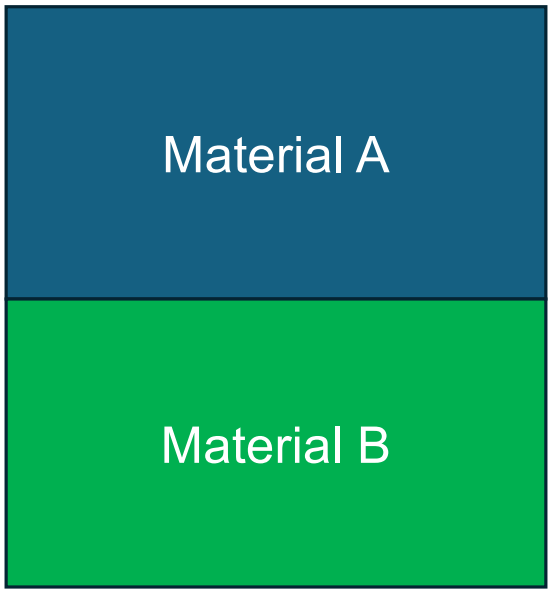
Acoustic and Diffuse Mismatch Model

Yucheng Yang

https://github.com/micromechanic/InterfacialPhononTransport

Thermal boundary conductance



Scenario:

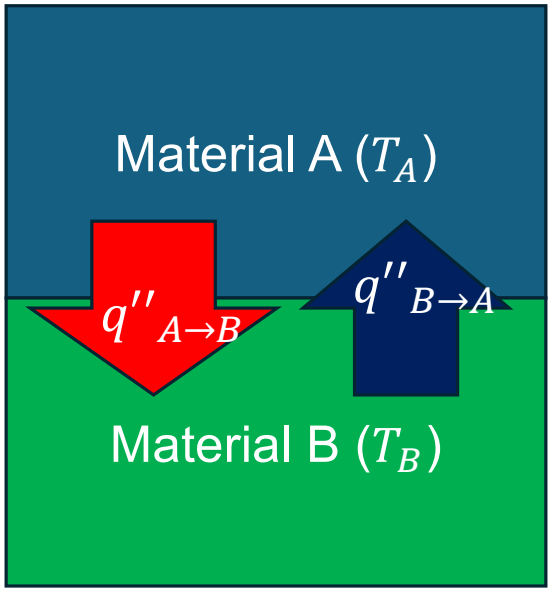
1. Material A is conformal deposited onto Materials: Thermal boundary conductance is due to material mismatch rather than voids.
2. Material A is sitting at T_A and Material B is sitting at T_B. At the interface, the difference between T_A and T_B is small.

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



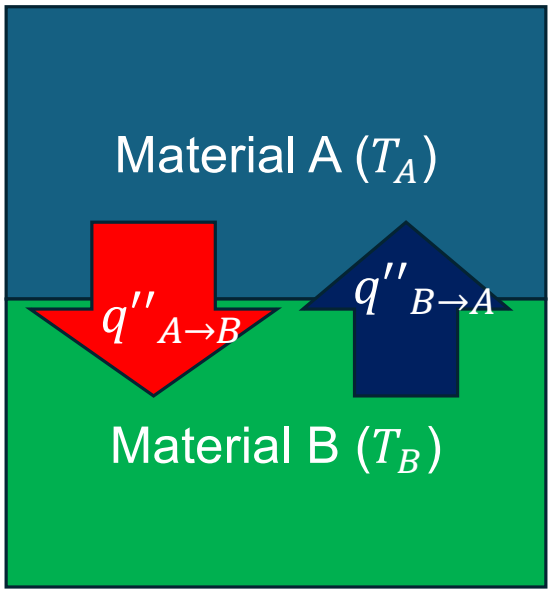
Net heat current density (q'' has a unit of W m^{-2}):

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

Thermal boundary conductance:

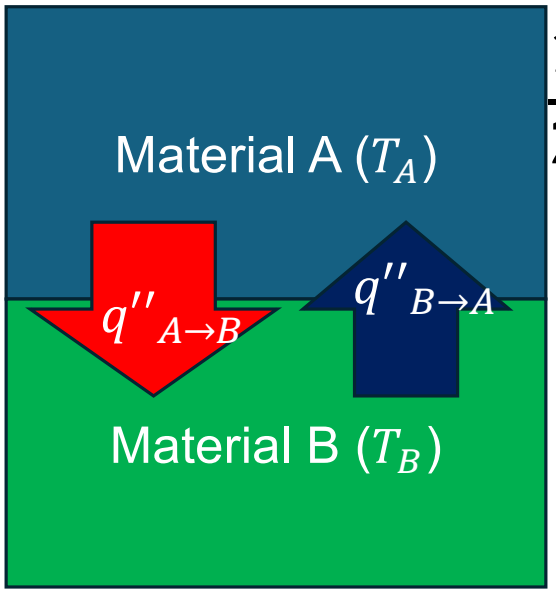
$$G = \frac{q''_{A\to B}(T_A) - q''_{B\to A}(T_B)}{T_A - T_B}$$

Landour formalism for phononic transport



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

Landour formalism for phononic transport



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

$\hbar\omega$: Energy of each phonons

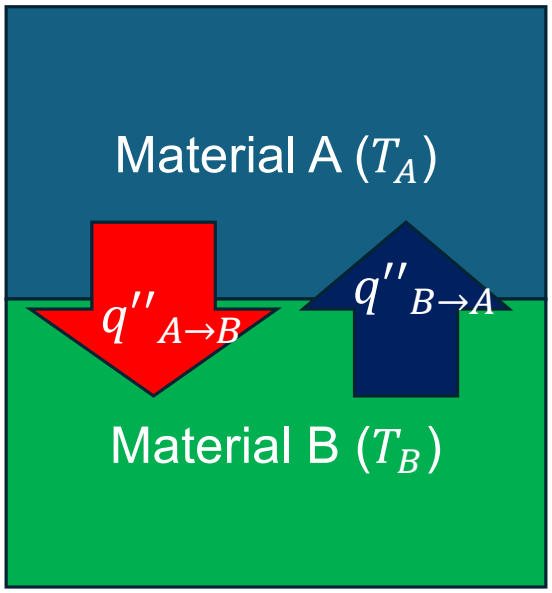
$v_{A,j}(\omega)$: The speed of these phonons

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

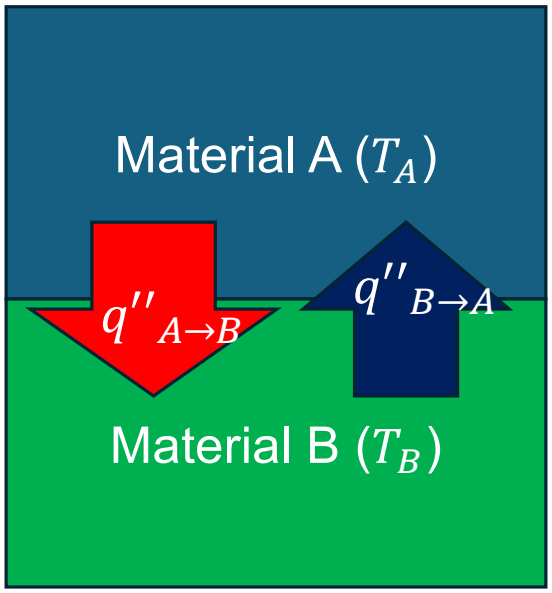


$$q''_{A\to B}(T_A) - q''_{B\to A}(T_B)$$
$$= \frac{1}{2}\sum_j \left[\int_0^{\omega_D} \hbar\omega v_{A,j}(\omega)\tau_{A\to B,j}(\omega)\, f_{BE}(T_A,\omega)D_{A,j}(\omega)d\omega\right.$$
$$\left. - \int_0^{\omega_D} \hbar\omega v_{B,j}(\omega)\tau_{B\to A,j}(\omega)\, f_{BE}(T_B,\omega)D_{B,j}(\omega)d\omega\right]$$

$$\boldsymbol{T_A = T_B}\textbf{:}$$

$$v_{A,j}(\omega)\tau_{A\to B,j}(\omega)D_{A,j}(\omega) =$$
$$v_{B,j}(\omega)\tau_{B\to A,j}(\omega)D_{B,j}(\omega)$$

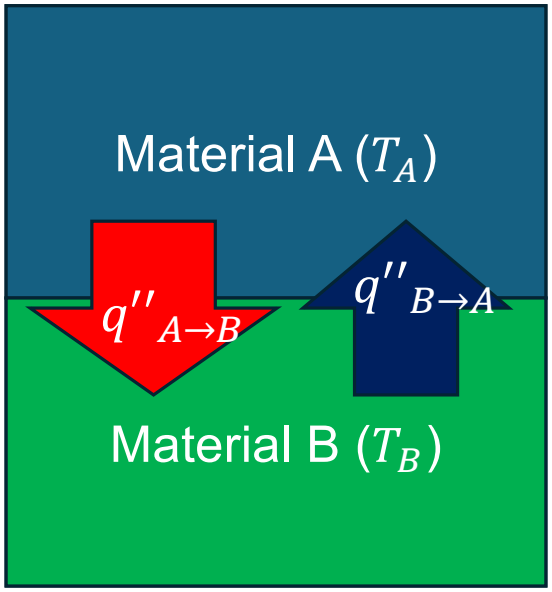
Simplified Landour formalism



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

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

Phononic window



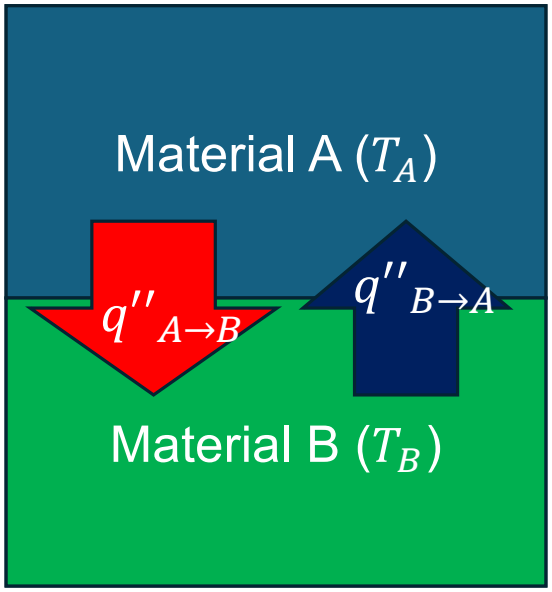
$$q''_{A\to B}(T_A) - q''_{A\to B}(T_B)$$
$$= \frac{1}{2}\sum_j \int_0^{\omega_D} \hbar\omega v_{A,j}\tau_{A\to B,j}(\omega)\, D_{A,j}(\omega)[f_{BE}(T_A,\omega) - f_{BE}(T_B,\omega)]d\omega$$

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



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

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

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

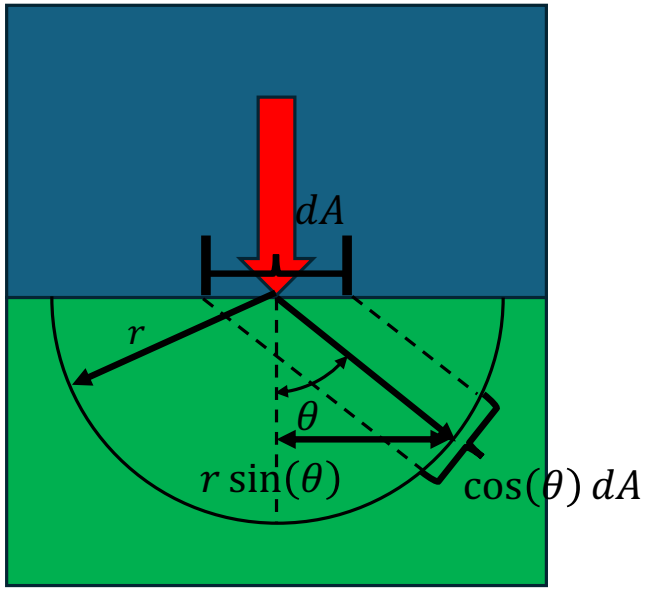
Equation for thermal conductance:

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

Mismatch Models

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

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



Average transmission coefficient:

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

$\alpha_{A\to B,j}(\omega,\theta)$: angle dependent transmission coefficient.
$\cos(\theta)$: from the projected area.
$\sin(\theta)$: from the spherical integral

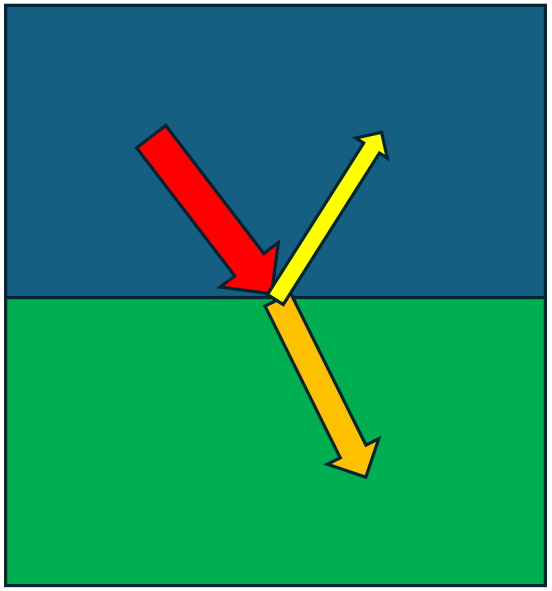
Regimes where AMM and DMM is applicable

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

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

T is small.

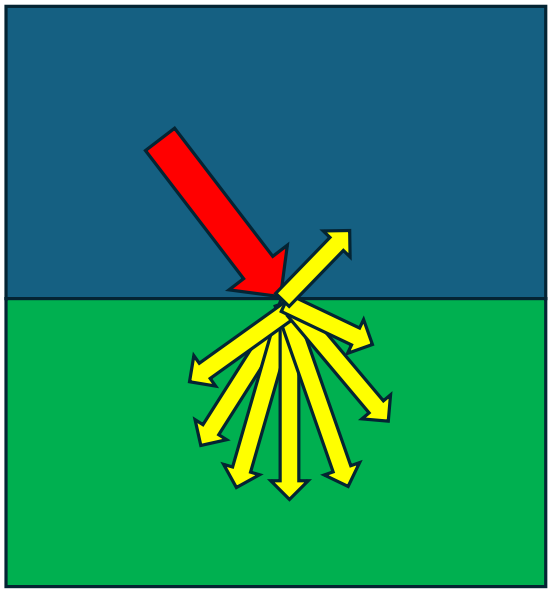
Acoustic Mismatch Model (AMM):



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

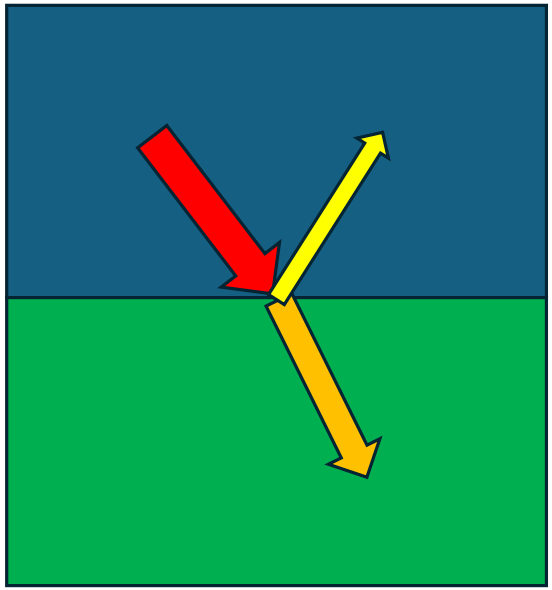
T is large.

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.

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

Acoustic Impedance:

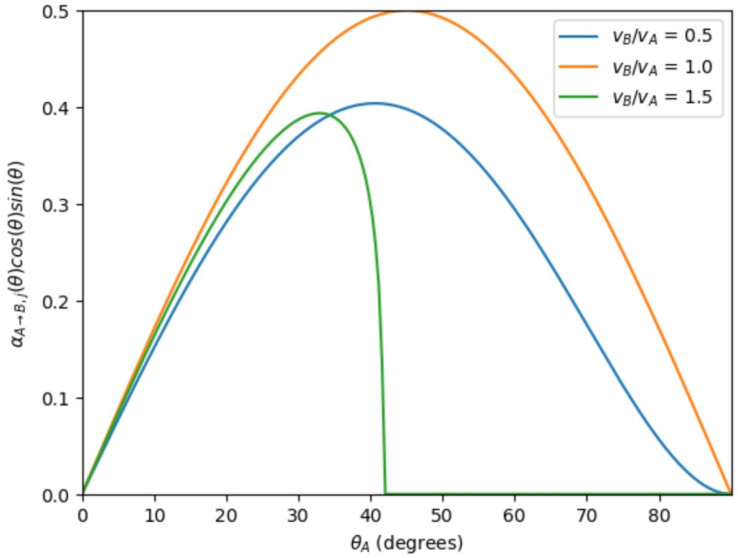
$$Z_A = \frac{\rho v_{A,j}}{\cos(\theta_A)} \qquad Z_B = \frac{\rho v_{B,j}}{\cos(\theta_B)}$$

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

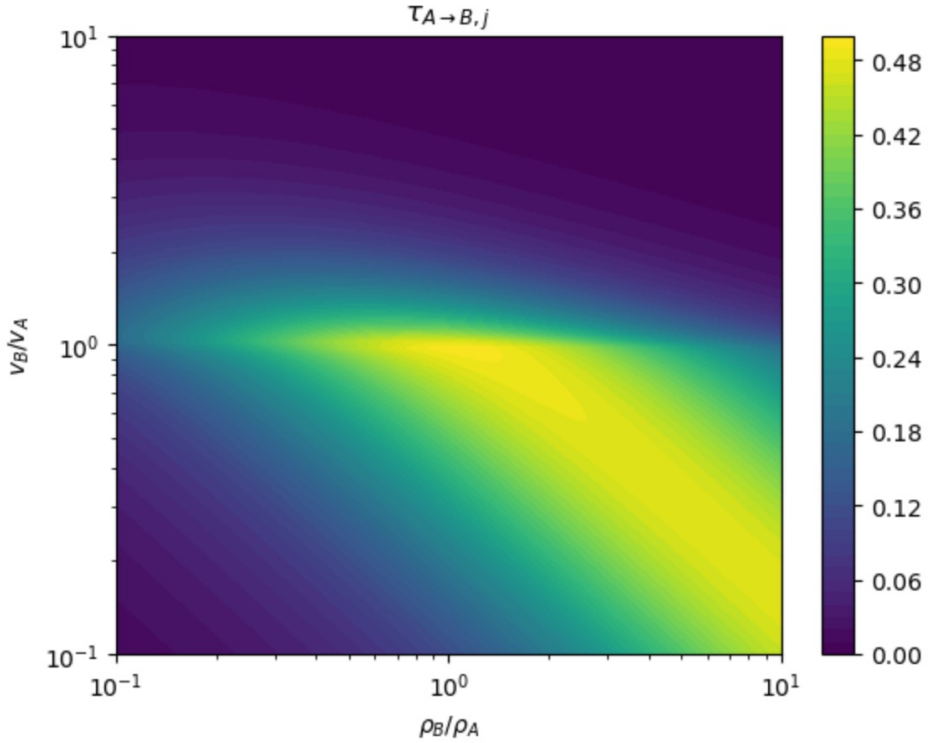
$$\alpha_{A\to B,j}(\theta)\cos(\theta)\sin(\theta)$$



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

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

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



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 ($\tau_{A\to B,j}$) 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:

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

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:

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

Simplify the equation to get a close formed solution

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

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

There are two important observations:

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

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

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:

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

	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.d
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.d
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
```

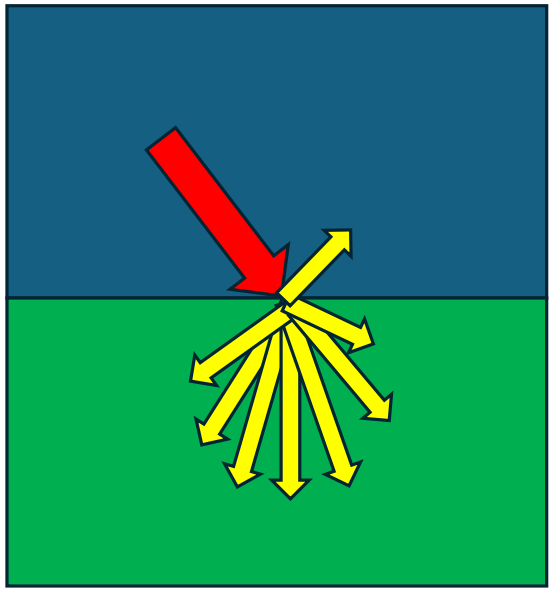
Gold to Silicon Interface

```
g_go_si= g_AMM(gold.v_l, silicon.v_l, gold.v_t, silicon.v_t, gold.density, silicon.dens
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 the come from so $\alpha_{A\to B,j}$ is not a function of θ_A.
- The phonon does not know which mode it came from $\alpha_{A\to B,j} \rightarrow \alpha_{A\to B}$.
- We assume that there is no absorption at the boundary.

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

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

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

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

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

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 $\alpha_{A\to B}$:

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

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

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

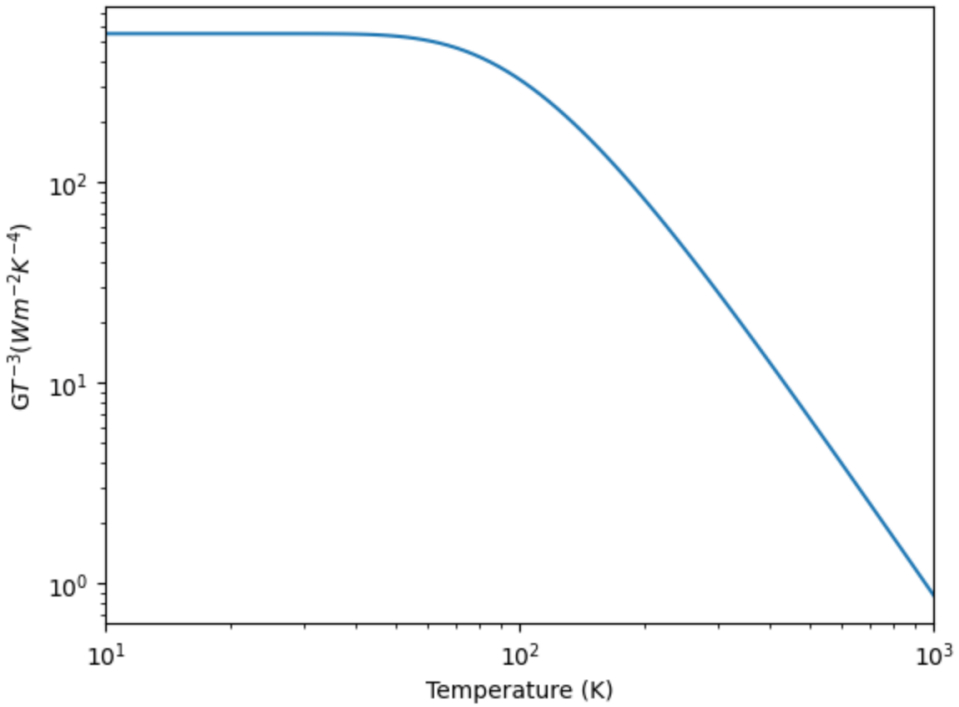
$$\tau_{A\to B} = \frac{1}{2} \frac{\sum_j v_{B,j}^{-2}}{\sum_j v_{B,j}^{-2} + \sum_j v_{A,j}^{-2}}$$

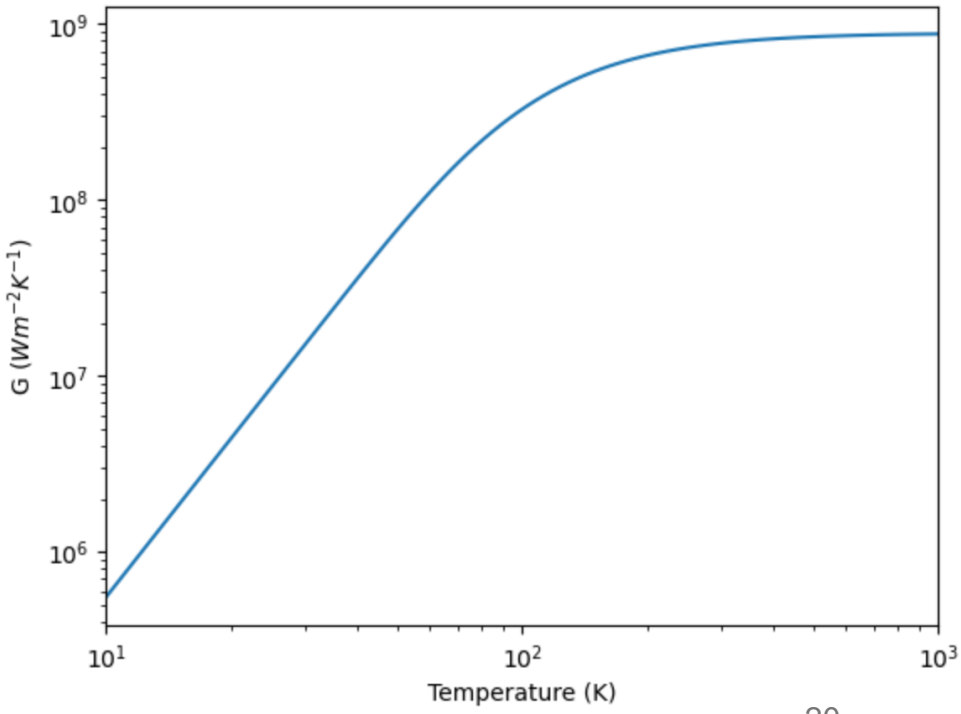
$$G = \frac{\tau_{A\to B} k_B^4 T^3}{4\pi^2 \hbar^3} \left[\frac{1}{v_{A,l}^2} + \frac{2}{v_{A,t}^2} \right] \int_0^{x_D} x^4 \frac{e^x}{(e^x - 1)^2}\, dx$$

Temperature dependent DMM

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

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





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.d
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
```

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.dens
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
```

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/m^2/K^4
```

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")
```

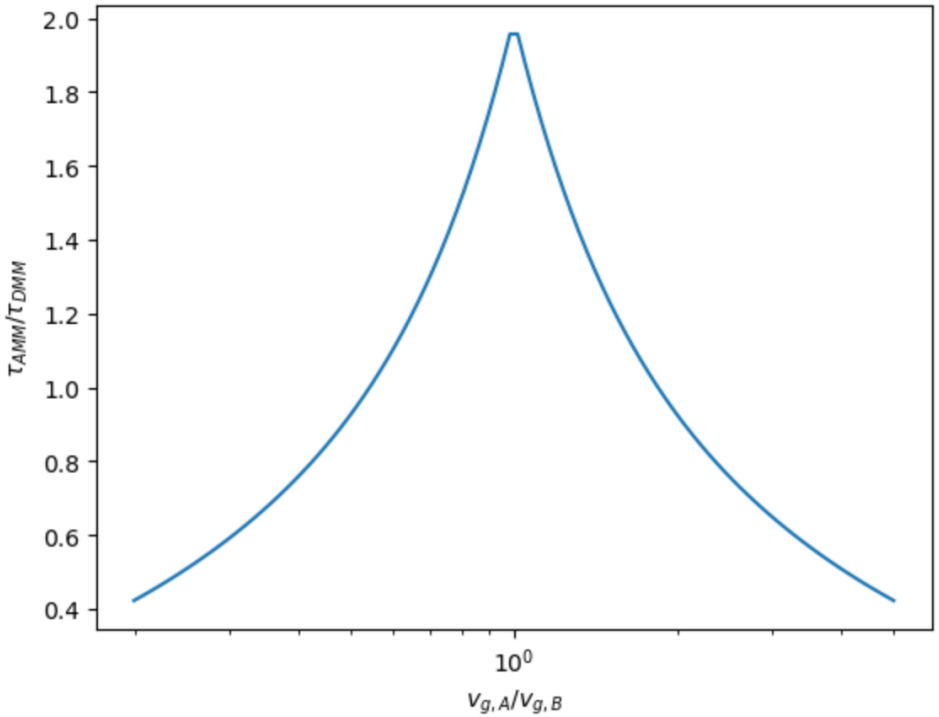
```
Gold to Quartz interface: 1336.20 W/m^2/K^4
```

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")
```

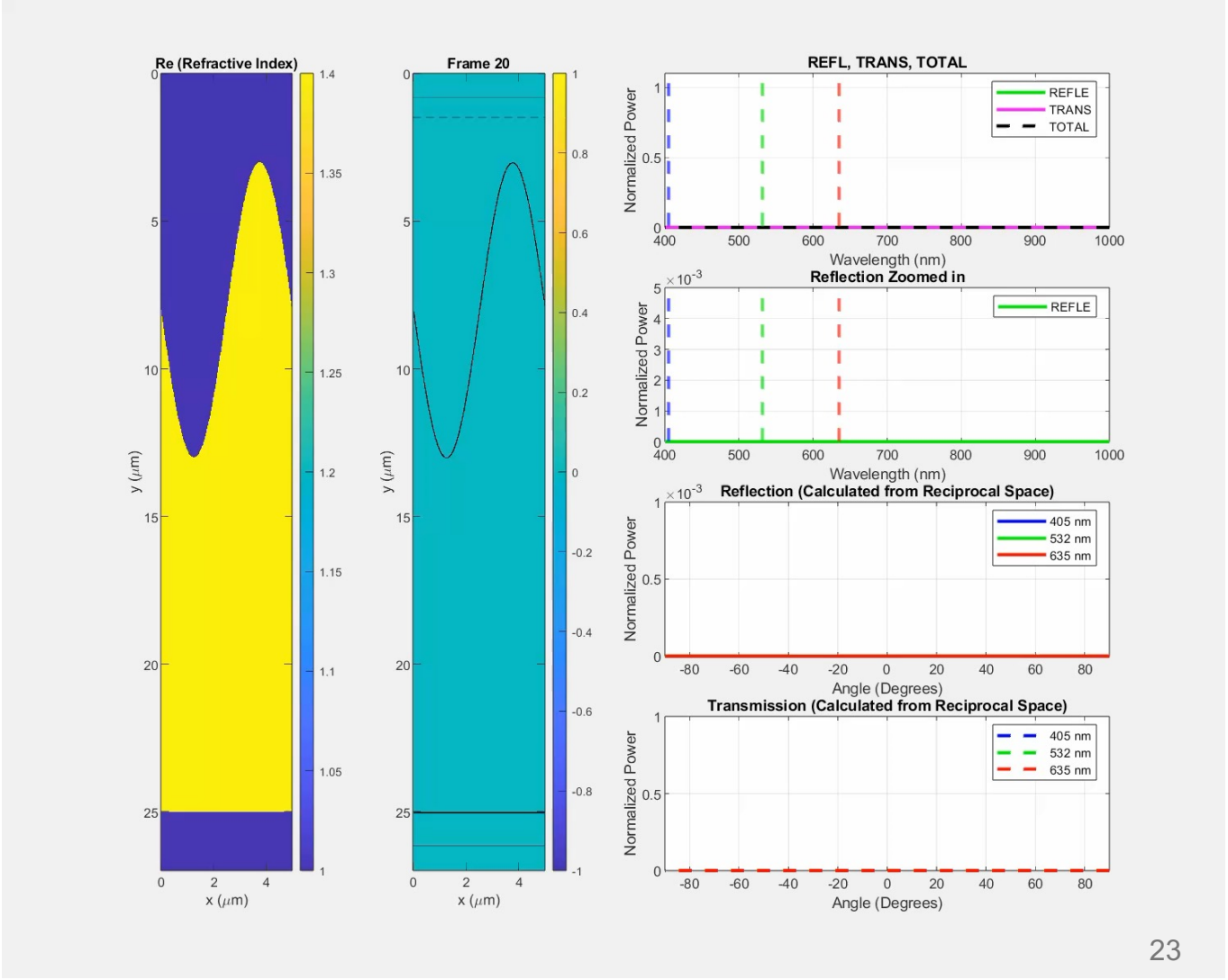
```
Gold to Silicon interface: 792.78 W/m^2/K^4
```

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


Re (Refractive Index)
Frame 20
REFL, TRANS, TOTAL
REFLE
TRANS
TOTAL
Normalized Power
Wavelength (nm)
Reflection Zoomed in
Reflection (Calculated from Reciprocal Space)
405 nm
532 nm
635 nm
Angle (Degrees)
Transmission (Calculated from Reciprocal Space)
y (μm)
x (μm)

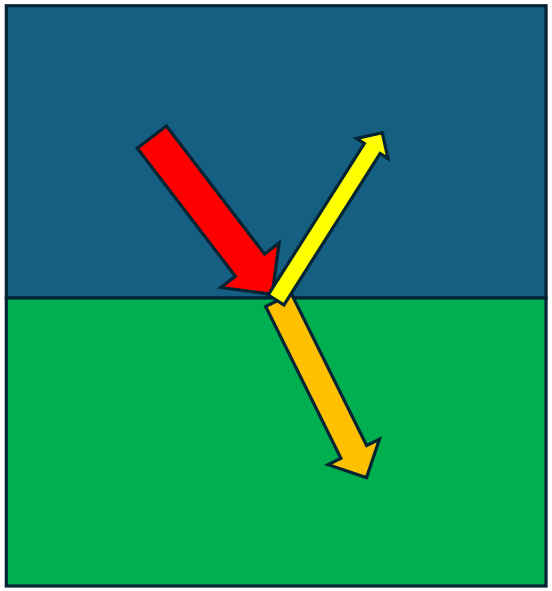
Additional Slides

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.

$$R_s = \left|\frac{Z_2\cos(\theta_i) - Z_1\cos(\theta_t)}{Z_2\cos(\theta_i) + Z_1\cos(\theta_t)}\right|^2 \qquad T_s = 1 - R_s$$

$$R_p = \left|\frac{Z_2\cos(\theta_t) - Z_1\cos(\theta_i)}{Z_2\cos(\theta_t) + Z_1\cos(\theta_i)}\right|^2 \qquad T_p = 1 - R_p$$

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 simply it to grasp basic understanding.
- This assumption does not allow total internal reflection. However, it is a huge simplification but necessary.

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

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