frac{S}{L}\left(T^+ - T^-\right)\kappa_{\text{ballistic}} = \Delta T_{\text{local}}\, G_{\text{ballistic}}$$

→ It gives a **link between T, T^+ and T^-**

$$Q = \Delta T_{local}.G_{ballistic} = S.\kappa_{diffusive}.\frac{dT}{dx}.$$

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3 New thermal parameters

Size dependent conductivity

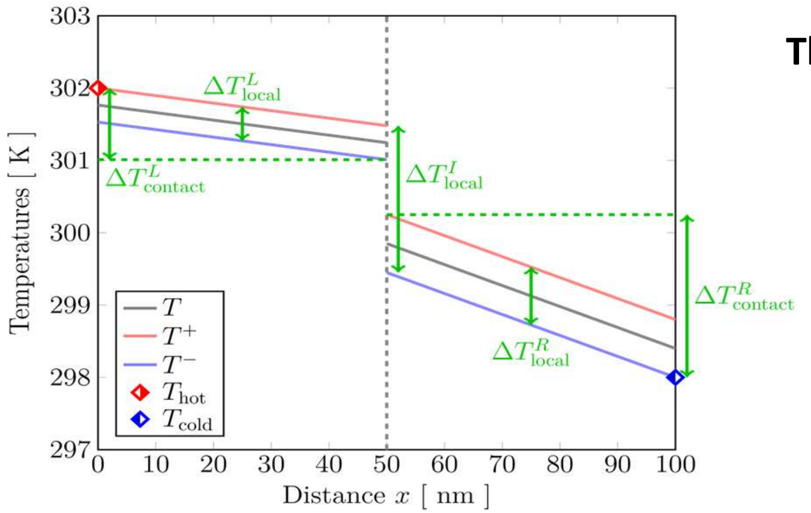
$$Q = \kappa_{\text{effective}} \frac{\Delta T_{\text{contacts}}}{L} \quad \text{with } \Delta T_{contacts} = T^+(0) - T^-(L)$$

New interface conductivity

$$G_{Inter} = Q.\Delta T_{\text{local}}{}^{I} \quad \text{with } \Delta T^{I}_{\text{local}} = T^+(x^I - \epsilon) - T^-(x^I + \epsilon)$$

Ballistic conductivity
(only material dependent)

$$\kappa_{\text{ballistic}} = \frac{\Omega}{(2\pi)^3} \sum_s \hbar\omega_s \left|v_{s,x}\right| \frac{L}{2} \frac{\partial f_{\text{BE}}}{\partial T}(\omega_s, \bar{T}) = L\, G_{\text{ballistic}}$$



This work: *(IJMHT, Davier, 2022)*

$$Q = \frac{\kappa^{L/R}_{\text{effective}}}{L^{L/R}} \Delta T^{L/R}_{\text{contact}} = G^I.\Delta T^I = \boldsymbol{G^{L/R}_{ballistic}}.\boldsymbol{\Delta T^{L/R}_{local}}$$

$$Q_{\text{th}} \left[\frac{L^L}{S.\kappa^L} - \frac{1}{G^L_{\text{ballistic}}} + \frac{1}{G_{inter}} + \frac{L^R}{S.\kappa^R} - \frac{1}{G^R_{\text{ballistic}}} \right] = \Delta T$$

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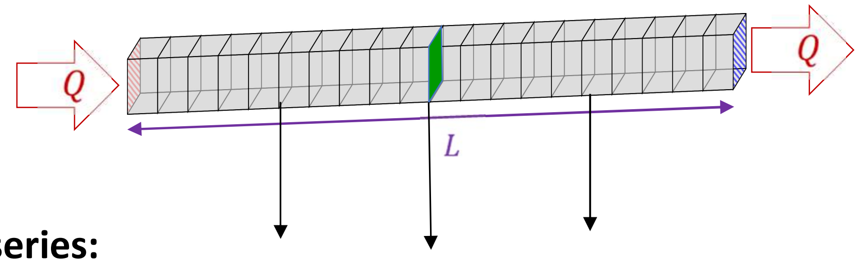
Application in analytical modeling: Standard vs. New approaches



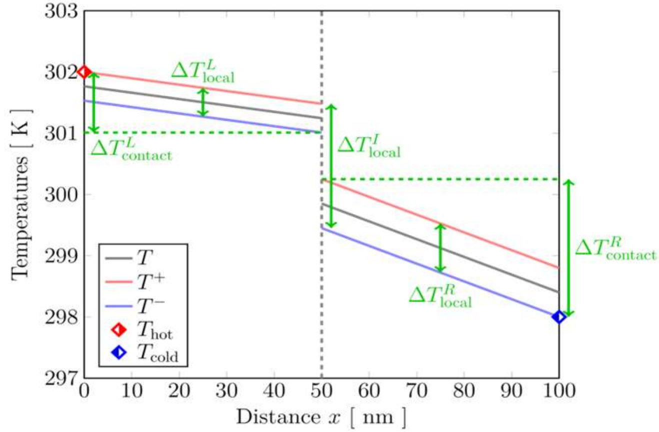
3 resistances in series:

$$Q_{\text{th,"diffusive"}} \left[\frac{L^L}{S.\kappa^L_{\text{diffusive}}} + \frac{1}{G_{inter}} + \frac{L^R}{S.\kappa^R_{\text{diffusive}}} \right] = \Delta T$$

This work: *(IJMHT, Davier, 2021)*

$$Q = \frac{\kappa^{L/R}_{\text{effective}}}{L^{L/R}} \Delta T^{L/R}_{\text{contact}} = G^I . \Delta T^I = G^{L/R}_{\text{ballistic}} . \Delta T^{L/R}_{\text{local}}$$

$$Q_{\text{th}} \left[\frac{L^L}{S.\kappa^L} - \frac{1}{G^L_{\text{ballistic}}} + \frac{1}{G_{inter}} + \frac{L^R}{S.\kappa^R} - \frac{1}{G^R_{\text{ballistic}}} \right] = \Delta T$$



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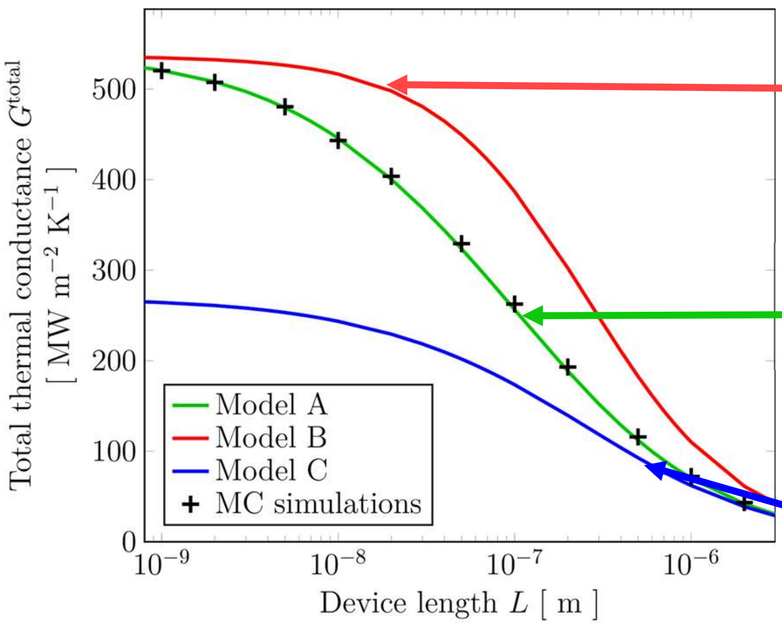
Homojunction



$$Q_{th,"diffusive"}\left[\frac{L^L}{S.\kappa^L_{diffusive}}+\frac{1}{G_{inter}}+\frac{L^R}{S.\kappa^R_{diffusive}}\right]=\Delta T$$

$$Q_{th}\left[\frac{L^L}{S.\kappa^L}-\frac{1}{G^L_{ballistic}}+\frac{1}{G_{inter}}+\frac{L^R}{S.\kappa^R}-\frac{1}{G^R_{ballistic}}\right]=\Delta T$$

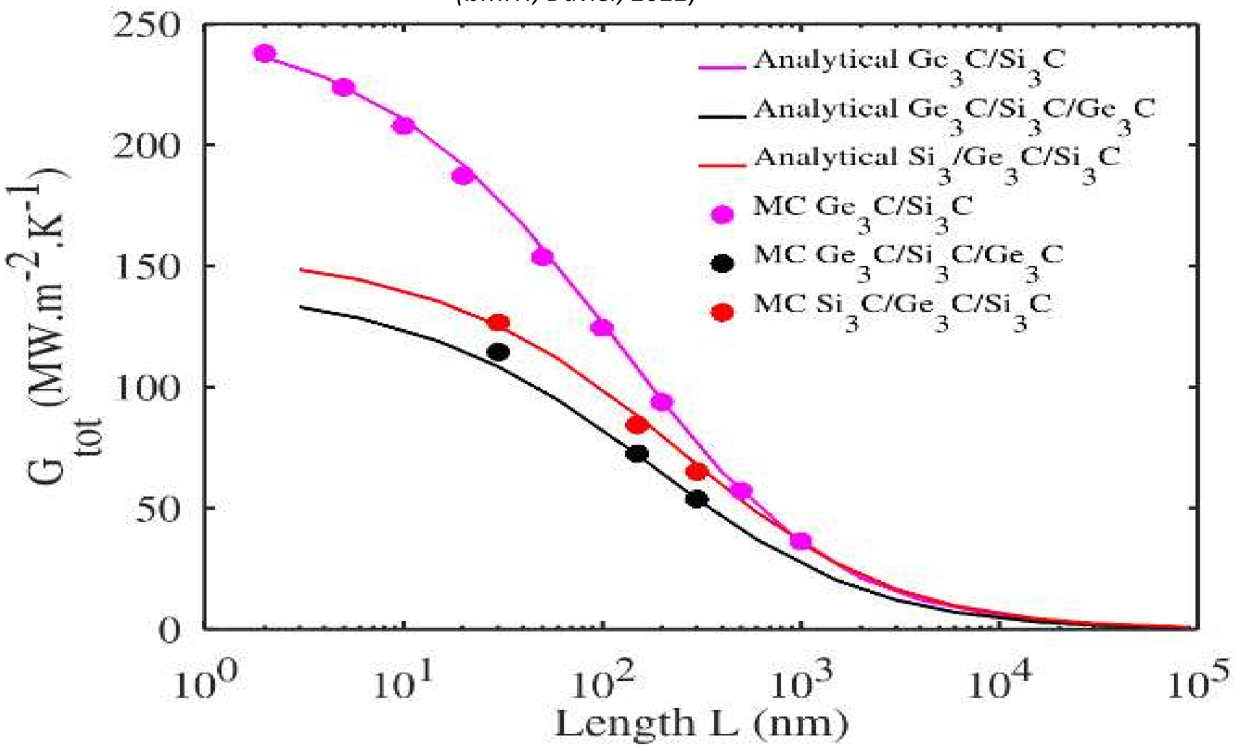
$$G^{total}_{std}=\left[\frac{L^L}{\kappa^L_{effective}}+\frac{1}{G^I}+\frac{L^R}{\kappa^R_{effective}}\right]^{-1}$$

$\rightarrow$ **Good agreement between MC and analitycal model**

$\rightarrow$ ***3 resistance in series using k$_{effective}$*** **is very disappointing**

Simple and double Si/Ge heterostructures

(IJMHT, Davier, 2022)



→ Good agreement between MC and analitycal model

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Conclusion

☞ At thermal interface, the use of temperatures T+ and T- considering incident phonons is relevant

☞ It could be used to define a new set of 3 thermal parameters

$$Q = \kappa_{\text{effective}} \frac{\Delta T_{\text{contacts}}}{L} \quad \text{with } \Delta T_{contacts} = T^{+}(0) - T^{-}(L)$$

cf. Davier at al, International Journal of Heat and Mass Transfer Volume 183, Part A, February 2022, 122056

$$G_{Inter} = Q.\Delta\, T_{\text{local}}{}^{I} \quad \text{with } \Delta T_{\text{local}}^{I} = T^{+}(x^{I} - \epsilon) - T^{-}(x^{I} + \epsilon)$$

$$\kappa_{\text{ballistic}} = \frac{\Omega}{(2\pi)^3} \sum_{s} \hbar\omega_s \left|v_{s,x}\right| \frac{L}{2} \frac{\partial f_{\text{BE}}}{\partial T}(\omega_s, \bar{T}) = L\, G_{\text{ballistic}}$$

☞ The resulting analytical model is efficient to reproduce advanced Monte Carlo results in all phonon transport regimes even in complex structures

Special thanks to:

- Brice Davier, former PhD student, now in Toulon university

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