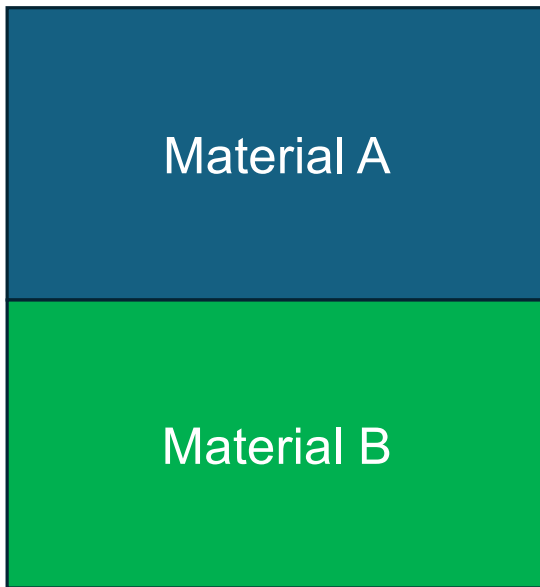


Acoustic and Diffuse Mismatch Model

<https://github.com/micromechanic/InterfacialPhononTransport>

Thermal boundary conductance



Scenario:

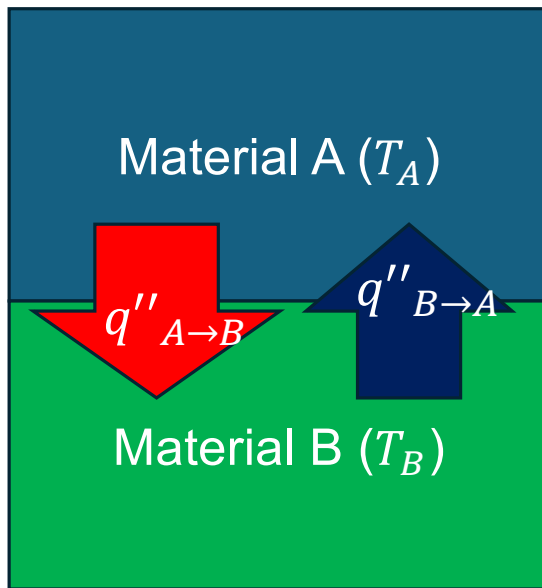
1. Material A is conformal deposited onto Materials:
Thermal boundary conductance is due to material mismatch rather than voids.
2. Material A is sitting at T_A and Material B is sitting at T_B . At the interface, the difference between T_A and T_B is small.

Question: what is the thermal boundary conductance at the interface between Material A and Material B?

Thermal boundary resist:

- Voids
- Material mismatch

Definition of thermal boundary conductance



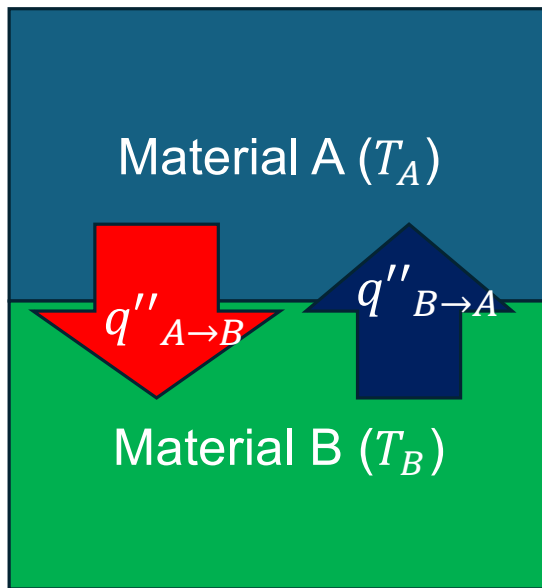
Net heat current density (q'' has a unit of W m^{-2}):

$$G(T_A - T_B) = q''_{A \rightarrow B}(T_A) - q''_{B \rightarrow A}(T_B)$$

Thermal boundary conductance:

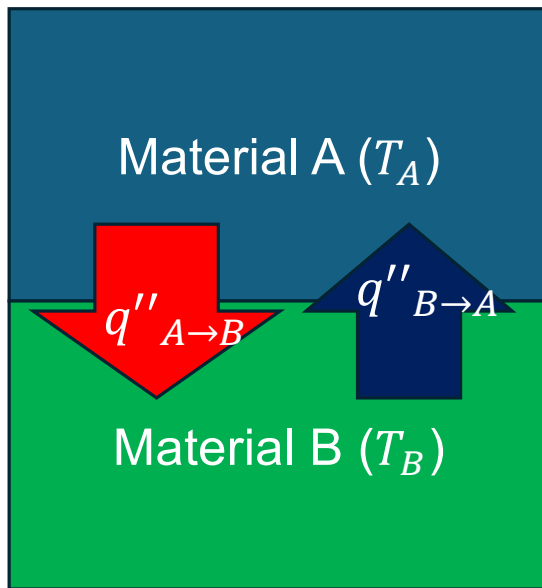
$$G = \frac{q''_{A \rightarrow B}(T_A) - q''_{B \rightarrow A}(T_B)}{T_A - T_B}$$

Landour formalism for phononic transport



$$\begin{aligned}
 & q''_{A \rightarrow B}(T_A) - q''_{B \rightarrow A}(T_B) \\
 &= \frac{1}{2} \sum_j \left[\int_0^{\omega_D} \hbar \omega v_{A,j}(\omega) \tau_{A \rightarrow B,j}(\omega) f_{BE}(T_A, \omega) D_{A,j}(\omega) d\omega \right. \\
 & \quad \left. - \int_0^{\omega_D} \hbar \omega v_{B,j}(\omega) \tau_{B \rightarrow A,j}(\omega) f_{BE}(T_B, \omega) D_{B,j}(\omega) d\omega \right]
 \end{aligned}$$

Landour formalism for phononic transport



$$\frac{1}{2} \sum_j \int_0^{\omega_D} \hbar \omega v_{A,j}(\omega) \tau_{A \rightarrow B,j}(\omega) f_{BE}(T_A, \omega) D_{A,j}(\omega) d\omega$$

$\hbar \omega$: Energy of each phonons

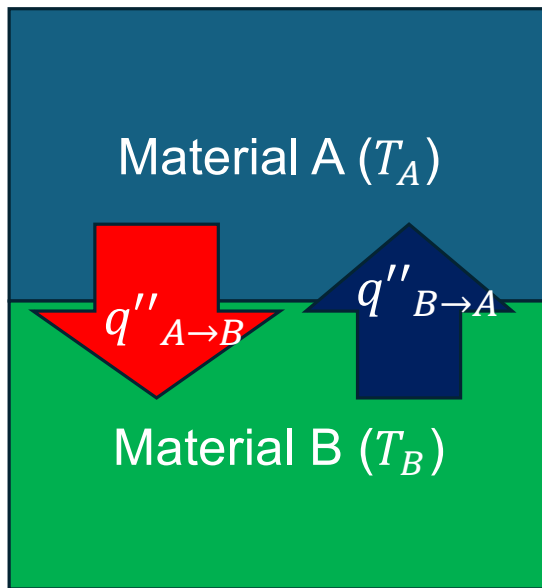
$v_{A,j}(\omega)$: The speed of these phonons

$\tau_{A \rightarrow B,j}(\omega)$: The probability the phonons will move from medium $A \rightarrow B$ of mode j .

$f_{BE}(T_A, \omega)$: The distribution of phonon population.

$D_{A,j}(\omega)$: The density of phonons at each state.

Simplifications

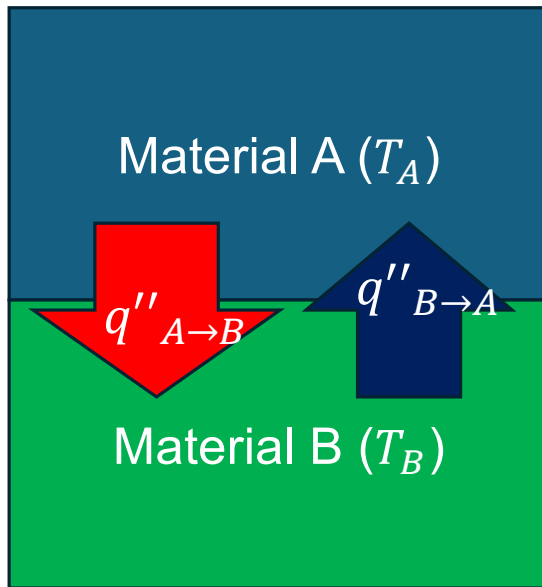


$$\begin{aligned}
 & q''_{A \rightarrow B}(T_A) - q''_{B \rightarrow A}(T_B) \\
 &= \frac{1}{2} \sum_j \left[\int_0^{\omega_D} \hbar \omega v_{A,j}(\omega) \tau_{A \rightarrow B,j}(\omega) f_{BE}(T_A, \omega) D_{A,j}(\omega) d\omega \right. \\
 & \quad \left. - \int_0^{\omega_D} \hbar \omega v_{B,j}(\omega) \tau_{B \rightarrow A,j}(\omega) f_{BE}(T_B, \omega) D_{B,j}(\omega) d\omega \right]
 \end{aligned}$$

$$T_A = T_B:$$

$$\begin{aligned}
 & v_{A,j}(\omega) \tau_{A \rightarrow B,j}(\omega) D_{A,j}(\omega) = \\
 & v_{B,j}(\omega) \tau_{B \rightarrow A,j}(\omega) D_{B,j}(\omega)
 \end{aligned}$$

Simplified Landour formalism

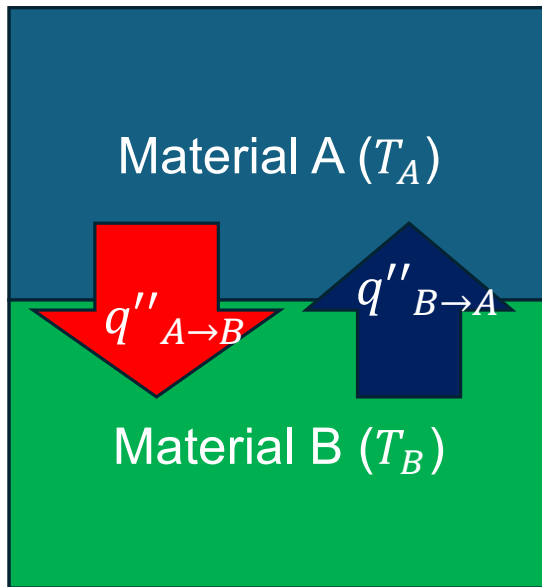


$$\begin{aligned}
 & q''_{A \rightarrow B}(T_A) - q''_{B \rightarrow A}(T_B) \\
 &= \frac{1}{2} \sum_j \left[\int_0^{\omega_D} \hbar \omega v_{A,j}(\omega) \tau_{A \rightarrow B,j}(\omega) f_{BE}(T_A, \omega) D_{A,j}(\omega) d\omega \right. \\
 & \quad \left. - \int_0^{\omega_D} \hbar \omega v_{B,j}(\omega) \tau_{B \rightarrow A,j}(\omega) f_{BE}(T_B, \omega) D_{B,j}(\omega) d\omega \right]
 \end{aligned}$$



$$\begin{aligned}
 & q''_{A \rightarrow B}(T_A) - q''_{A \rightarrow B}(T_B) \\
 &= \frac{1}{2} \sum_j \int_0^{\omega_D} \hbar \omega v_{A,j} \tau_{A \rightarrow B,j}(\omega) D_{A,j}(\omega) [f_{BE}(T_A, \omega) \\
 & \quad - f_{BE}(T_B, \omega)] d\omega
 \end{aligned}$$

Phononic window



$$q''_{A \rightarrow B}(T_A) - q''_{A \rightarrow B}(T_B)$$

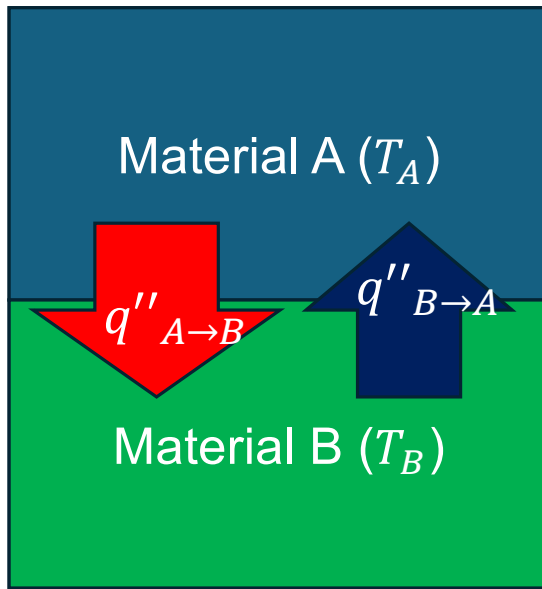
$$= \frac{1}{2} \sum_j \int_0^{\omega_D} \hbar \omega v_{A,j} \tau_{A \rightarrow B,j}(\omega) D_{A,j}(\omega) [f_{BE}(T_A, \omega) - f_{BE}(T_B, \omega)] d\omega$$

Assume the difference between T_A and T_B is small:

$$f_{BE}(T_A, \omega) - f_{BE}(T_B, \omega) = f_{BE}(T_A, \omega) - f_{BE}(T_A - \Delta T, \omega)$$

$$f_{BE}(T_A, \omega) - f_{BE}(T_B, \omega) = \frac{\partial f_{BE}(T_A, \omega)}{\partial T} \Delta T$$

Thermal boundary conductance equation



$$q''_{A \rightarrow B}(T_A) - q''_{A \rightarrow B}(T_B) = \frac{1}{2} \sum_j \int_0^{\omega_D} \hbar \omega v_{A,j} \tau_{A \rightarrow B,j}(\omega) D_{A,j}(\omega) [f_{BE}(T_A, \omega) - f_{BE}(T_B, \omega)] d\omega$$

$$q''_{A \rightarrow B}(T_A) - q''_{A \rightarrow B}(T_B) = \frac{1}{2} \sum_j \int_0^{\omega_D} \hbar \omega v_{A,j} \tau_{A \rightarrow B,j}(\omega) D_{A,j}(\omega) \frac{\partial f_{BE}(T_A, \omega)}{\partial T} \Delta T d\omega$$

Review of Modern Physics, Vol.61, No. 3, July 1989

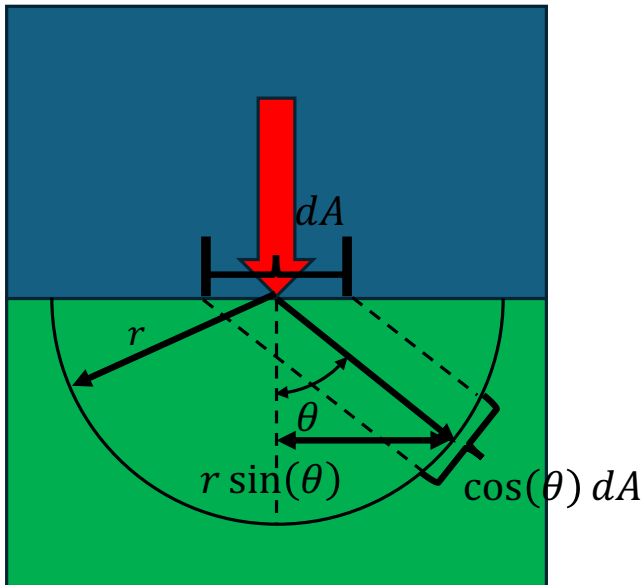
Equation for thermal conductance:

$$G = \frac{q''_{A \rightarrow B}(T_A) - q''_{A \rightarrow B}(T_B)}{T_A - T_B} = \frac{1}{2} \sum_j \int_0^{\omega_D} \hbar \omega v_{A,j} \tau_{A \rightarrow B,j}(\omega) D_{A,j}(\omega) \frac{\partial f_{BE}(T_A, \omega)}{\partial T} d\omega$$

Mismatch Models

$$G = \frac{\dot{q}}{\Delta T} = \frac{1}{2} \sum_j \int_0^{\omega_D} \hbar \omega v_{A,j} \tau_{A \rightarrow B,j}(\omega) D_{A,j}(\omega) \frac{\partial f_{BE}(T_A, \omega)}{\partial T} d\omega$$

We know everything, except $\tau_{A \rightarrow B,j}(\omega)$.



Average transmission coefficient:

$$\tau_{A \rightarrow B,j}(\omega) = \int_0^{\pi/2} \alpha_{A \rightarrow B,j}(\omega, \theta) \cos(\theta) \sin(\theta) d\theta$$

$\alpha_{A \rightarrow B,j}(\omega, \theta)$: angle dependent transmission coefficient.

$\cos(\theta)$: from the projected area.

$\sin(\theta)$: from the spherical integral

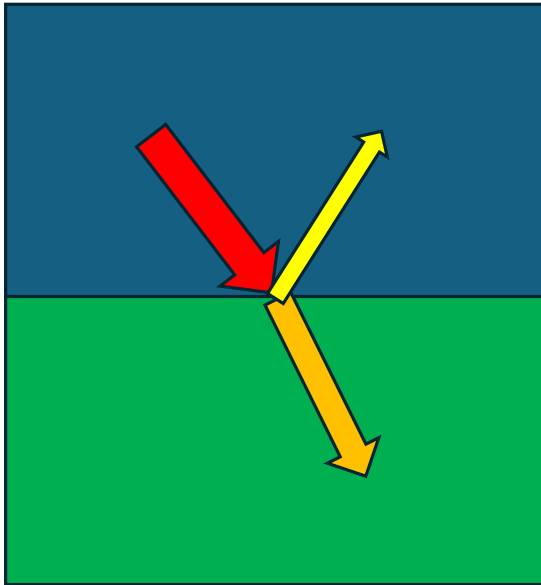
Regimes where AMM and DMM is applicable

$$\alpha_{A \rightarrow B, j}(\omega, \theta)$$

Interface roughness is very small compared to the De Broglie wavelength of the phonons.

T is small.

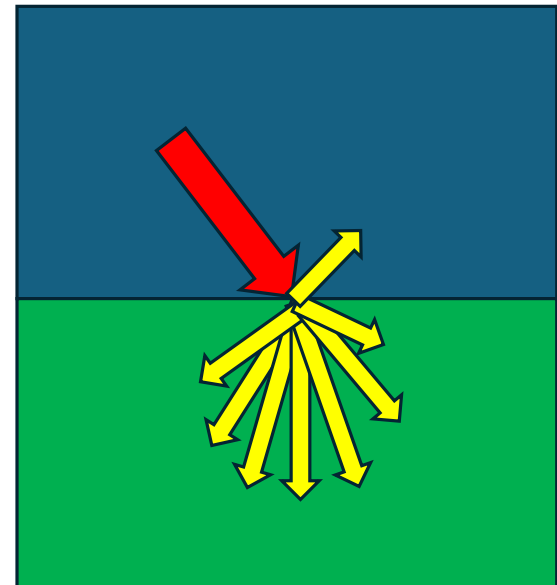
Acoustic Mismatch Model (AMM):



Interface roughness is very large compared to the De Broglie wavelength of the phonons.

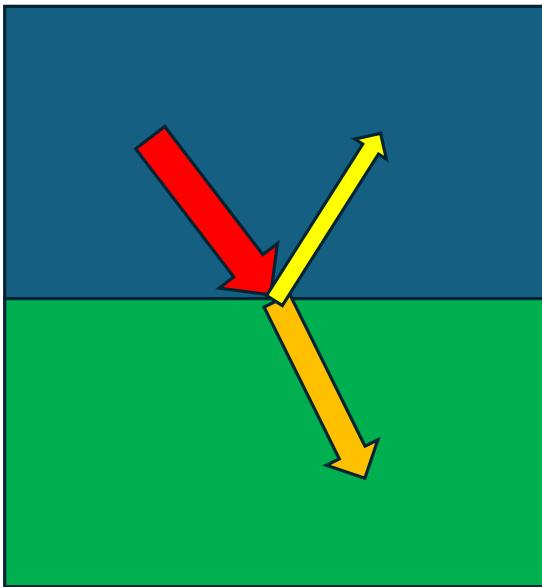
T is large.

Diffuse Mismatch Model (DMM):



Highly simplified scenario for AMM

Acoustic Mismatch Model (AMM):



- Do not allow mode conversion. Transverse mode stay transverse. Longitudinal stay Longitudinal.
- The only angle dependence is the velocity component that is perpendicular to the interface.
- The only differences between different branches (transverse vs. longitudinal) are the speed of sound.
- No frequency dependence.

$$\alpha_{A \rightarrow B,j}(\theta_A) = \frac{4Z_A Z_B}{(Z_A + Z_B)^2}$$

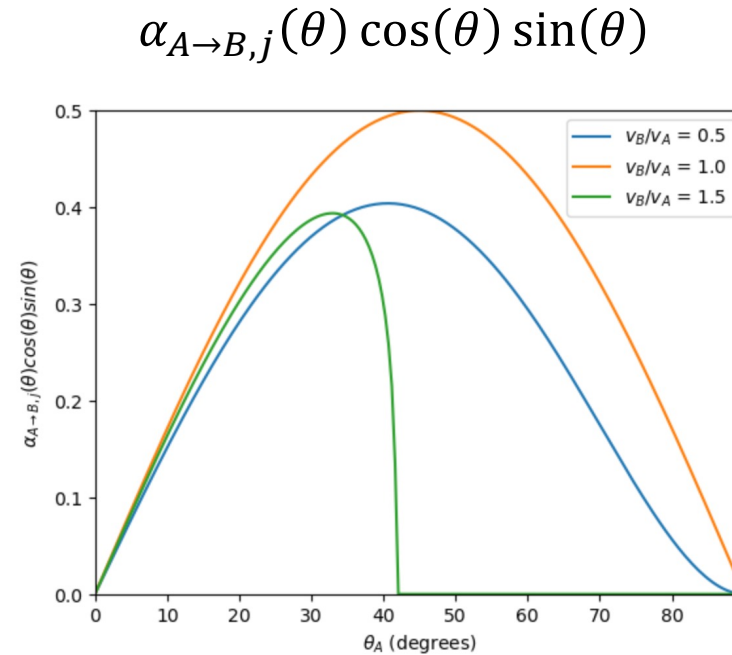
Acoustic Impedance:

$$Z_A = \frac{\rho v_{A,j}}{\cos(\theta_A)} \quad Z_B = \frac{\rho v_{B,j}}{\cos(\theta_B)}$$

Snell's Law (relating θ_A and θ_B):

$$\frac{\sin(\theta_A)}{v_{A,j}} = \frac{\sin(\theta_B)}{v_{B,j}}$$

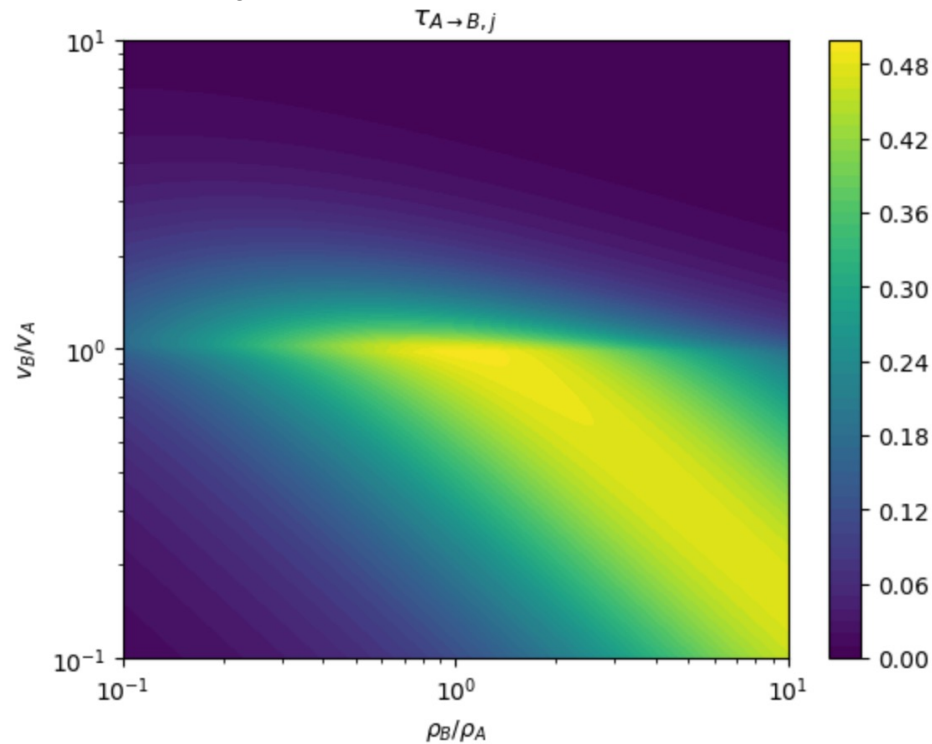
In side of the transmission coefficient for AMM



By looking at the $\alpha_{A \rightarrow B,j}(\theta) \cos(\theta) \sin(\theta)$, it is intuitive that $\tau_{A \rightarrow B,j}$ is the largest when $v_b/v_A = 1$ and smallest when $v_B/v_A = 1.5$ due to total internal refraction. The maximum $\alpha_{A \rightarrow B,j}(\theta) \cos(\theta) \sin(\theta)$ is 0.5 for $v_b/v_A = 1$.

Density and v_g ratio impact on $\tau_{A \rightarrow B, j}$

$$\tau_{A \rightarrow B, j} = \int_0^{\pi/2} \alpha_{A \rightarrow B, j}(\theta) \cos(\theta) \sin(\theta) d\theta$$



Reproducing the results from: Can. J. Phys. Vol. 37 (1959)

Solving the thermal boundary conductance

Calculation for Thermal Boundary Conductance using AMM

since the average transmission coefficient ($\tau_{A \rightarrow B,j}$) and phonon propagation velocity ($v_{A,j}$) is assumed to be independent to the phonon frequency (ω), the previous thermal boundary conductance (G) equation simplifies to:

$$G = \frac{1}{2} \sum_j v_{A,j} \tau_{A \rightarrow B,j} \int_0^{\omega_D} \hbar \omega D_{A,j}(\omega) \frac{\partial f_{BE}(T, \omega)}{\partial T} d\omega$$

Under Debye's assumption of linear phonon dispersion, the phonon density of state ($D_{A,j}(\omega)$) is:

$$D_{A,j}(\omega) = \frac{\omega^2}{2\pi^2 v_{A,j}^3}$$

Thus, G simplifies to:

$$G = \frac{1}{4\pi^2} \left[\frac{\tau_{A \rightarrow B,l}}{v_{A,l}^2} + \frac{2\tau_{A \rightarrow B,t}}{v_{A,t}^2} \right] \int_0^{\omega_D} \hbar \omega^3 \frac{\partial f_{BE}(T, \omega)}{\partial T} d\omega$$

Simplify the equation to get a close formed solution

To improve numerical stability, we introduce the dimensionless variable x for $\frac{\hbar\omega}{k_B T}$. This substitution improves numerical stability, because it rescales the integration variable to be dimensionless and of order unity near the dominant contribution.

$$G = \frac{k_B^4 T^3}{4\pi^2 \hbar^3} \left[\frac{\tau_{A \rightarrow B,l}}{v_{A,l}^2} + \frac{2\tau_{A \rightarrow B,t}}{v_{A,t}^2} \right] \int_0^{x_D} x^4 \frac{e^x}{(e^x - 1)^2} dx$$

There are two important observations:

1. The integral is unitless. Thus, G is positively correlated with T^3 .
2. When $T \ll \Theta_D$, $x_D \rightarrow \infty$, the integral has a solution of $\frac{4}{15}\pi^4$:

$$G = \frac{\pi^2 k_B^4 T^3}{15 \hbar^3} \left[\frac{\tau_{A \rightarrow B,l}}{v_{A,l}^2} + \frac{2\tau_{A \rightarrow B,t}}{v_{A,t}^2} \right]$$

At low temperature which is the applicable regime of AMM, the G is only dependent on the v_A , v_B , ρ_A , ρ_B , and T . However, at ultralow temperature ($T < 1K$), the AMM model underestimates G , for more detail refer to the review paper: Reviews of Modern Physics, Vol. 61, No. 3, July 1989.

Creating a database for the material properties

AMM Thermal Boundary Conductance:

One common way to show the thermal boundary conductance is to show the T independent terms:

$$\frac{G}{T^3} = \frac{\pi^2 k_B^4}{15 \hbar^3} \left[\frac{\tau_{A \rightarrow B, l}}{v_{A, l}^2} + \frac{2\tau_{A \rightarrow B, t}}{v_{A, t}^2} \right]$$

	material	density	v_l	v_t
0	gold	19300	3390.0	1290.0
1	quartz	2660	6090.0	4100.0
2	sapphire	3970	10890.0	6450.0
3	silicon	2330	8970.0	5332.0

The result is similar but not exactly the same:
Reviews of Modern Physics, Vol. 61, No. 3, July 1989

Gold to Sapphire Interface

```
T = 10; # Kelvin
g_go_sa = g_AMM(gold.v_l, sapphire.v_l, gold.v_t, sapphire.v_t, gold.density, sapphire.density)
g_go_sa_T = g_go_sa/T**3;
print(f"Gold to sapphire interface: {g_go_sa_T:.2f} W/m^2/K^4")
```

Gold to sapphire interface: 526.39 W/m^2/K^4

Sapphire to Gold Interface

```
g_sa_go = g_AMM(sapphire.v_l, gold.v_l, sapphire.v_t, gold.v_t, sapphire.density, gold.density)
g_sa_go_T = g_sa_go/T**3;
print(f"Sapphire to gold interface: {g_sa_go_T:.2f} W/m^2/K^4")
```

Sapphire to gold interface: 526.40 W/m^2/K^4

Gold to Quartz Interface

```
g_go_qz = g_AMM(gold.v_l, quartz.v_l, gold.v_t, quartz.v_t, gold.density, quartz.density)
g_go_qz_T = g_go_qz/T**3;
print(f"Gold to Quartz interface: {g_go_qz_T:.2f} W/m^2/K^4")
```

Gold to Quartz interface: 1327.14 W/m^2/K^4

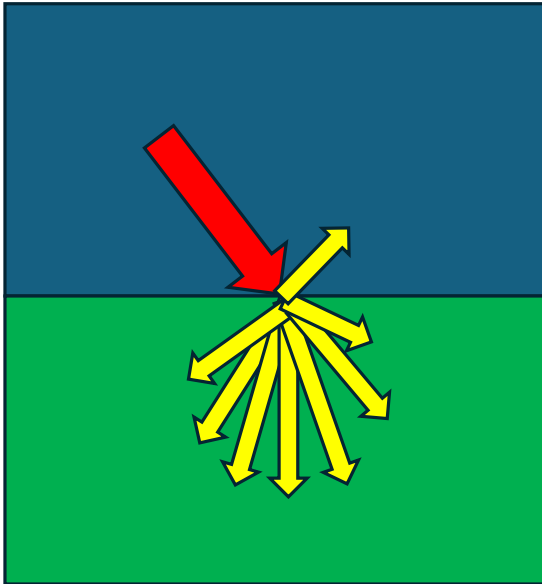
Gold to Silicon Interface

```
g_go_si = g_AMM(gold.v_l, silicon.v_l, gold.v_t, silicon.v_t, gold.density, silicon.density)
g_go_si_T = g_go_si/T**3;
print(f"Gold to Silicon interface: {g_go_si_T:.2f} W/m^2/K^4")
```

Gold to Silicon interface: 780.96 W/m^2/K^4

High temperature: diffuse mismatch model

Diffuse Mismatch Model (DMM):



- The phonon does not know where it came from so $\alpha_{A \rightarrow B, j}$ is not a function of θ_A .
- The phonon does not know which mode it came from $\alpha_{A \rightarrow B, j} \rightarrow \alpha_{A \rightarrow B}$.
- We assume that there is no absorption at the boundary.

$$\alpha_{A \rightarrow B} = 1 - \alpha_{B \rightarrow A}$$

Thus, the number of phonons that leaving from A to B must equal to the phonon leaving from B to A.

$$\sum_j v_{A,j} D_{A,j} f_{BE} \alpha_{A \rightarrow B} = \sum_j v_{B,j} D_{B,j} f_{BE} (1 - \alpha_{A \rightarrow B})$$

We can solve for $\alpha_{A \rightarrow B}$:

$$\alpha_{A \rightarrow B} = \frac{\sum_j v_{B,j} D_{B,j} f_{BE}}{\sum_j v_{B,j} D_{B,j} f_{BE} + \sum_j v_{A,j} D_{A,j} f_{BE}}$$

Solving for the average transmission coefficient

In the Debye model, the only difference in the density of state between material A and material B is the phonon group velocity. We can solve for $\alpha_{A \rightarrow B}$:

$$\alpha_{A \rightarrow B} = \frac{\sum_j v_{B,j}^{-2}}{\sum_j v_{B,j}^{-2} + \sum_j v_{A,j}^{-2}}$$

$$\tau_{A \rightarrow B,j} = \int_0^{\pi/2} \alpha_{A \rightarrow B,j}(\theta) \cos(\theta) \sin(\theta) d\theta$$

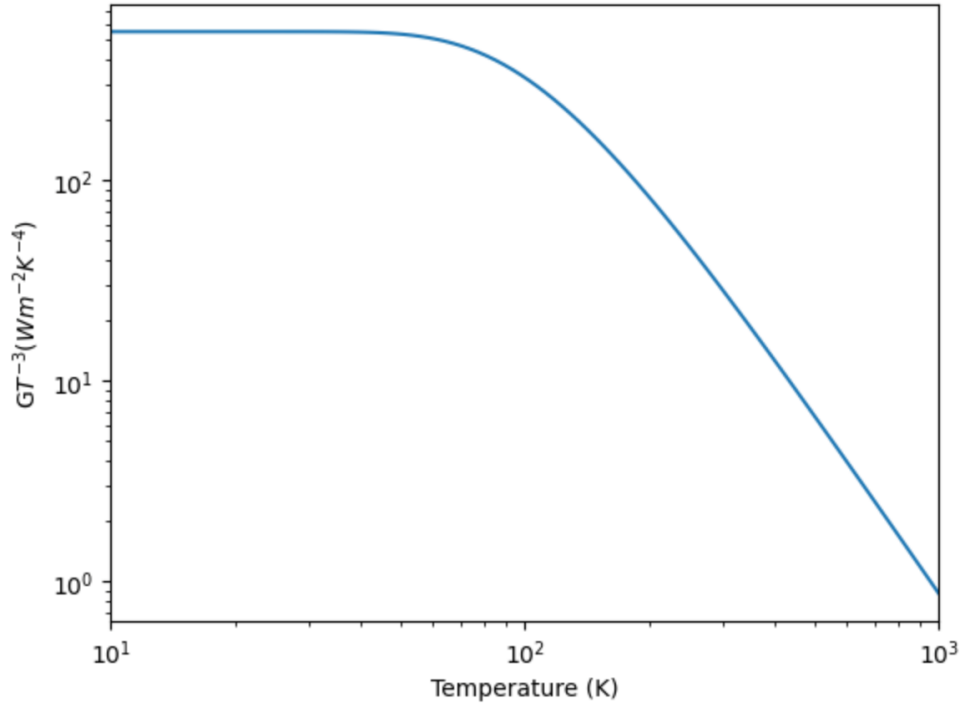
Since $\alpha_{A \rightarrow B}$ is independent of θ_A , so the angle integral becomes 1/2:

$$\tau_{A \rightarrow B} = \frac{1}{2} \frac{\sum_j v_{B,j}^{-2}}{\sum_j v_{B,j}^{-2} + \sum_j v_{A,j}^{-2}}$$

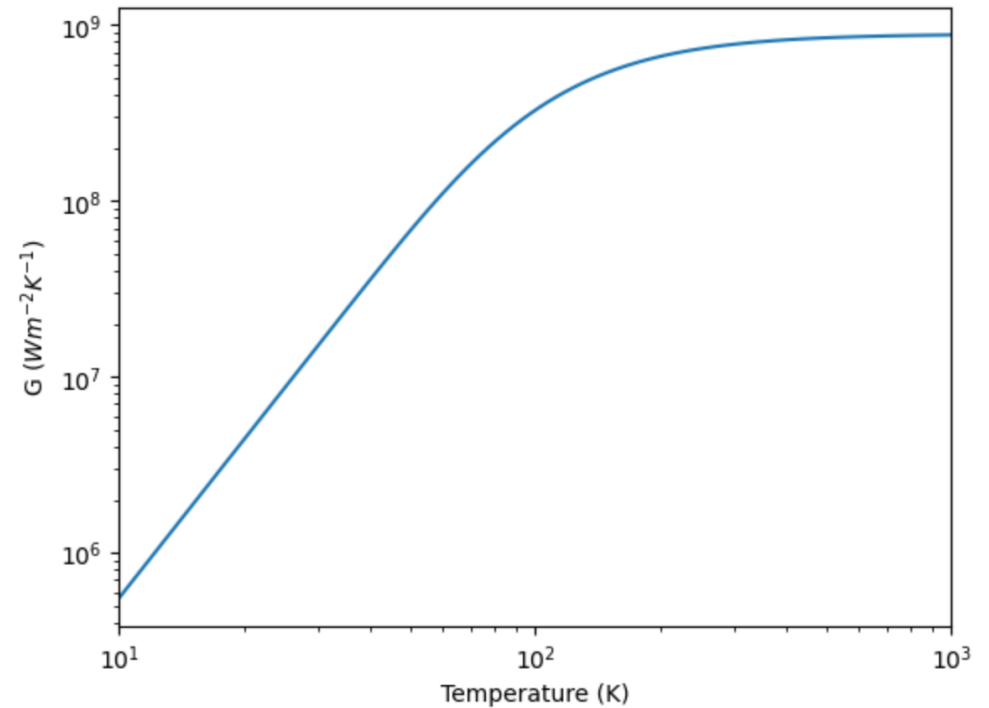
$$G = \frac{\tau_{A \rightarrow B} k_B^4 T^3}{4\pi^2 \hbar^3} \left[\frac{1}{v_{A,l}^2} + \frac{2}{v_{A,t}^2} \right] \int_0^{x_D} x^4 \frac{e^x}{(e^x - 1)^2} dx$$

Temperature dependent DMM

$$\int_0^{x_D} x^4 \frac{e^x}{(e^x - 1)^2} dx$$



$$G = \frac{\tau_{A \rightarrow B} k_B^4 T^3}{4\pi^2 \hbar^3} \left[\frac{1}{v_{A,l}^2} + \frac{2}{v_{A,t}^2} \right] \int_0^{x_D} x^4 \frac{e^x}{(e^x - 1)^2} dx$$



For a solid-solid interface, AMM and DMM is similar

Gold to Sapphire Interface

```
T = 10; # Kelvin
g_go_sa = g_AMM(gold.v_l, sapphire.v_l, gold.v_t, sapphire.v_t, gold.density, sapphire.density)
g_go_sa_T = g_go_sa/T**3;
print(f"Gold to sapphire interface: {g_go_sa_T:.2f} W/m^2/K^4")
```

Gold to sapphire interface: 526.39 W/m²/K⁴

Gold to Quartz Interface

```
g_go_qz = g_AMM(gold.v_l, quartz.v_l, gold.v_t, quartz.v_t, gold.density, quartz.density)
g_go_qz_T = g_go_qz/T**3;
print(f"Gold to Quartz interface: {g_go_qz_T:.2f} W/m^2/K^4")
```

Gold to Quartz interface: 1327.14 W/m²/K⁴

Gold to Silicon Interface

```
g_go_si = g_AMM(gold.v_l, silicon.v_l, gold.v_t, silicon.v_t, gold.density, silicon.density)
g_go_si_T = g_go_si/T**3;
print(f"Gold to Silicon interface: {g_go_si_T:.2f} W/m^2/K^4")
```

Gold to Silicon interface: 780.96 W/m²/K⁴

Gold to Sapphire Interface

```
T = 10
g_go_sa = g_DMM_Tind(gold.v_l, sapphire.v_l, gold.v_t, sapphire.v_t, T_debye, T, 1000)
print(f"Gold to sapphire interface: {g_go_sa:.2f} W/m^2/K^4")
```

Gold to sapphire interface: 551.75 W/m²/K⁴

Gold to Quartz Interface

```
g_go_qz = g_DMM_Tind(gold.v_l, quartz.v_l, gold.v_t, quartz.v_t, T_debye, T, 1000)
print(f"Gold to Quartz interface: {g_go_qz:.2f} W/m^2/K^4")
```

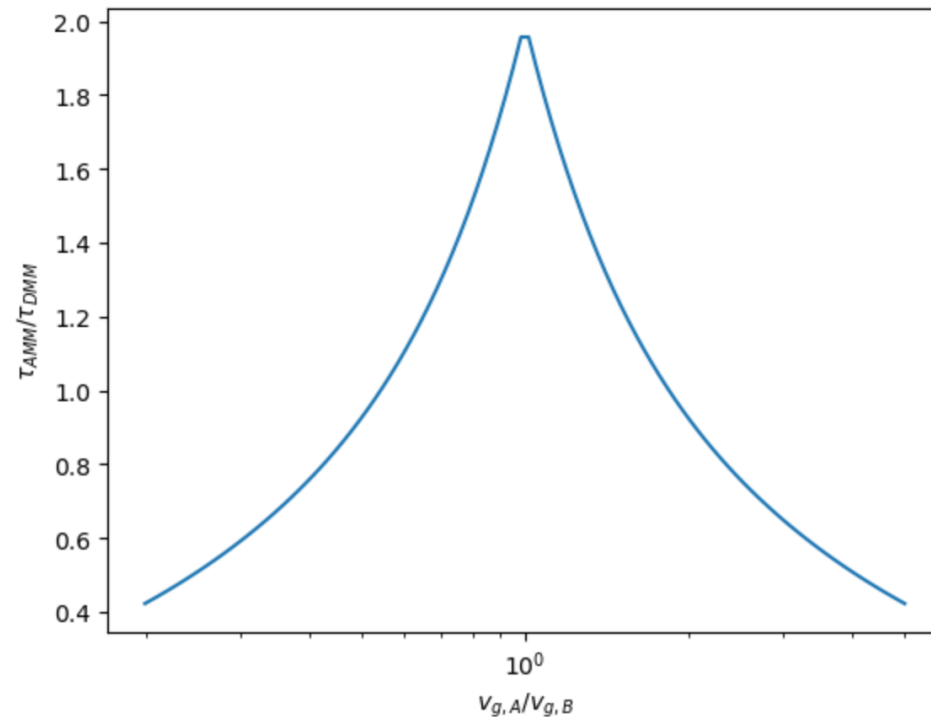
Gold to Quartz interface: 1336.20 W/m²/K⁴

Gold to Quartz Interface

```
g_go_si = g_DMM_Tind(gold.v_l, silicon.v_l, gold.v_t, silicon.v_t, T_debye, T, 1000)
print(f"Gold to Silicon interface: {g_go_si:.2f} W/m^2/K^4")
```

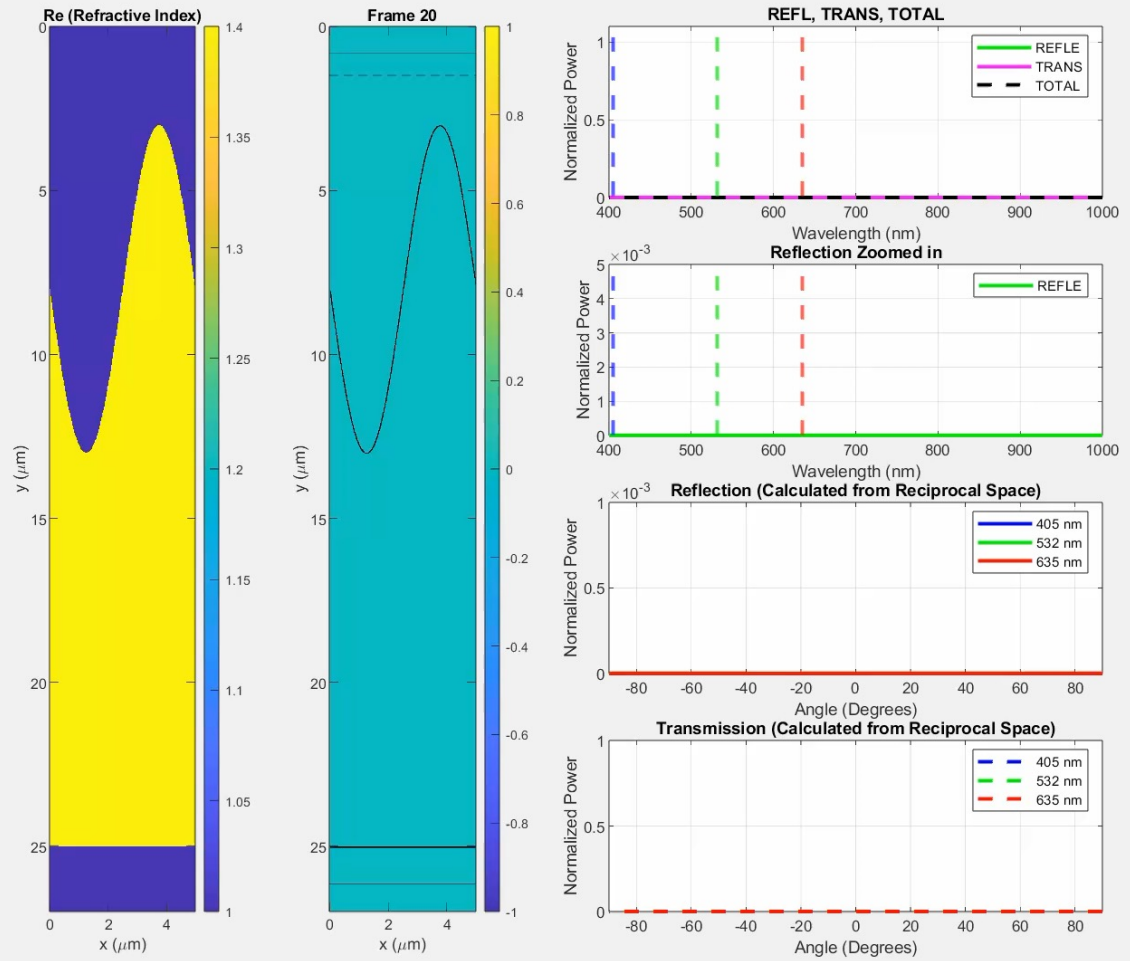
Gold to Silicon interface: 792.78 W/m²/K⁴

Why does DMM and AMM is different



This result shows that when two materials are very similar, the $\tau_{AMM} > \tau_{DMM}$. However, whenever the group velocity varies dramatically, $\tau_{AMM} < \tau_{DMM}$. For most of the solid-solid interfaces, the phonon group velocity is so different that the transmission is significantly different.

Questions



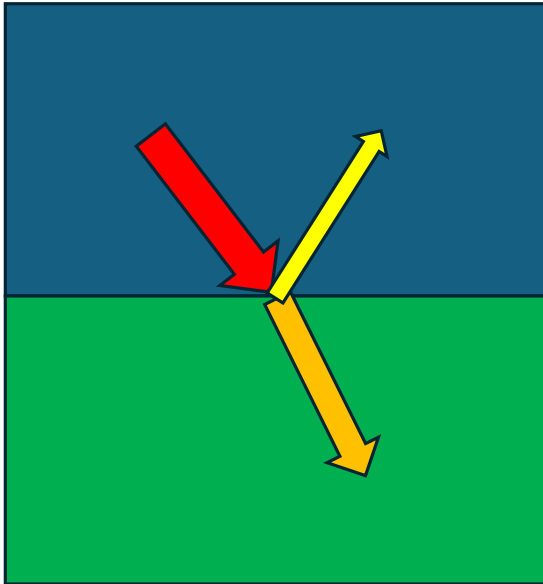
Additional Slides

Phononic window plot

$$f_{BE}(T_A, \omega) - f_{BE}(T_B, \omega) = \frac{\partial f_{BE}(T_A, \omega)}{\partial T} \Delta T$$

Phonons is analogous to photons

Acoustic Mismatch Model (AMM):



- Photons and phonons are both bosonic particles which follows the same Bose – Einstein distribution.
- Under Debye approximation, both photons and phonons follow the same density of states.

Photon's behavior at the interface under specular reflection:

1. Photon's specular reflection and transmission of an interface can be derived from Maxwell's equations.
2. The derivations will not be shown here, due to time limitations. However, it is known as **Fresnel's equation**.
3. Fresnel's equation says:
Transmission is dependent on the **angle** of the incident light, **polarization**, and the **refractive index** (optical impedance) of the two media.

Frensel Equation (Photons)

All these equations can be derived; They are **NOT** constitutive equations.
They are derived from Maxwell's equation with proper boundary conditions at the interfaces.

$$R_s = \left| \frac{Z_2 \cos(\theta_i) - Z_1 \cos(\theta_t)}{Z_2 \cos(\theta_i) + Z_1 \cos(\theta_t)} \right|^2$$

$$T_s = 1 - R_s$$

$$R_p = \left| \frac{Z_2 \cos(\theta_t) - Z_1 \cos(\theta_i)}{Z_2 \cos(\theta_t) + Z_1 \cos(\theta_i)} \right|^2$$

$$T_p = 1 - R_p$$

Wave Impedance:

$$Z_1 = \frac{Z_0}{n_1}, Z_2 = \frac{Z_0}{n_2}$$

Snell's Law:

$$\frac{\sin(\theta_i)}{n_1} = \frac{\sin(\theta_t)}{n_t}$$

Phonon simplifications

Phonon branches are derived from the theory of elasticity which is very different E&M:

➤ Simplification 1:

We are only

$$R_s = \left| \frac{Z_2 \cos(\theta_i) - Z_1 \cos(\theta_t)}{Z_2 \cos(\theta_i) + Z_1 \cos(\theta_t)} \right|^2$$

Phonons are different from photons (branches)

Phonon branches are derived from the theory of elasticity which is very different E&M.

- This result that phonons has three branches rather than two polarizations; We have to significantly simplify it to grasp basic understanding.
- This assumption does not allow total internal reflection. However, it is a huge simplification but necessary.

$$\tau_{A \rightarrow B}(\omega) = \tau_{B \rightarrow A}(\omega)$$

$$R_s = \left| \frac{Z_2 \cos(\theta_i) - Z_1 \cos(\theta_t)}{Z_2 \cos(\theta_i) + Z_1 \cos(\theta_t)} \right|^2$$