Monte Carlo Simulation Study of Cs_2Te

PITZ (DESY)

Gowri Adhikari

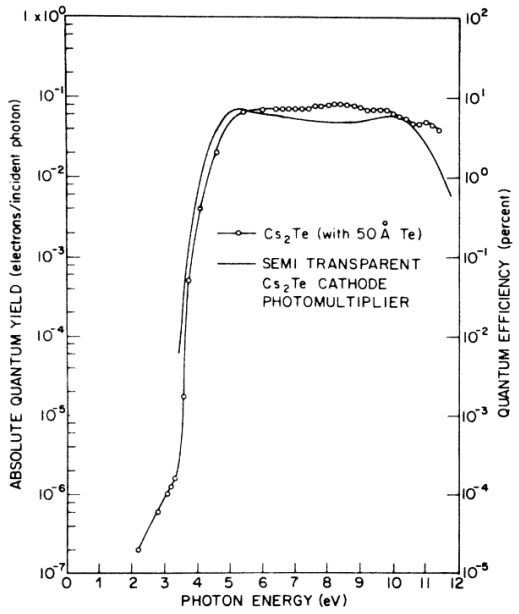
U.S. DEPARTMENT OF ENERGY
Office of Science

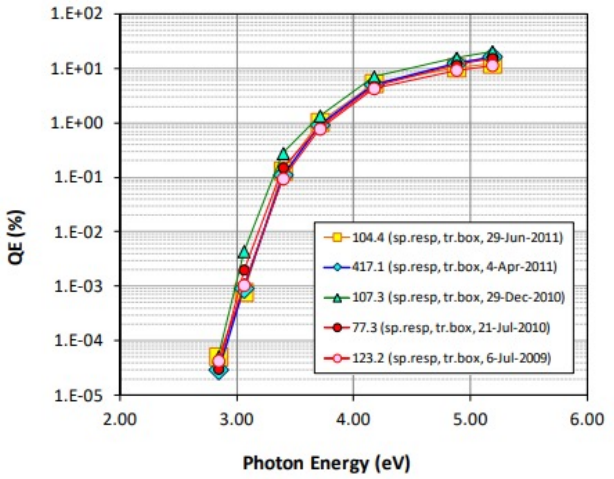
SLAC NATIONAL ACCELERATOR LABORATORY

Outline

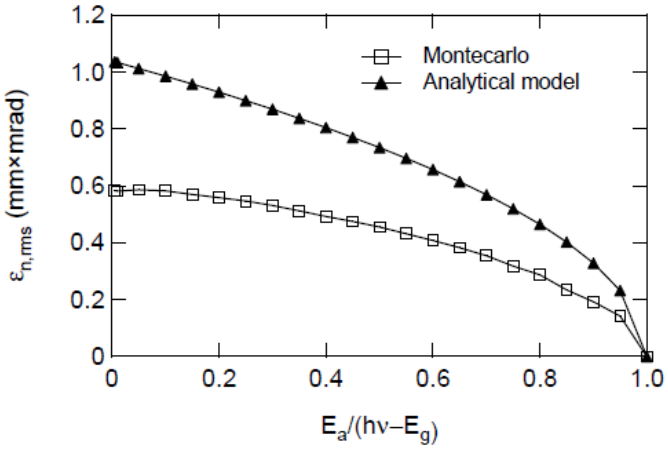
- Introduction
- Density Functional Theory (DFT)
  - Band structure
  - Effective mass
- Three-step model
- Absorption profile
- Initial parameters for the emission
- Phonon scattering
- Transmission probability
- Quantum efficiency
- Thermal emittance
- Simulation results

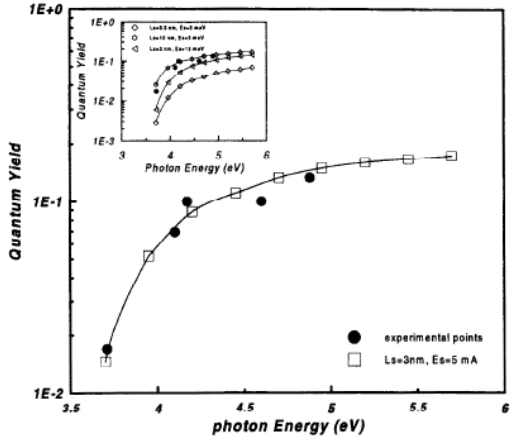
Introduction





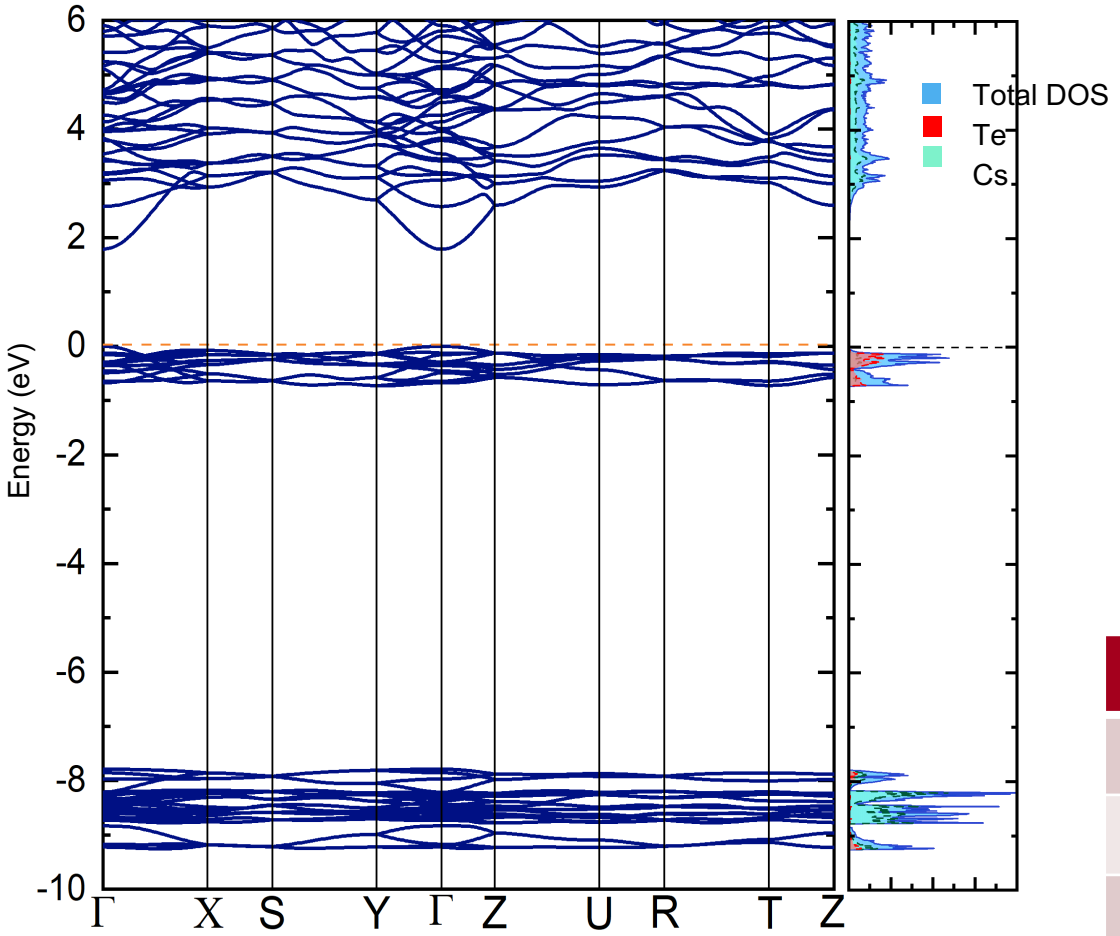
Several experiments have been devoted to characterizing Cs_2Te photocathodes in terms of quantum yield and thermal emittance.

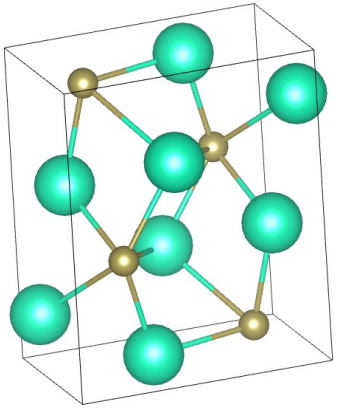




Monte Carlo simulation was applied to simulate the quantum yield dependence on photon energy in Cs_2Te and the transverse emittance dependence on the electron affinity.

Band structure and Density of states – Cs_2Te





Orthorhombic crystal structure
Space group pnma (62)

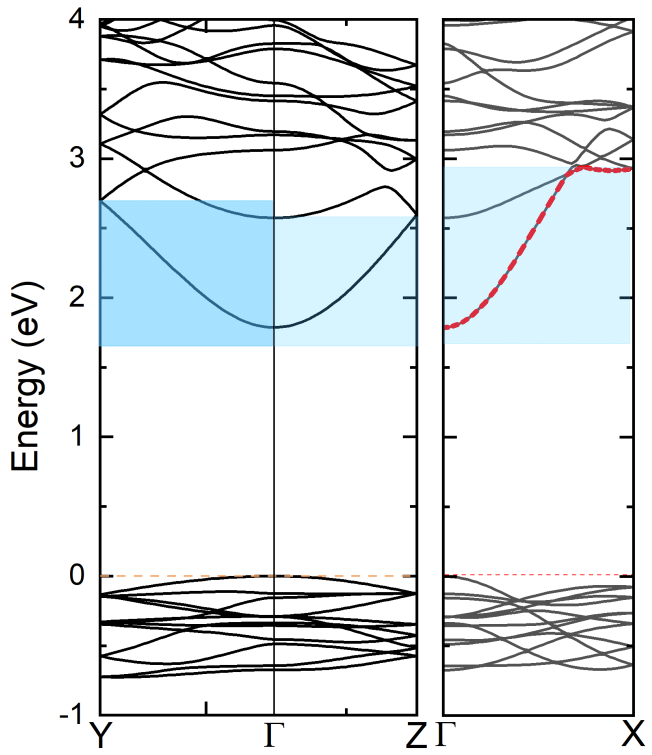
	DFT	Ref (6)	EXP (5)
a (Å)	5.844	5.845	5.871
b (Å)	9.415	9.542	9.109
c (Å)	11.663	11.591	11.474

Band structure and Density of states – Cs_2Te

- A parabolic fit was used to calculate the effective mass using the curvature of the fit.
- The effective mass at the Fermi energy can calculate using

$$m^* = \hbar^2 \left(d^2E \Big/ dk^2 |_{k=k_f} \right)^{-1}$$

Direction	ΓX direction
ΓX direction	0.27 m_0
$Y\Gamma$ direction	0.25 m_0
ΓZ direction	0.27 m_0



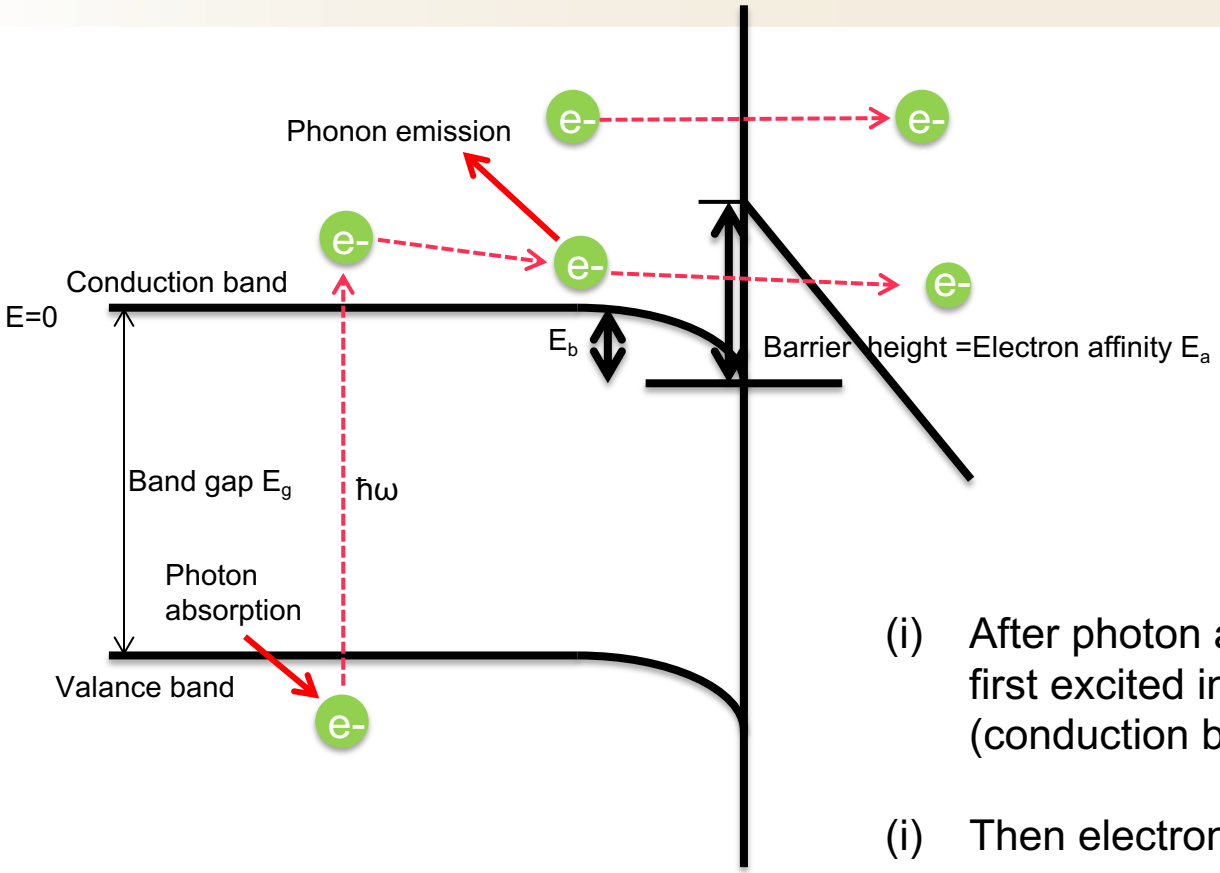
- Electron effective mass roughly estimated using

$$m^* = \frac{E_g m_0}{R_\infty},$$

where m_0- electron effective mass and R_∞ - Rydberg Constant 13.606 eV E_g - band gap.

- According to the above equation m^* is 0.2425 and this value is very close to the DFT calculated effective mass.

Three-step model

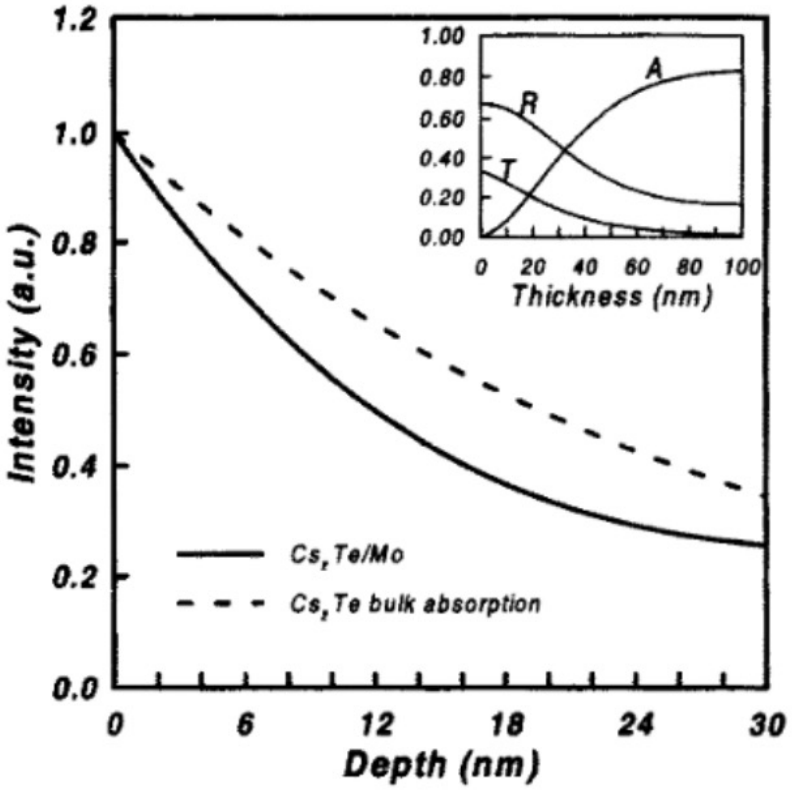


(i) After photon absorption, the electrons are first excited into a higher energy state (conduction band).

(i) Then electrons transfer to the surface with or without scattering.

(i) Finally, the electrons escape into the vacuum.

Absorption profile – Cs_2Te



Absorption profile curve for Cs_2Te bulk and Cs_2Te/Mo interface with a Cs_2Te thickness of 30nm.
Inset- reports the reflectance (R), transmission (T), and absorption (A) of Cs_2Te/Mo as function of Cs thickness.

- The absorbed laser energy decays exponentially along the cathode's thickness.

$$F(s) = F_0 e^{-\alpha(\omega)s}$$

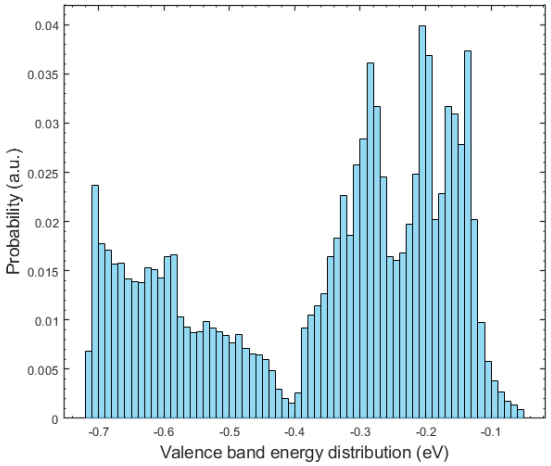
- Absorption coefficient $\alpha(\omega)$ depends on the wavelength.
- The absorption coefficient $\alpha(\omega)$ - 0.0577 was obtained by interpolating the figure on the left side [03].
- In this simulation, I consider 15 nm thickness.
- Assumption 1 – The absorption coefficient is constant for all photon energies.
- Far from the threshold region, the absorption should not vary significantly.

Initial parameters for an electron

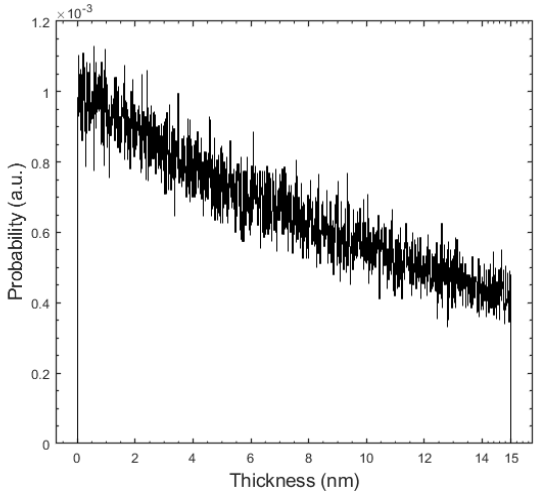
- Assumption 2 - Each photon (no photon=$2*10^5$) emits an electron from the valence band.
- The Density of states (DOS) of the valence band is used to select the number of electrons.
- Conduction band minimum set as the energy zero point.
- This simulation uses the experimental band gap energy (3.3 eV) value.
- Conduction band energy = VB energy + Photon energy - Band gap.
- The position of an electron is calculated using the Monte Carlo simulation.
- $F(s) = \alpha(\omega)e^{-\alpha(\omega)s}$ is the distribution of the position of excited electrons.
- The initial direction was selected using the Monte Carlo simulation assuming all the directions are isotropic.

Distributions for initial variables

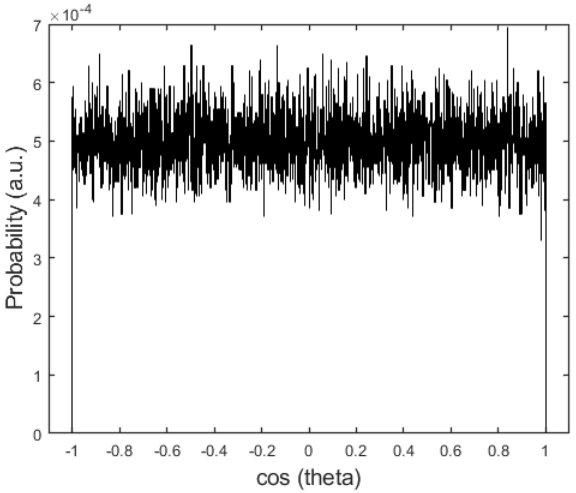
Valence Band Energy, Longitudinal Position, and cos(θ)



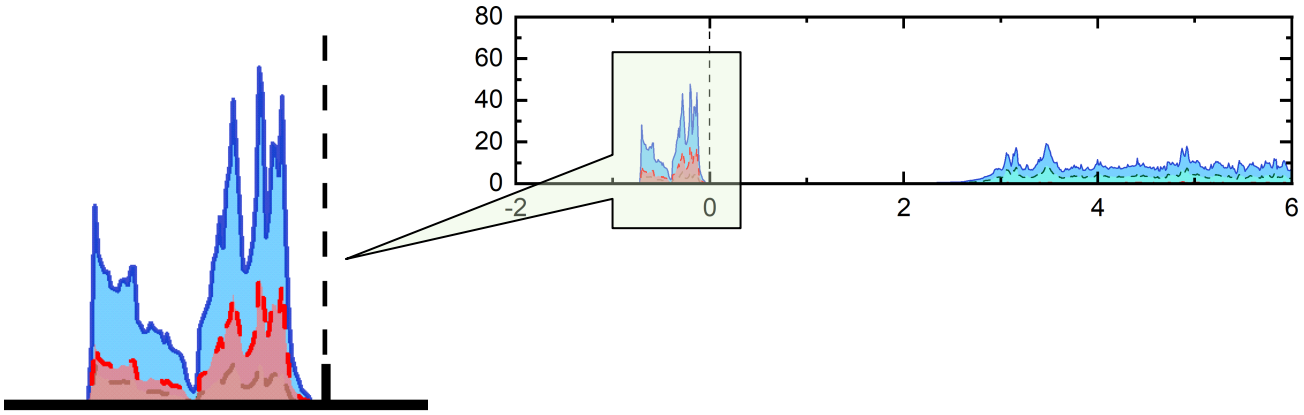
Valence band energy distribution. The bin size is 0.01 eV.



Electron position distribution. The bin size is 0.01 nm.



Cos (θ) distribution. The bin size is 1×10^{-4}.



Phonon Scattering – Cs_2Te

SLAC

Inter valley scattering

- If photon energy is greater than 2*band gap (E_g) the electron-electron scattering dominates.
- For photon energies less than $2E_g$ e-e scattering has a very low probability and electron energy reduces due to electron-phonon scattering.
- For simplicity, only optical phonon scattering and inter valley phonon scattering considered.
- When electrons' energy is high enough to scatter into other valleys, inter valley scattering dominates.
- Inter valley scattering rate

$$\lambda_{i\pm}(E) = \frac{{D_i}^2 {m^*}^{\frac{3}{2}} (N_q + \frac{1}{2} \mp \frac{1}{2})}{\sqrt{2}\pi\hbar^2 \rho E_{ph}} (E \pm E_{ph})^{\frac{1}{2}}$$

+/- - absorption and emission

E_{ph} – phonon energy

D_i – deformation potential 1x10^9 eV/cm

ρ – density of material

Phonon scattering rates

SLAC

Polar optical phonons

- Electrons lie in one band; polar optical phonon scattering is the dominant process.

- Polar optical phonon scattering rate

$$\lambda_{0\pm}(E) = \frac{e^2 m^{*\frac{1}{2}} E_{ph}\left(N_q + \frac{1}{2} \mp \frac{1}{2}\right)}{4\sqrt{2}\pi\hbar^2 \varepsilon_0 \varepsilon_p E^{\frac{1}{2}}} ln \left| \frac{(E \pm E_{ph})^{\frac{1}{2}} + E^{\frac{1}{2}}}{(E \pm E_{ph})^{\frac{1}{2}} - E^{\frac{1}{2}}} \right|$$

$$\varepsilon_p = \frac{1}{1/\varepsilon_\infty - 1/\varepsilon_s}$$

- The Occupation number of the phonon follows the Bose-Einstein statics,

$$N_q = \frac{1}{\exp\left(E_{ph}/k_B T\right) - 1}$$

+/- - absorption and emission

E_{ph} – phonon energy

$\varepsilon_\infty, \varepsilon_s$ - high frequency and static dielectric constant

Phonon scattering cont.

- Scattering rate $\lambda(E)$=$\lambda_{0-} + \lambda_{0+}$, for electrons with energy lower than the minimum of the second lowest band.
  - λ_{0-}/λ, is the possibility of emitting an electron and energy loss E_{ph}.
  - λ_{0+}/λ, is the possibility of absorbing an electron and energy absorption E_{ph}.

- Scattering rate $\lambda(E)$=$\lambda_{0-} + \lambda_{0+}$+ $\lambda_{i-} + \lambda_{i+}$, for electrons with higher energy.
  - $(\lambda_{0-}+\lambda_{i-})/\lambda$, is the possibility of emitting an electron and energy loss E_{ph}.
  - $(\lambda_{0+}+\lambda_{i+})/\lambda$, is the possibility of absorbing an electron and energy absorption E_{ph}.

- The probability for an electron to travel a distance d without suffering a scattering event is $P(\lambda) = \exp\left(-\frac{d}{\lambda}\right)$, where λ is the electron's mean free path.

- After scattering, the change of direction is not isotropic.

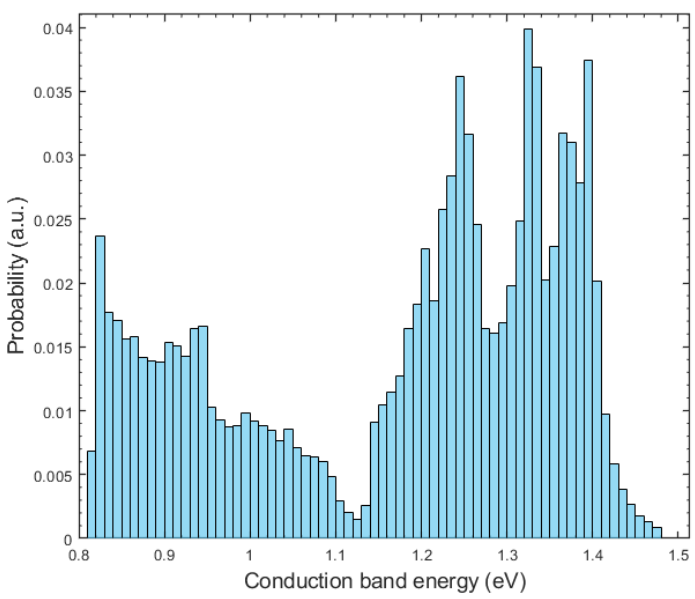
- The polar angle θ between the original and the new trajectory and the azimuthal angle φ will follow the distributions,

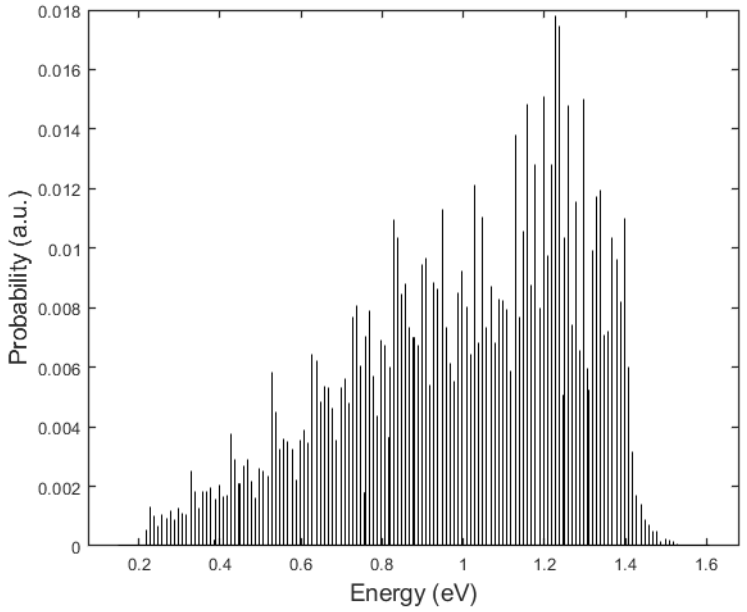
$$g_1(\theta) \propto \frac{\sin\theta}{E+(E\pm E_{ph})-2\sqrt{(E(E\pm E_{ph})cos\theta)}},$$

$$g_2(\varphi) = \frac{1}{2\pi}.$$

Energy Distribution

Photon energy =4.83 eV





The left side picture represents the energy distribution in the conduction band before scattering. The right-side figure represents the energy distribution after scattering.

Transmission probability

$$T(E,s,x,\xi,E_a) = D\big((E-\Delta E)x^2 + E_b,\xi,E_a\big)$$

$$D(E,\xi,E_a) = \frac{2}{1+\frac{(H(E)+E)}{2\sqrt{EH(E)}}\left[e^{\theta(E)} - \frac{1}{4}(1-e^{-\theta(E)})\right]}$$

$$\theta(E) = \begin{cases} 0 & E > E_a \\ \frac{2}{\hbar e\xi}\sqrt{2m^*(E_a-E)^3} & E \le E_a \end{cases}$$

$$H(E) = \sqrt{(E-E_a)^2 + ({f_0}^2\hbar^2(e\xi)^2/2m^*)^{\frac{2}{3}}},$$

f_0-dimensionless number 0.51697
ξ- electric field
$\alpha(\omega)$- absorption coefficient
ΔE – energy loss

Quantum Efficiency

- When the electrons approach the surface, they will traverse the band bending region and obtain extra E_b in the longitudinal direction and the Schottky reduction E_{sch}.
- The quantum efficiency is calculated using the number of scattered electrons and the no of photons.
- Reflection, absorption, and transmission possibilities are considered to calculate the number of electrons.

$$QE = \frac{(1-R) * (1-\exp(\alpha T)) * scatterd\ and\ emitted\ elctrons}{No\ of\ photons\ absorbed}$$

Thermal Emittance

- The transverse momentum conservation law at the surface,

$$P_{trans}^{in} = P_{trans}^{out}$$

$$P^{out} = \sqrt{(2m_0(E + E_b + E_{sch})}$$

$$P_{trans}^{out} = \sqrt{(2m_0(E + E_b + E_{sch})}sin\theta cos\phi$$

$$E_{sch}\ (eV) = 0.038\sqrt{E(MV/m)}$$

$$P^{out} > P_{trans}^{out}$$

- The normalized transverse rms emittance may be deduced by measuring the rms beam divergence at the cathode for a given beam spot size.

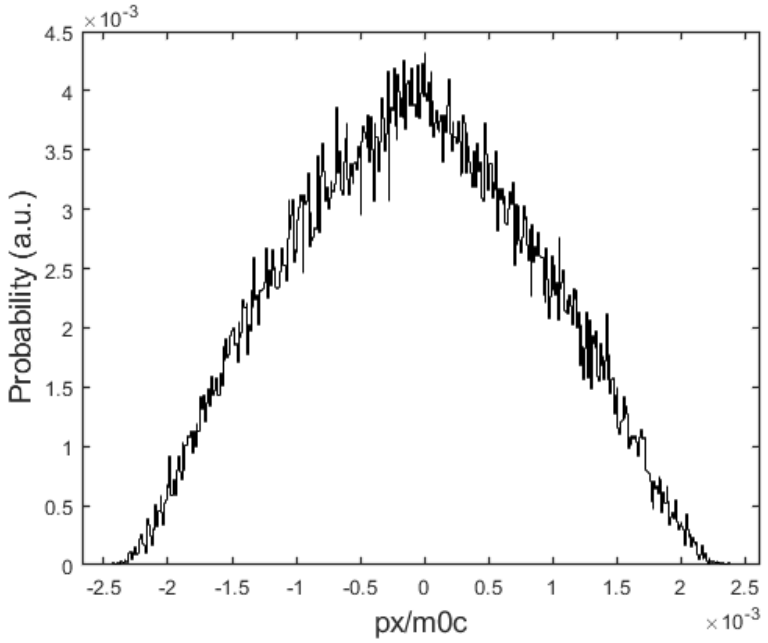
- The normalized transverse rms emittance is defined as

$$\epsilon_{n,rms} = \frac{1}{m_0 c}\sqrt{\sigma^2(x)\sigma^2(p_x) - \sigma^2(xp_x)}$$

- The correlation term $\sigma^2(xp_x)$ vanishes at the source since the quantities x and p_x are uncorrelated.

$$\epsilon_{n,rms} = \frac{1}{m_0 c} p_{x,rms} \times x_{rms}$$

Normalized Transverse Momentum Distribution



The probability distribution for the normalized transverse momentum at the cathode for photo-emitted electrons. A bin of 1×10^{-5} is used for the normalized transverse momentum. Laser spot size 1.5 mm.

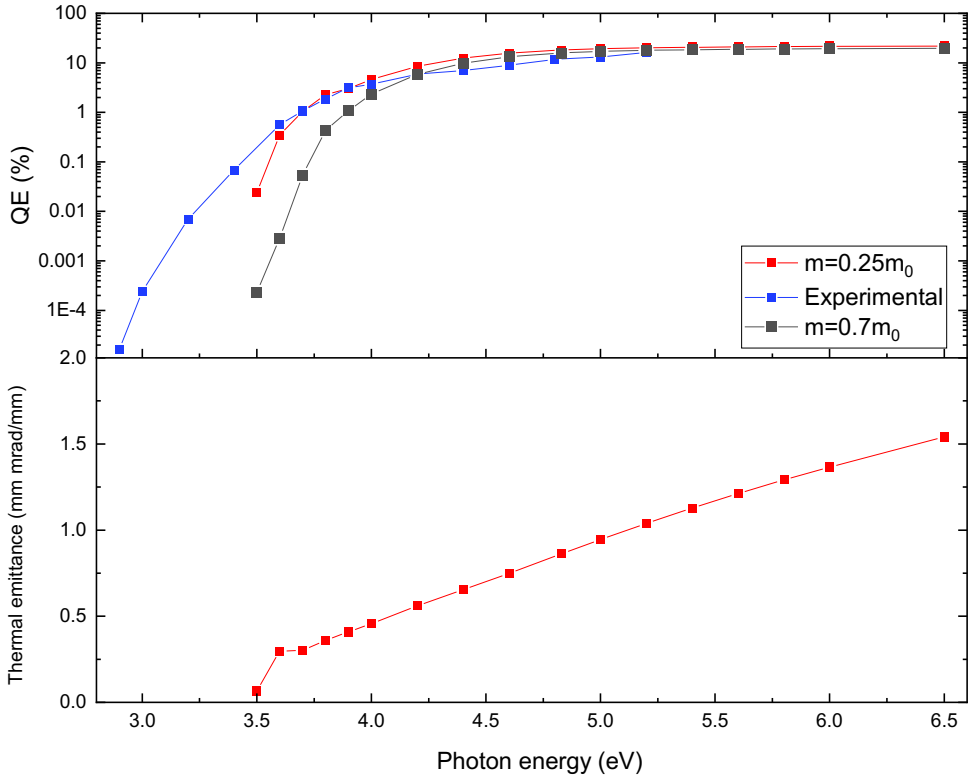
Constants used in this simulation

SLAC

Band gap E_g	3.3 eV
Electron affinity E_a	0.25 eV
Band bending energy E_b	0.05 eV
Effective mass m*	0.7 m_0
Reflectivity R	20 %
Thickness l	15 nm
Phonon energy E_{ph}	0.04 eV
Static dielectric constant ε_∞	3
High frequency dielectric constant ε_s	5.76
Density of material ρ	3.99 gcm^{-3}

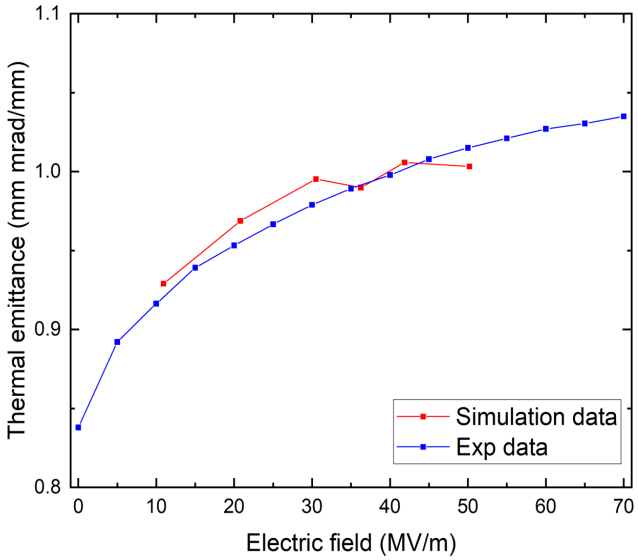
Quantum Efficiency and Thermal Emittance

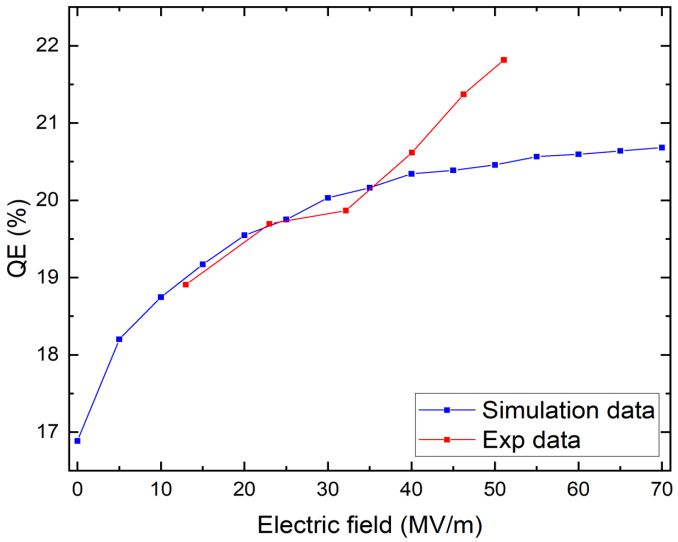
Electric Field= 0 MVm^{-1}



Thermal emittance and QE at 15 nm

Photon Energy =4.83 eV

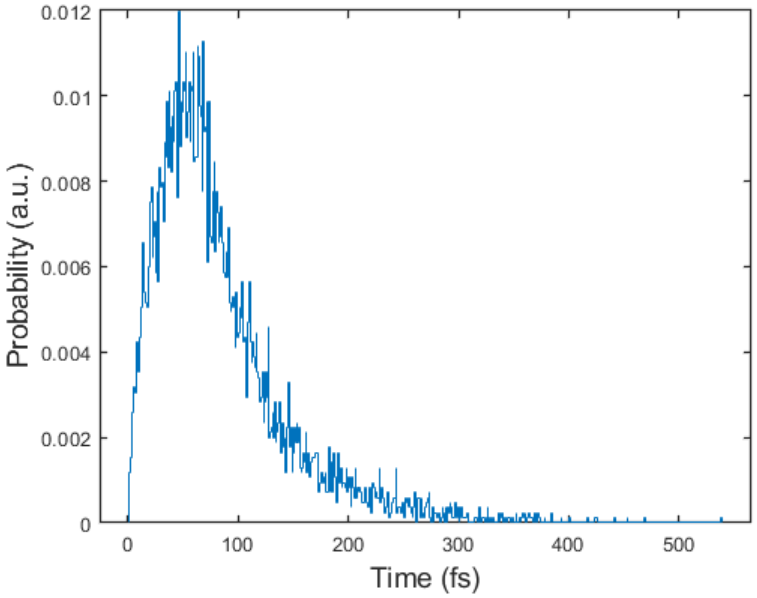


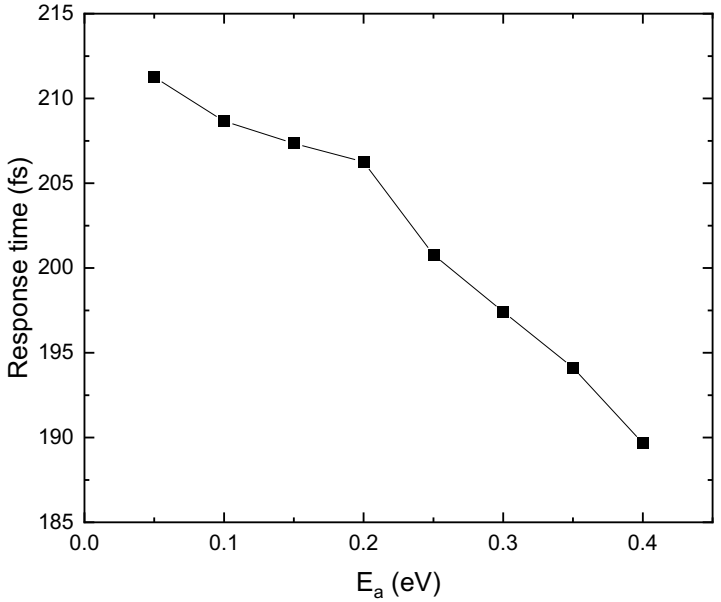


Comparison between the simulation results, and the experimental data in Thermal emittance and QE for Cs_2Te at 4.83 eV. The thickness of the photocathode is 15 nm.

Response time- Cs_2Te

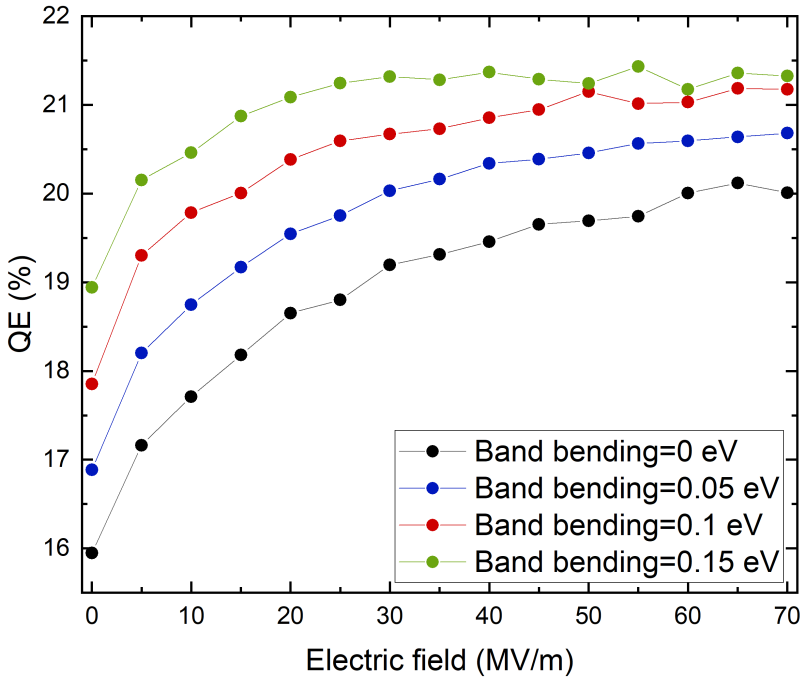
Electric Field = 20 MVm^{-1} and Photon Energy= 4.83 eV

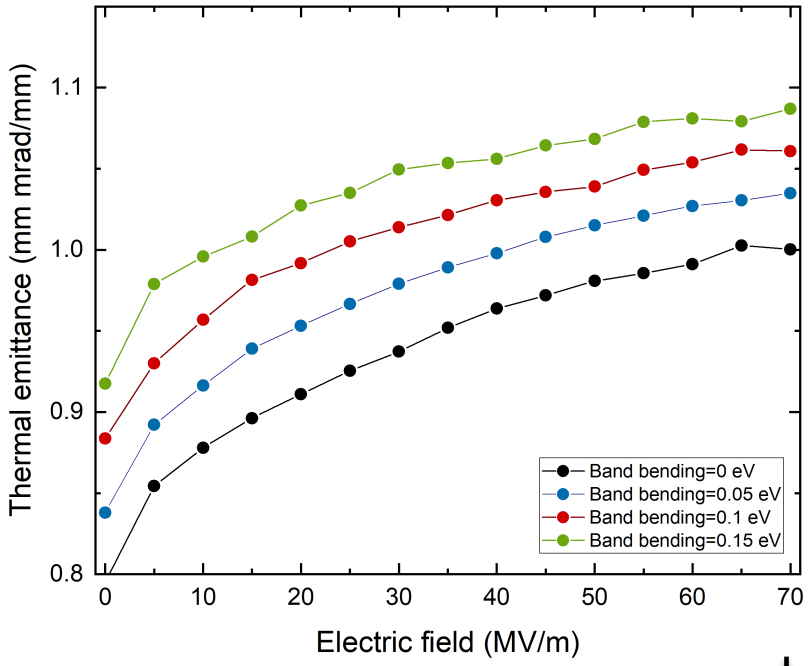


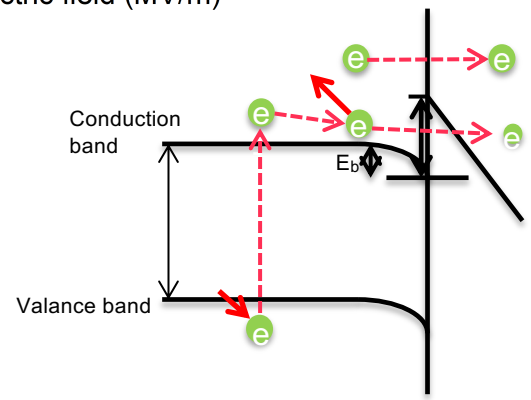


Band Bending Effect

Photon Energy = 4.83 eV

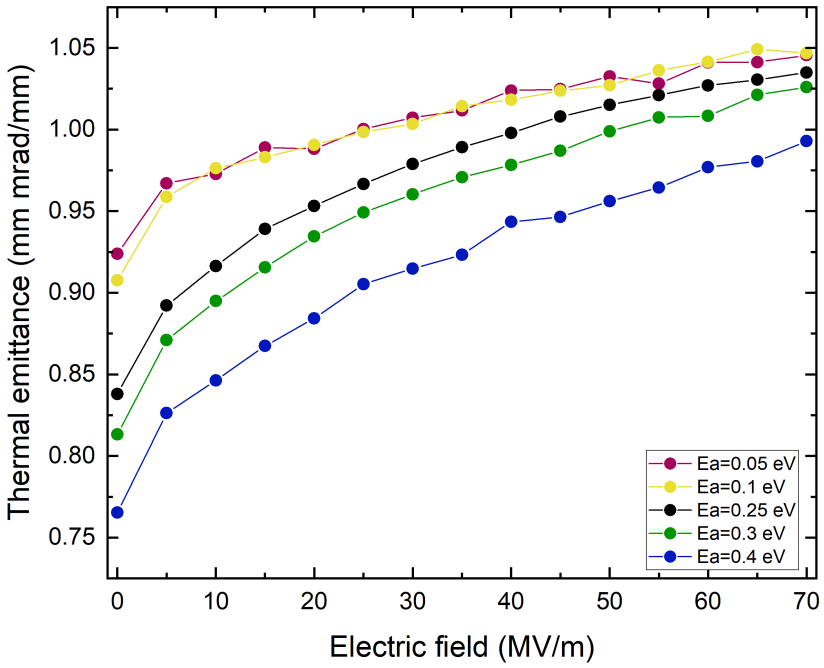


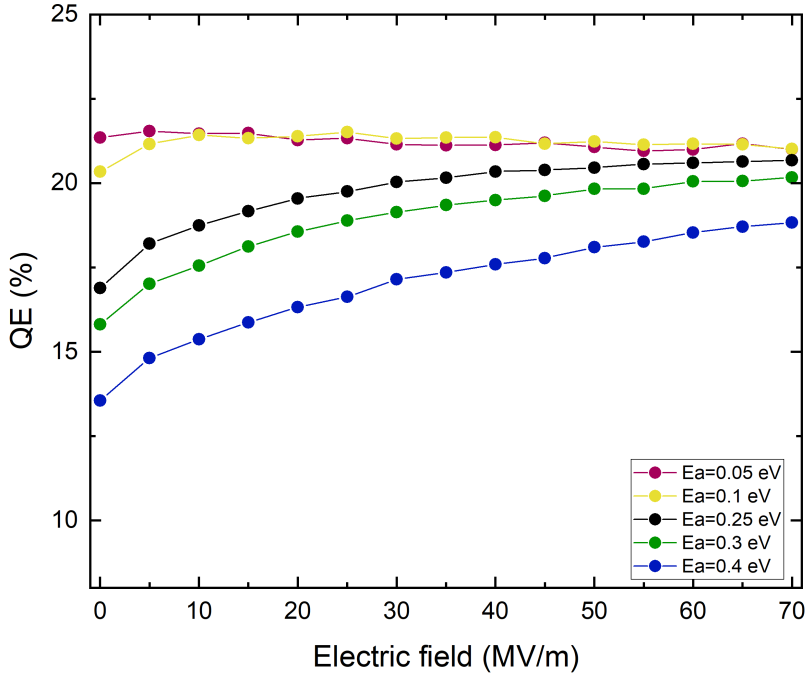


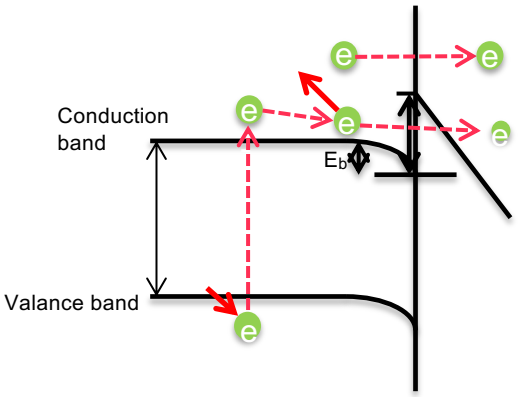


Electron affinity effect

Photon Energy =4.83 eV







Summary

SLAC

- Monte Carlo Simulation was used to calculate quantum efficiency and thermal emittance
- The density functional theory calculated DOS distribution incorporated in the simulation.
- The direction change after each scattering event considered in the simulation.
- e- ph scattering is considered and mainly focused on polar optical phonon scattering and intervalley phonon scattering.
- Calculated thermal emittance values and quantum efficiency values agree with the experimental values.
- The response time is 200.7 fs at a 20 MVm^{-1} electric field and 4.83 eV photon energy.

References

1. A. Jain*, S.P. Ong*, G. Hautier, W. Chen, W.D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, K.A. Persson *(*=equal contributions) The Materials Project: A materials genome approach to accelerating materials innovation* APL Materials, 2013, 1(1), 011002.

2. I. Schewe-Miller and P. Bottcher, Synthesis and crystal structures of K5Se3 , Cs 5 Te 3 and Cs 2 Te, Z. Kristallogr.196, 137 (1991).

3. G. Fernini, P. Michelato, F. Parmigiani, "A monte carlo simulation of low energy photoelectron scattering in Cs_2Te" Solid State Comm. **106**, 21 (1998).

4. F. Banfi, G. Ferrini, and et. al. "Monte carlo transverse emittance study on Cs2Te", 27th International free electron laser conference 21-26 (2005)

5. H. Xie, I. Ben-Zvi, and et.al. "Experimental measurements and theoretical model of the cryogenic performance of bialkali photocathode and characterization with Monte Carlo simulation".Phys. Rev. ST. Accel. Beams 19 103401 (2016)

6. P. Huang, H. Qian, et. al. "Photoemission and degradation of semiconductor photocathode" Phys. Rev. ST. Accel. Beams 22, 123403 (2019)

7. R.A. Powell, W.E. Spicer, et.al. "Photoemission studies of Cs2Te", Phys.rev.B. 8 8 (1973)

8. H. Xie, I. Ben-Zvi, and et.al. "Experimental measurements and theoretical model of the cryogenic performance of bialkali photocathode and characterization with Monte Carlo simulation".Phys. Rev. ST. Accel. Beams 19 103401 (2016)

9. L. Monaco et.al "Growing and characterization of Cs_2Te photocathodes with different thickness at INFN LASA" 39th Free Electron Laser conf. (2019)

10. P. Huang, H. Qian, et.al. "Test of Cs_2Te thickness on cathode performance at PITZ", 39th Free electron conf. (2019)

Thank you

PITZ, DESY, Zeuthen

Houjun Qian, Mikhail Krasilnikov, Matthias Gross, Frank Stephan

Department of Engineering Physics, Tsinghua University

Peng-Wei Huang

DESY, Hamburg

Sven Lederer, Pavel Juarez

Physics Department, Carl von Ossietzky University

Caterina Cocchi, Holger-Dietrich Sassnick

Istituto Nazionale di Fisica Nucleare – LASA

Daniele Sertore, Laura Monaco