Light absorption and electron-phonon scattering in Cs_2Te photocathodes

1. Optical properties and models
2. Electron-phonon scattering effects and calculations
3. Contribution of scattering effects to QE in the presence of penetrating fields
4. Next steps

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Motivation

→ "**Single electron emission**" (without collective effects) not well fitting to photoemission measurements in **space charge dominated regime**

→ Understanding of **slice emittance formation** and optimization of projected transverse emittance requiring improved photoemission modeling

→ Field effects (previously) considered for **"electron escape"** (3^{rd} step of Spicer's) to the vacuum (close to but outside of surface), but not yet for **"electron transport"** (2^{nd} step) to the cathode surface (beneath it)

To dos:

→ Establish modeling approaches for **light absorption** and **electron scattering** (first without fields)

→ Evaluation of (optical + band structural) property parameters for Cs_2Te (missing in general)

→ Introduce **field (RF + SP-CH + laser) dependencies** to electron scattering process (first with RF fields)

→ Characterize improved emission model by **measurements**

→ Simplify the model for **PIC simulations** and implement it with a suitable numerical tool

Photoemission in a nutshell

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Work function Φ
- Band gap E_g
- Electron affinity E_a
- Schottky(-like) effects
- Any other factors that may affect E_g and E_a

Note that,
$\Delta E_g \rightarrow \Delta m_{eff} \rightarrow \Delta \mu \rightarrow \Delta v_d \rightarrow \Delta E_k$

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Relaxation time τ
- Electron-electron scattering
- Electron-phonon scattering
  - Acoustic phonon
  - Polar optical phonon
- Electron-impurity scattering

Electron energy E_k

Electric fields E_{in}

Note that, temperature plays.

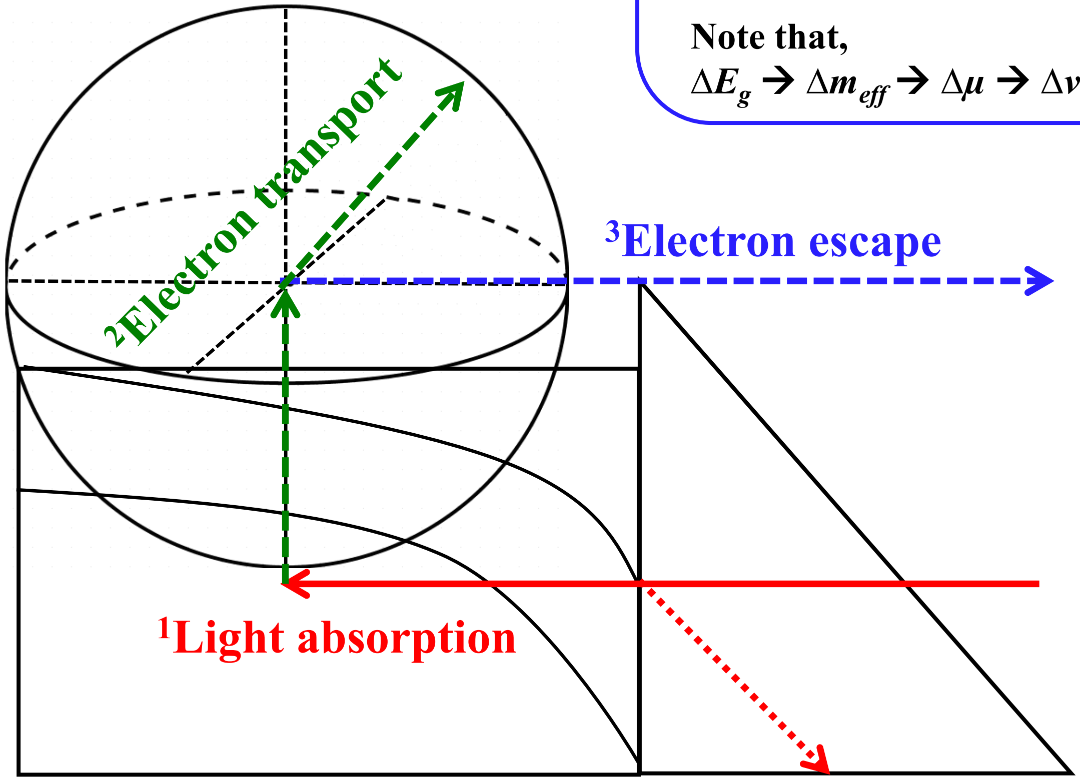
E_k

m_{eff}/τ
$(1/\mu)$

1

Reflectivity R
Penetration depth δ
Dielectric constant ε

All can be determined from (n-k) data. n: refraction index; k: extinction coefficient



Analysis of measured optical property parameters of Cs_2Te

Refraction index n; Extinction coefficient k; Reflectivity coefficient R; Penetration depth δ; Permertivity ε_r

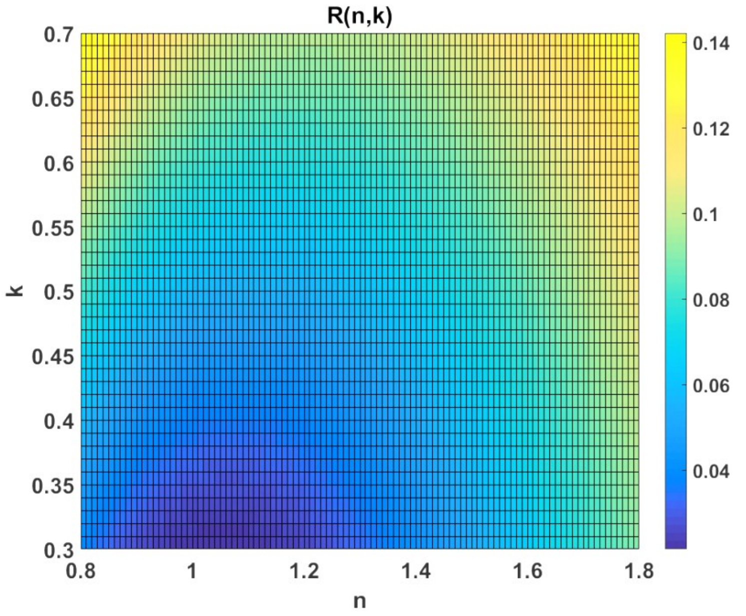
- ❑ Complex refraction coefficient of materials: $\hat{\boldsymbol{n}} = \boldsymbol{n} + \boldsymbol{ik}$
- ❑ Data* (λ ∈**[250 517]nm**) from sets of reflectivity measurements and dispersive analysis→ $\boldsymbol{n} \in$ **[0.8 1.8]**; $\boldsymbol{k} \in$ **[0.3 0.7]**;
- ❑ Numerical analysis with (n, k) data sets (250-517 nm)

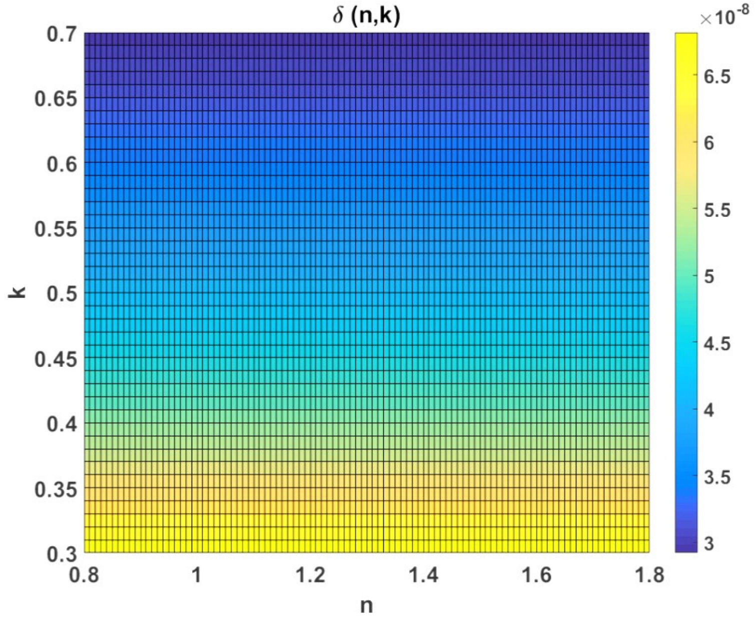
Cross-Refs: for CsI,
1. $\varepsilon_r \leq 9$ @ [113 310]nm
2. $\varepsilon_r \approx 5.65$ @1MHz, data for Cs_2Te missing!

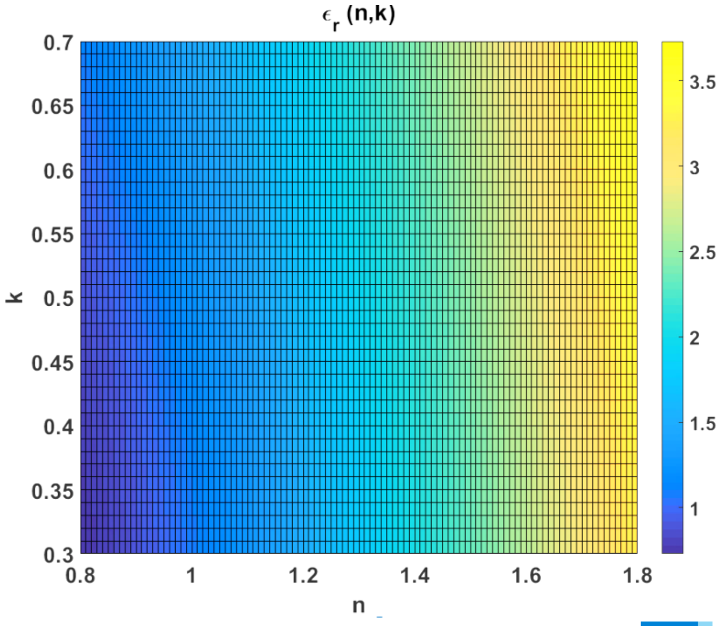
$$\boldsymbol{R} \approx \frac{(n-1)^2+k^2}{(n+1)^2+k^2} \in [2.15\ 14.21]\%$$

$$\boldsymbol{\delta} \approx \frac{\lambda}{4\pi k} \in [29\ 68]\text{nm} @\ 257\ \text{nm}$$

$$\boldsymbol{\varepsilon_r} \approx (n-ik)^2 \in [0.73\ 3.73]$$





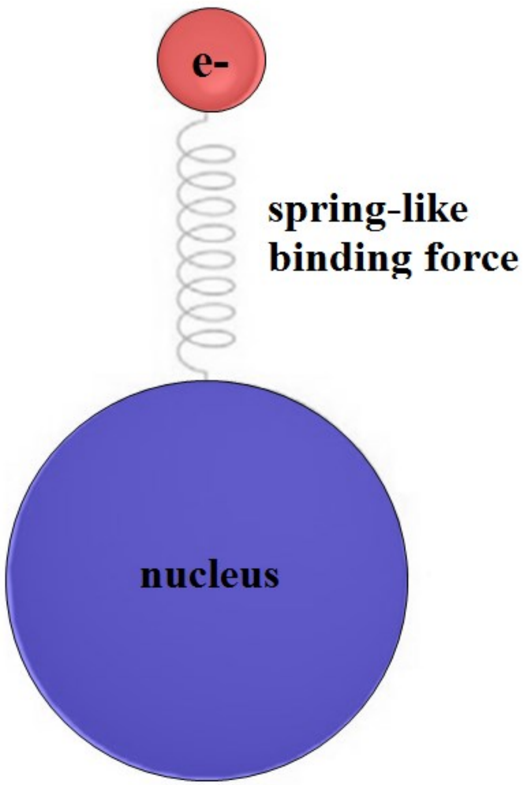


* D. Sertore, INFN Milano - LASA

Deep penetration depth for thin film cathode

Formulizing (n, k) dependencies based on the Drude-Lorentz model

n: refraction index; k: extinction coefficient; $\hat{n} = n + ik$ → optical properties



Lorentz oscillator model

- ❑ Dispersive response of materials to external driving force (fields) by influencing the intrinsic wave impedance
- ❑ Intrinsic wave impedance $\eta(\omega) = \frac{\eta_0}{n(\omega)}$ $\quad n(\omega) = \frac{c}{v_p}$
- ❑ Lorentz oscillator system
  - "**Dipole** motion" harmonically responding to the driving **field**
  - **Restoring** (Coulomb) force trying to maintain system equilibrium
  - Dampening term modeled by m_{eff}/τ

Formulizing (n, k) dependencies based on the Drude-Lorentz model

Mathematical description

Contributions of free carriers(τ)

$$\begin{cases} n^2 - k^2 \propto \omega, \tau(\omega, T, E_k, E_g), E_g \approx A_{static}\Psi + A_{hf}(1-\Psi) + DL_{sum} \\ 2nk \propto \omega, \tau(\omega, T, E_k, E_g), E_g \approx (A_{static} - A_{hf})\Phi - DL_{prod} \end{cases}$$

Contributions of lattice vibration (ω_T)

with

$$\Psi = \frac{\omega_T^2(\omega_T^2 - \omega^2)}{(\omega^2 - \omega_T^2)^2 + (\Upsilon\omega\omega_T)^2}, \quad \Phi = \frac{\Upsilon\omega\omega_T^3}{(\omega^2 - \omega_T^2)^2 + (\Upsilon\omega\omega_T)^2} \quad DL_{sum} = -\frac{(\omega_p\tau)^2}{1 + (\omega\tau)^2},$$

$$DL_{prod} = \frac{\tau\omega_p^2}{\omega[1 + (\omega\tau)^2]} \quad \omega_p = \sqrt{\frac{4\pi\rho\alpha_{fs}\hbar c}{m}} \quad m = \frac{E_g}{E_{Ry}} m_0$$

ω: light frequency
c: speed of light
$\hbar$: Planck constant, h/2π
E_g: band gap energy
E_{Ry}: Rydberg energy, ~13 e'
m_0: electron rest mass
m: electron effective mass
ρ: number density
τ: relaxation time
ω_T: transverse optical mode frequency
ω_p: plasma frequency
α_{fs}: fine structure constant
Υ: Lorentz coefficient
A_{static}: static (dielectric) constant
A_{hf}: high frequency (dielectric) constant

- Given **ω~10^{15}(laser),** ω_p~10^{13} for 10^{17}/cm^3, τ~100×10^{-15} contributions of free carriers **~10^{-4}**
- Given **ω~10^9(RF),** ω_p~10^{13} for 10^{17}/cm^3, **τ~100×10^{-15}** contributions of free carriers **~1**
- Given **ω~10^9(RF),** ω_p~10^{13} for 10^{17}/cm^3, **τ~50×10^{-15}** contributions of free carriers **~0.3**

Penetrating RF fields may affect τ and modify (n-k), thus influencing optical properties

A rough fit to the reflectivity measurements for Cs_2Te

Reflectivity coefficient R

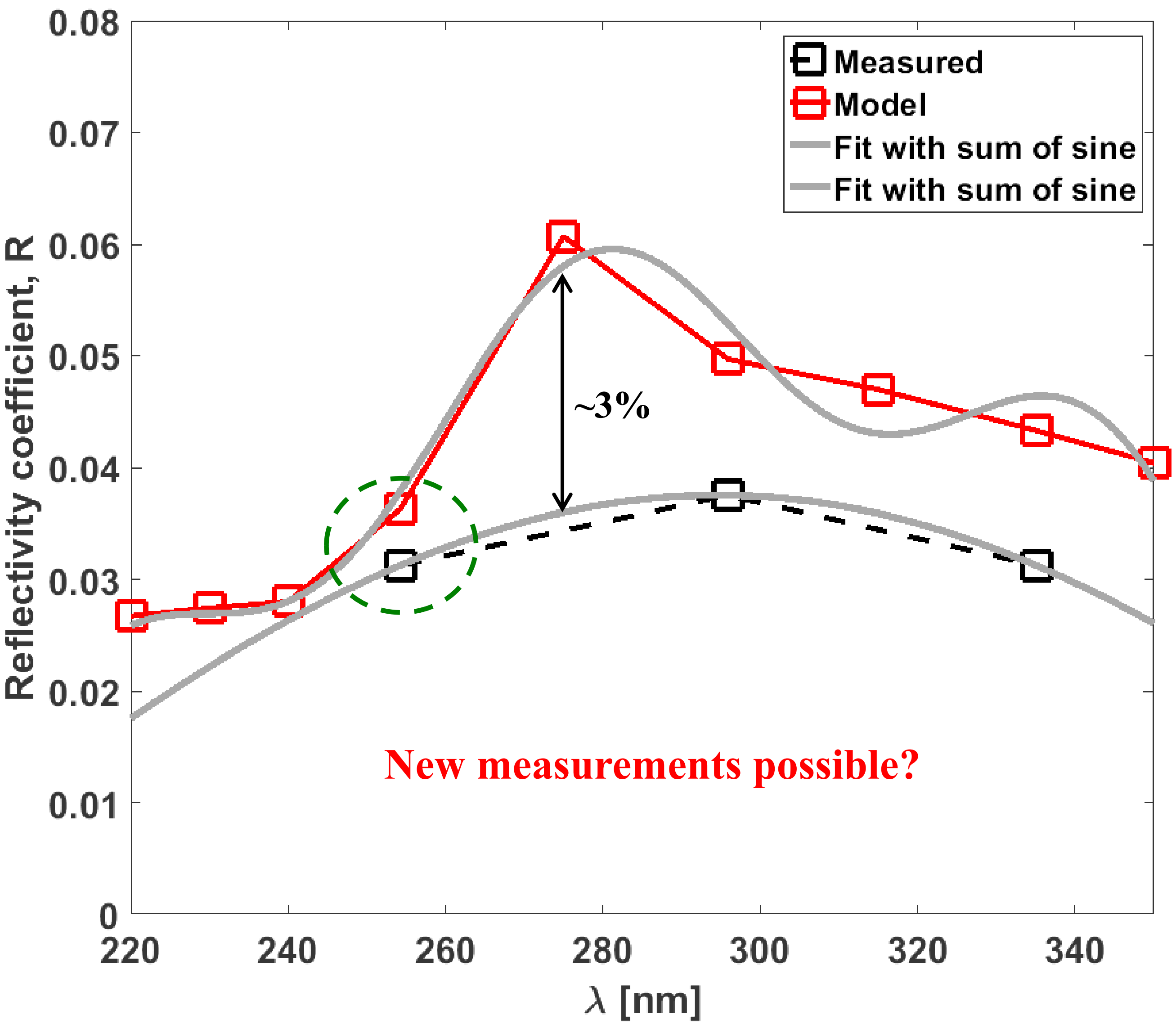
- No one to one data now from (n, k) to the reflectivity
- The fit done by scanning (n, k) range for smallest ΔR w.r.t. measurements satisfying the Drude-Lorentz's equation with lowest errors

$$@\ \lambda = 257\ nm$$

$$R \approx \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2} \approx 4\%$$

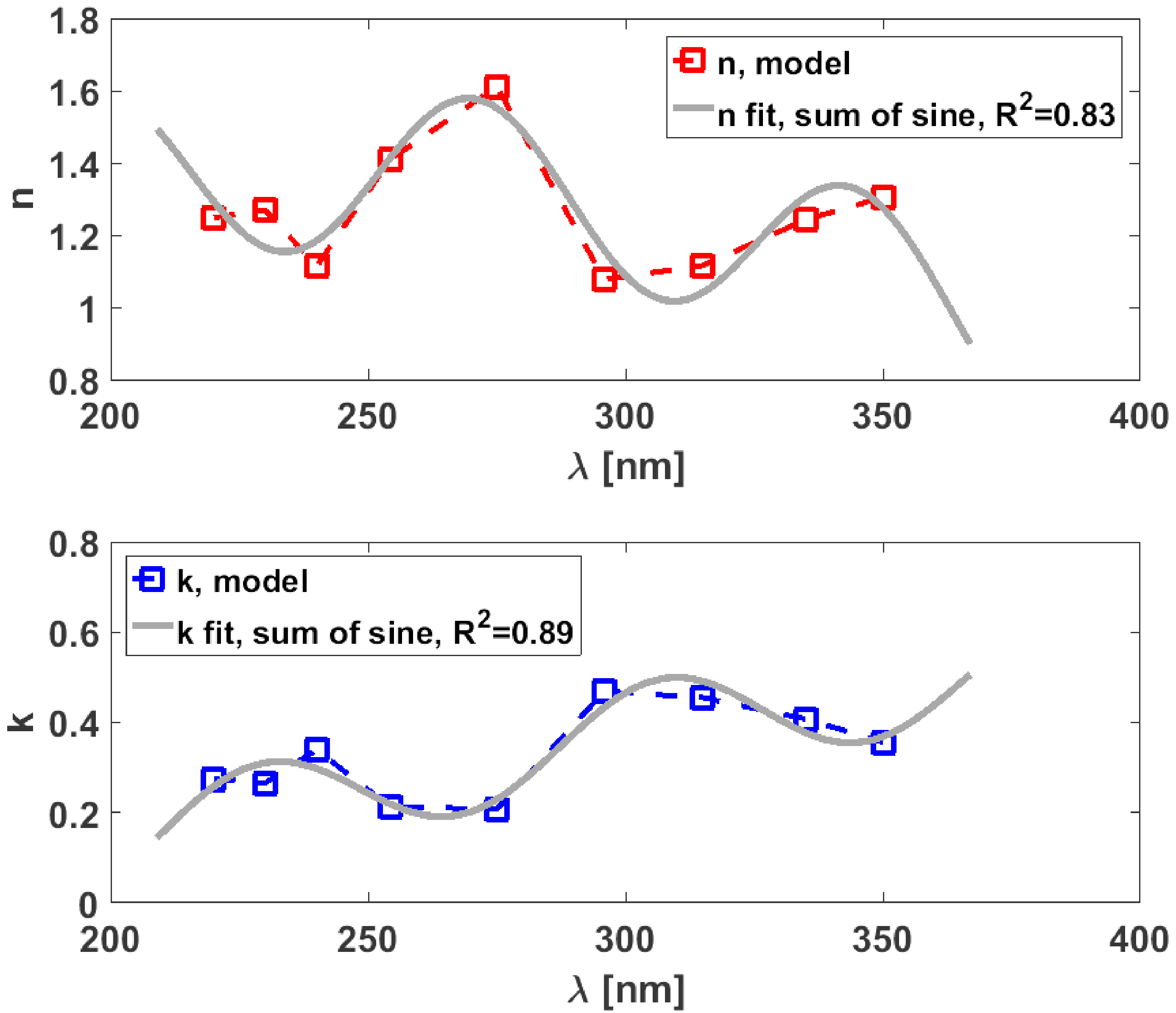
$$\delta \approx \frac{\lambda}{4\pi k} \approx 90\ nm$$

$$\varepsilon_r \approx (n - ik)^2 \approx 2$$



(n, k) data given by D-L model

Refraction index *n* and extinction coefficient *k*

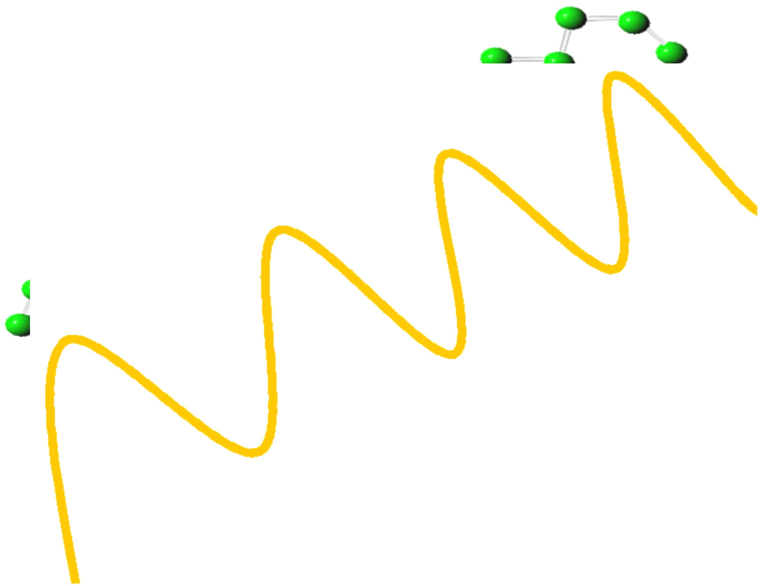


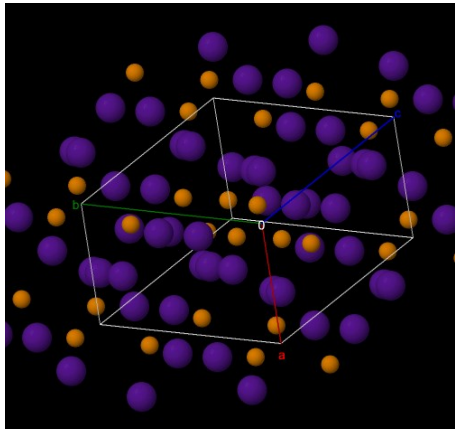
Scattering effects in Cs_2Te

- ❑ Electron-electron scattering → **dominating for metal cathodes**

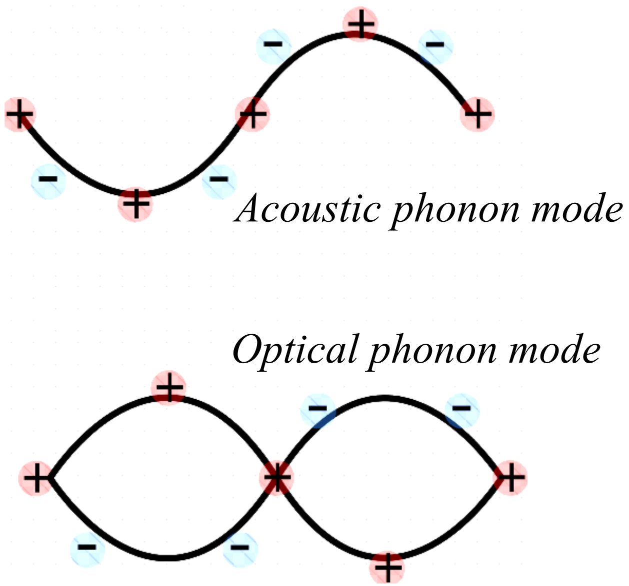
- ❑ **Electron-phonon scattering → dominating for semiconductor cathodes**
  - **Polar optical phonon** (vibration within a cell, v_g=0, standing…)
  - **Acoustic phonon (**vibration of a cell, v_g>0, travelling…**)**

- ❑ Electron-impurity(defect) scattering → presumably much weaker effect than others





Sketch of a 3D Cs_2Te lattice structure



Scattering effects in Cs_2Te

Acoustic phonon [a]

$$\frac{1}{\tau_{ac}} = \frac{4m\Xi^2 k(k_B T)}{\pi\hbar^3 \rho v_s^2}\left(\frac{T}{\Theta}\right)^5 W_-\left(5,\frac{\Theta}{T}\right) \propto E_k, E_g, T$$

Polar optical phonon [b]

$$\frac{1}{\tau_{pop}} = 2\omega_q \Delta\epsilon \left[2\frac{1}{\exp\left(\frac{\hbar\omega_q}{k_B T}\right)-1}+1\right]\frac{16u^2+18u+3}{3(1+2u)\sqrt{u(u+1)}} \propto E_k, E_g, T$$

Matthiessen's rule

$$\frac{1}{\mu} = \sum_i \frac{1}{\mu_j} \quad \rightarrow \quad \frac{1}{\tau} = \sum_i \frac{1}{\tau_j}$$

Band structural parameters of Cs_2Te need to be calculated for modeling the scattering effects.

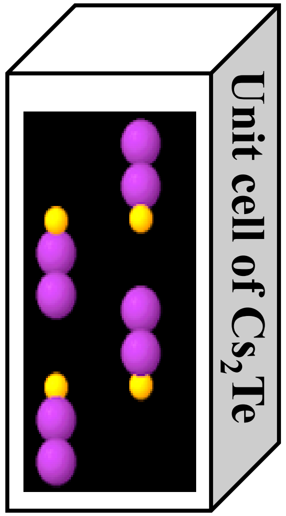
$$hk = 2\pi\sqrt{2mE_k} \qquad E_k = h\omega - E_g - E_a \qquad u = E_k/E_g$$

Note that, other scattering scheme may exist, but probably not significantly contributing

[a] K. Jensen 2007 ("emission from metals and cesiated surfaces")

[b] K. Jensen 2008 ("an alpha-semiconductor model")

Calculation of band structural parameters for Cs_2Te



Physical Property	Calculation for Cs_2Te	Reference to Cs_3Sb
Mass density	$\rho = \frac{4(2M_{Cs} + 1M_{Te})}{\Delta V} \approx \mathbf{3.99\ g/cm^3}$ *	$4.519\ g/cm^3$
Sound velocity	$v_s = \sqrt{\frac{c_{11}}{\rho}} \approx \mathbf{5484\, m/s}$ **	5153 m/s
Phonon energy (lowest mode)	$\hbar\omega_q = \frac{4\pi\hbar v_s}{\lambda_{pm}} \approx \mathbf{0.0767 eV}$	0.05 eV
Average ionic radii	$l \approx \mathbf{0.194\ nm}$ ***	0.14 nm
Deformation potential	$\Xi = Dl \approx \mathbf{9.7\ eV}$ ****	7 eV
Bloch–Grüneisen function	$W_{-}\left(5, \frac{\Theta}{T}\right) \approx (\frac{\Theta}{T})^4/4$	
Fine structure coefficient	$\alpha_{fs} = e^2/4\pi\epsilon_0\hbar c \approx 1/137.1$	
Effective mass	$m = \frac{E_g}{E_{Ry}} m_0 \approx \mathbf{0.24\ m_0}$	$0.1176\ m_0$

* Thermal expansion not considered

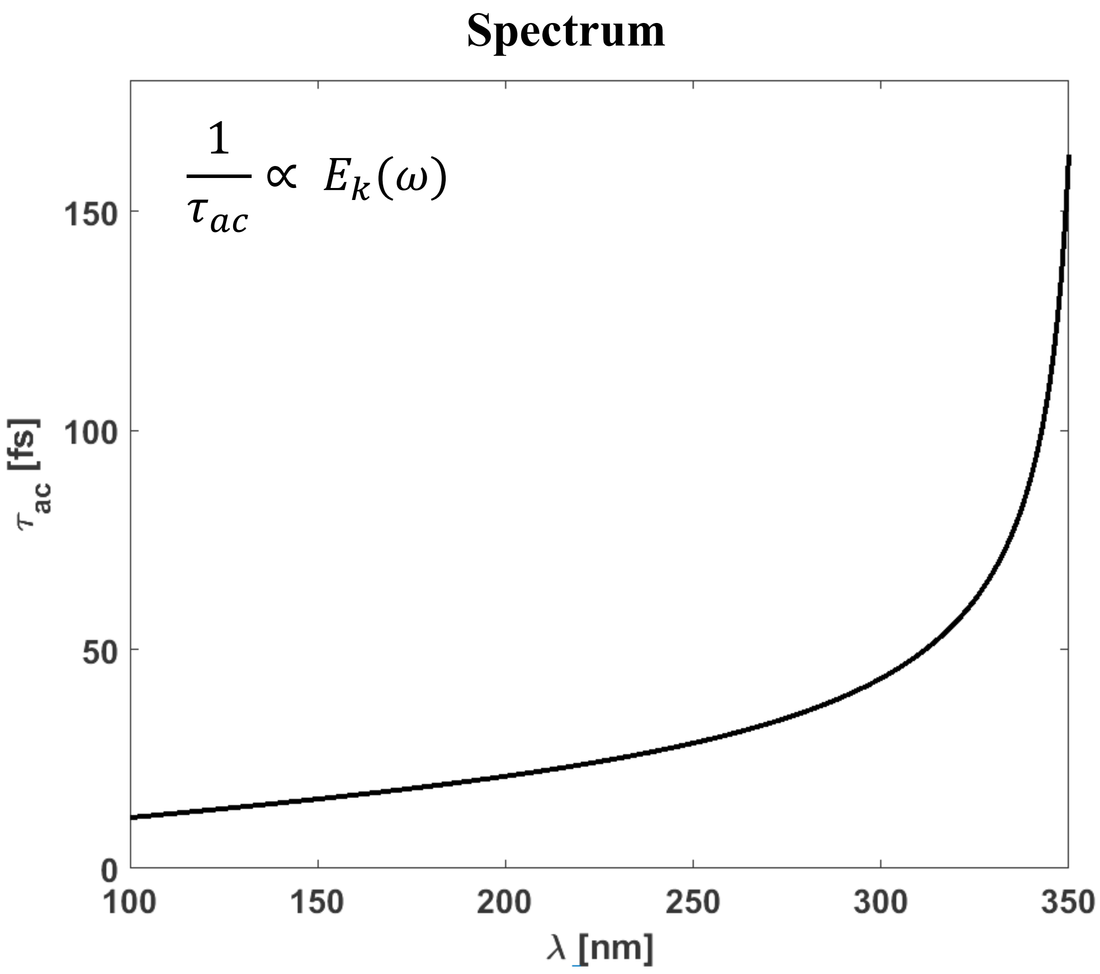
** Generic elastic constant, $c_{11} = 12\times10^{10}\ N/m^2$

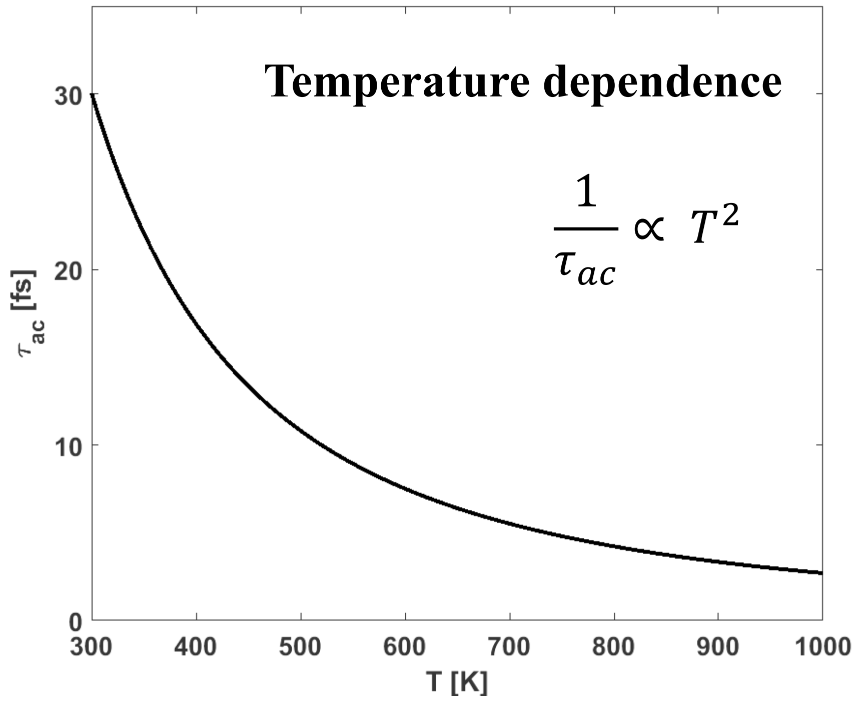
*** Average of the ionic radii of *Cs* and *Te*

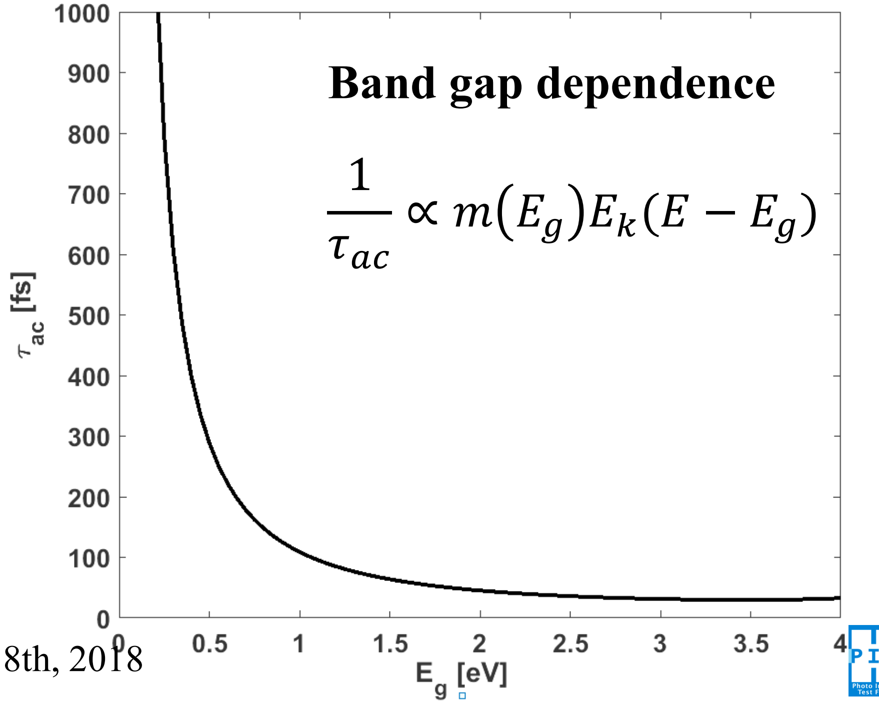
**** Mean deformation potential constant $D = 5\times10^8\ eV/cm$

Calculated effective relaxation time

Acoustic phonon scattering, τ_{ac}

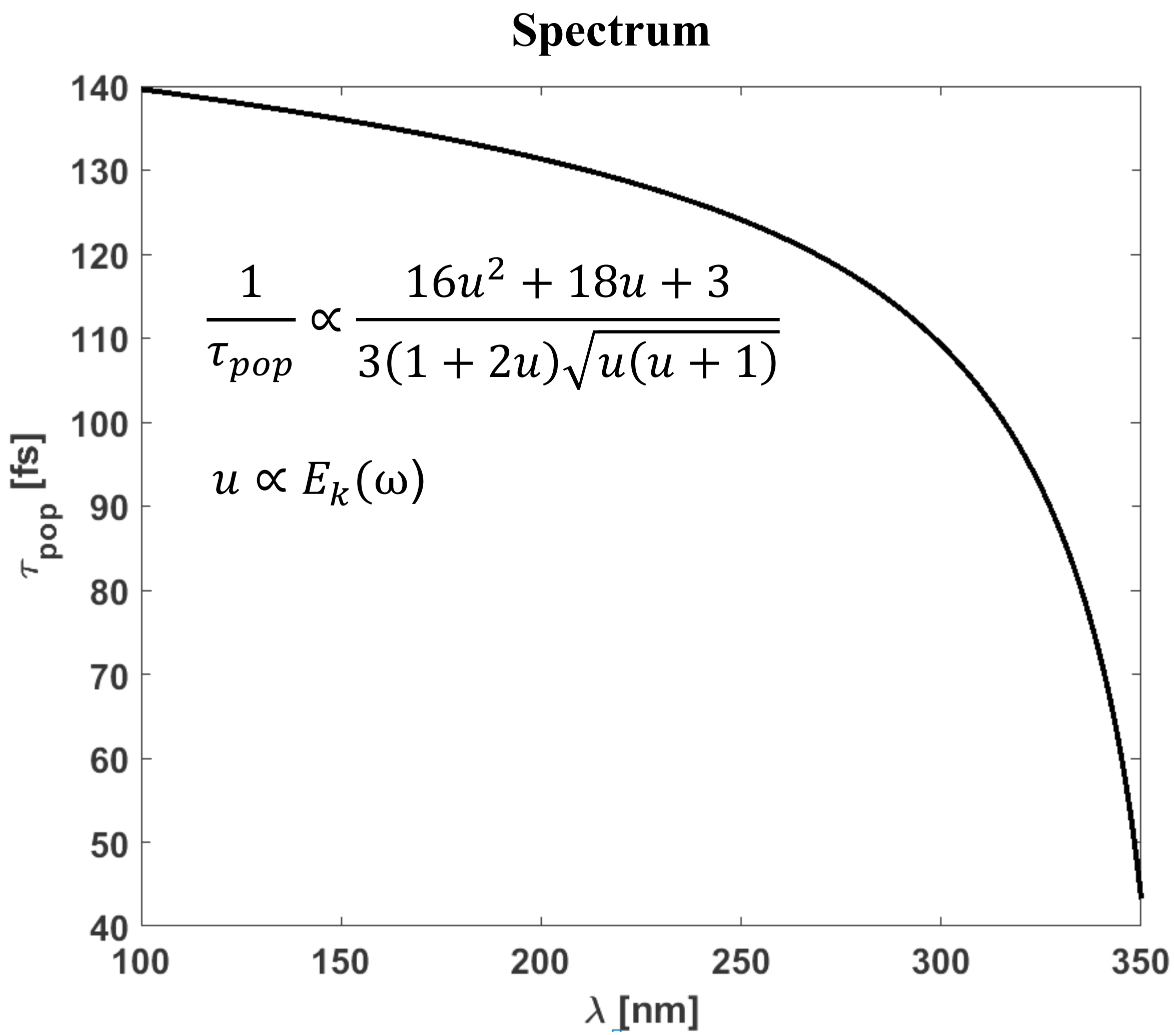


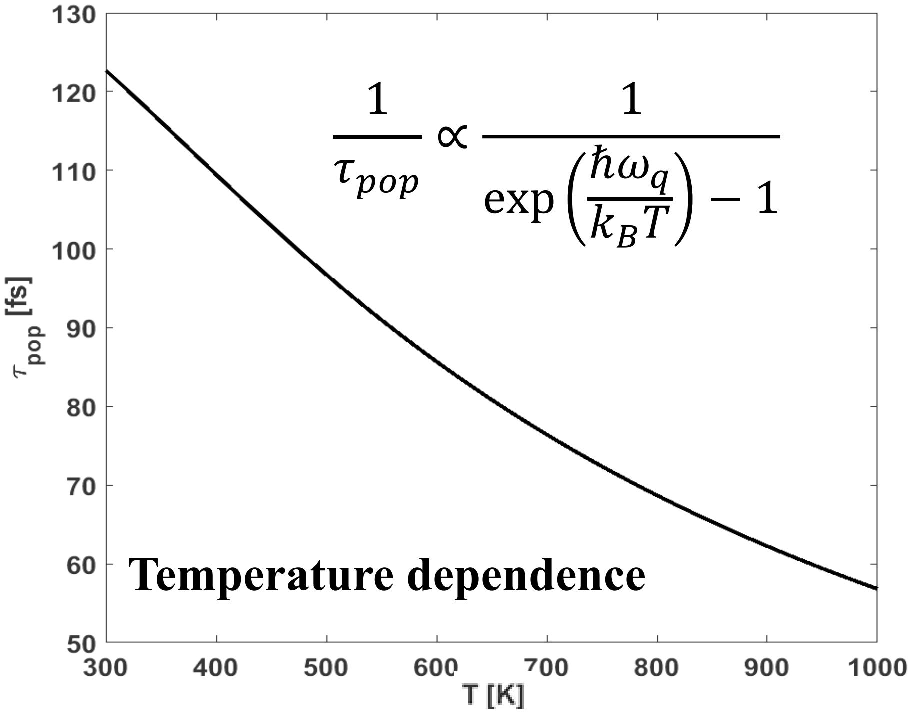


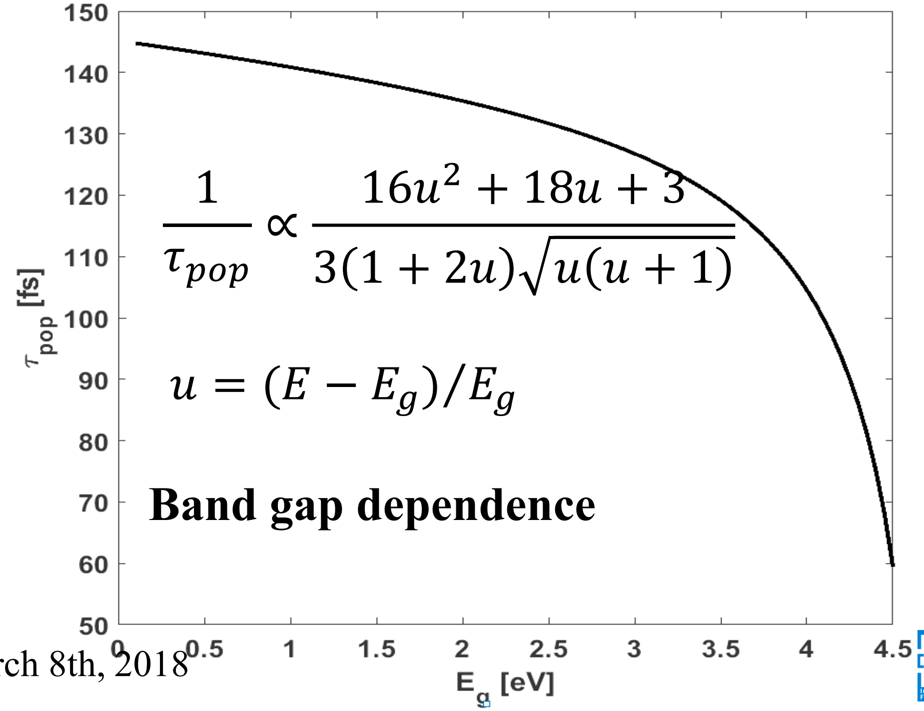


Calculated effective relaxation time

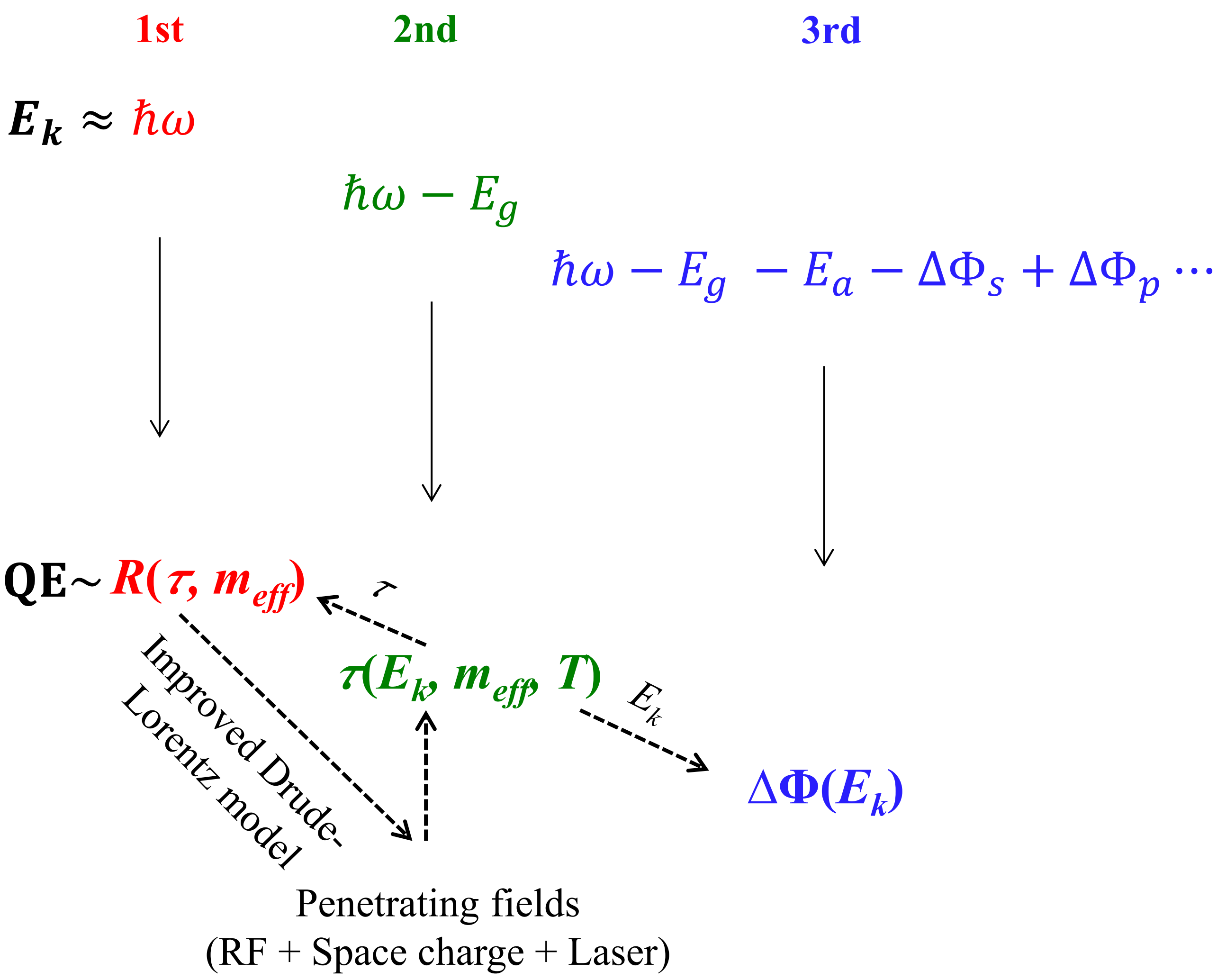
Optical phonon scattering, τ_{pop}







Modeling of electron mobility in presence of penetrating fields



$$\begin{cases} l(E_k) = \tau(E_k)v_d \\ v_d = \mu E_{in} \\ \mu = \dfrac{q}{m_{eff}(E_g)}\tau(E_k) \end{cases}$$

l : mean free path
v_d: drift velocity
E_{in}: penetrating fields
μ: electron mobility

$$\rightarrow l(E_k, E_g, t) = \frac{q\tau^2(E_k)}{m_{eff}(E_g)} E_{in}(t)$$

$$\rightarrow E_{in}(t) \quad \rightarrow E_{RF} \rightarrow E_{out}/\epsilon_r(f = 1.3\text{GHz})$$
$$\rightarrow E_{SPCH}$$
$$\rightarrow E_{Laser}\ (1.2\text{PHz}) \rightarrow E_0 e^{-\alpha z}$$

→ If laser and RF uncoupled, l can be calculated in x and z direction, respectively

How the modified mean free path integrated into the overall QE?

Contributions of each step to the overall QE

- ❑ Factor of reflectivity $\propto 1 - R(\omega, n(\tau), k(\tau))$

- ❑ Factor of work function $\propto \sqrt{1 + \frac{\hbar\omega - E_g - E_a(\pm\Delta E_k)}{E_a}}$

- ❑ **Factor of scattering effect** $\rightarrow l(E_k, E_g, t) = \frac{q\tau^2(E_k)}{m_{eff}(E_g)} E_{in}(t)$

integration over absorption depth

$$\rightarrow f_\lambda(cos\theta) = \frac{\int_0^\infty exp\left(-\frac{z}{\delta} - \frac{z}{lcos\theta}\right) dz}{\int_0^\infty \exp\left(-\frac{z}{\delta}\right) dz}$$

Fraction of surviving electrons from scattering

θ: escape cone angle, $x = cos\ \theta$

integration over escape angle and energy

$$\rightarrow \frac{\int_{E_a}^{\hbar\omega - E_g} E \int_{\sqrt{E_a/E}}^{1} x f_\lambda(x, p) dx dE}{\int_0^{\hbar\omega - E_g} E \int_0^1 x dx dE}$$

Next steps

- ✓ Light absorption modeling requires dispersive reflectivity measurements for determining optical parameters
- ✓ Relative permittivity @ 1.3GHz better determined from proper measurements (maybe already at HZDR) or (if no choice) considered as a fitting parameter
- ✓ Some principle test simulations on the scattering rates in the presence of RF fields can be done first