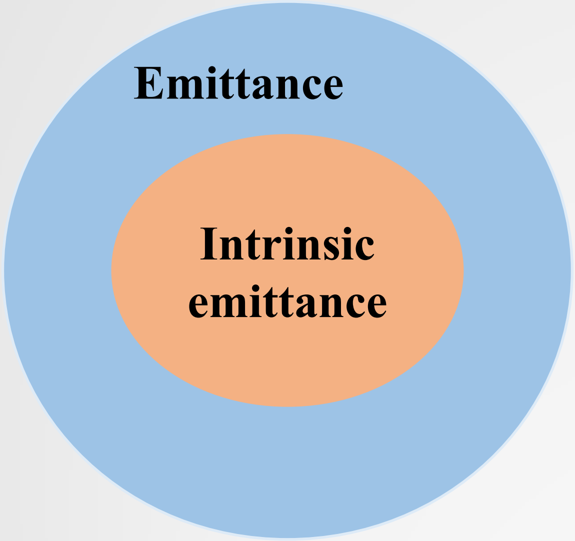
Model of Photoemission and degradation of semiconductor photocathode

Speaker: Peng-Wei Huang

April 04, 2019

CONTENTS

XFEL:
High brightness
High repetition rate
High peak current
……


Emittance

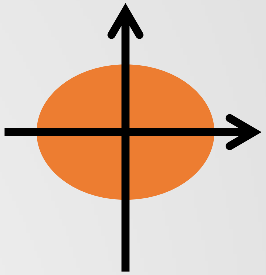
Intrinsic emittance

Photocathode:
High quantum efficiency
Low thermal emittance
……

$$\varepsilon_n = \frac{1}{m_0 c}\sqrt{\langle x^2\rangle\langle p_x^2\rangle - \langle x p_x\rangle^2}$$

$$= \frac{1}{m_0 c}\sqrt{\langle x^2\rangle\langle p_x^2\rangle}$$

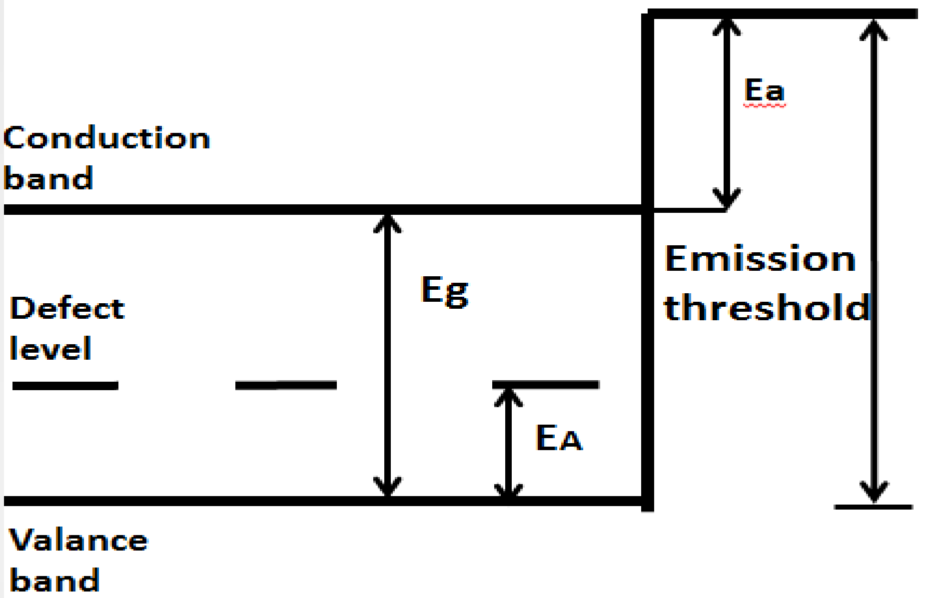
$$= \sigma_x\sqrt{\frac{\langle p_x^2\rangle}{m_0^2 c^2}} = \sigma_x\sqrt{\frac{\mathrm{MTE}}{m_0 c^2}}$$



MTE——mean transverse energy

- Low thermal emittance
- Semiconductor photocathode
- Photon energy near or below the threshold

Cathode	Threshold (eV)	Photon (eV)	Thermal emittance (mm.mrad/mm)	Quantum efficiency
GaAs[1]	1.42	1.44	0.24	~10^{-3}
Cs$_3$Sb[2]	1.9	1.8	0.27	~5×10^{-4}
Na$_2$KSb[3]	1.9	1.8	0.26	~10^{-4}



[1]Bazarov I V, Dunham B M, Li Y, et al. Thermal emittance and response time measurements of negative electron affinity photocathodes[J]. Journal of Applied Physics, 2008, 103(5): 054901.
[2]Cultrera L, Karkare S, Lee H, et al. Cold electron beams from cryocooled, alkali antimonide photocathodes[J]. Physical Review Special Topics-Accelerators and Beams, 2015, 18(11): 113401.
[3] Measurement of the tradeoff between intrinsic emittance and quantum efficiency from a NaKSb photocathode near threshold

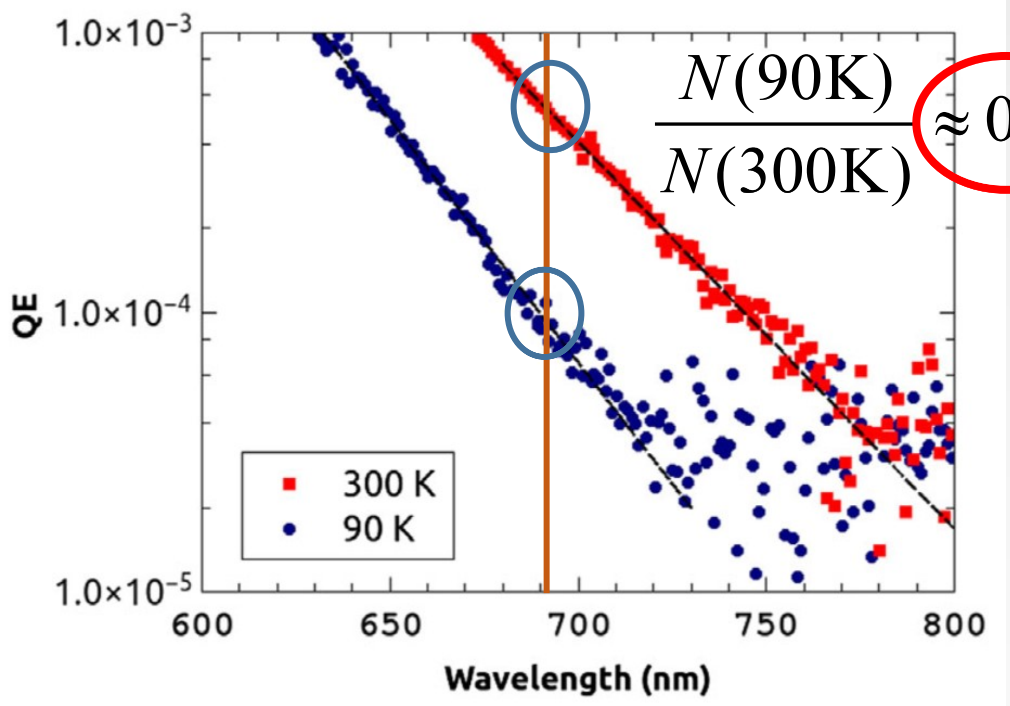
Suppose all the electrons come from defect level(e.g. 1.8eV Cs_3Sb)

$$\varepsilon_n = \sigma_x \sqrt{\frac{\text{MTE}}{m_e c^2}}$$

$$\text{MTE}=\frac{h\nu - E_g - E_a + E_A}{3}$$

$$= 0.133\text{eV} > 0.04\text{eV}$$

MTE is larger than the experimental data [1].



$$\frac{N(90\text{K})}{N(300\text{K})} \approx 0.1$$

Cultrera, PRSTAB 18, 113401(2015)

$$\frac{N(90\text{K})}{N(300\text{K})} = \frac{2\times\exp[\frac{E_A - E_F}{k_B\times 300}]+1}{2\times\exp[\frac{E_A - E_F}{k_B\times 90}]+1}$$

$$\approx 4.4\times 10^{-6}$$

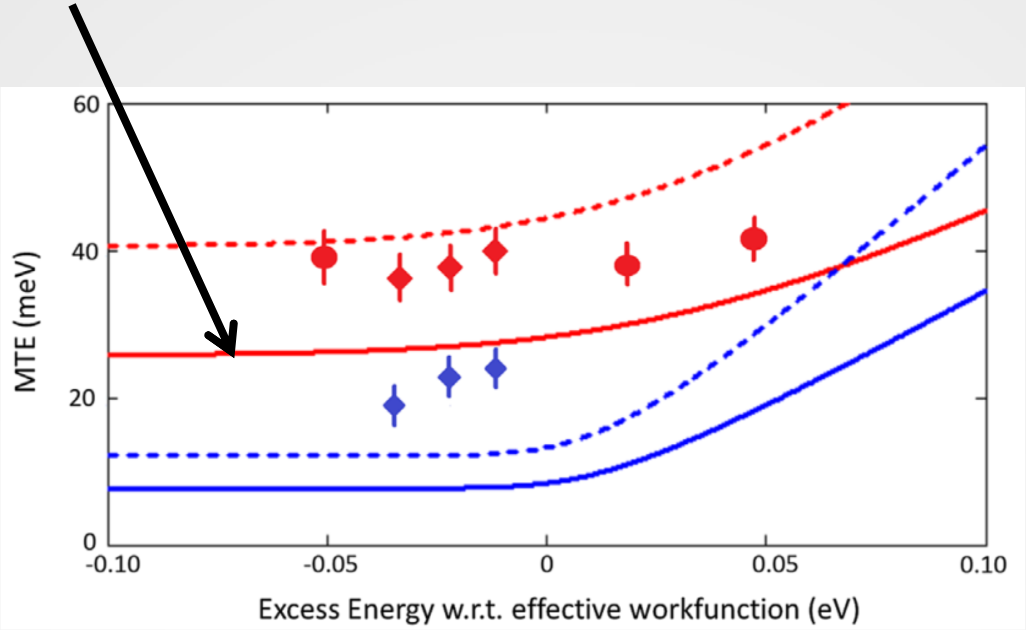
Thermal limit to the intrinsic emittance from metal photocathodes may not be applicable to semiconductors

$\hbar$

$$\varepsilon_x = \sigma_x \sqrt{\frac{kT}{mc^2}}$$

Tend to underestimate the thermal emittance

Surface roughness ?

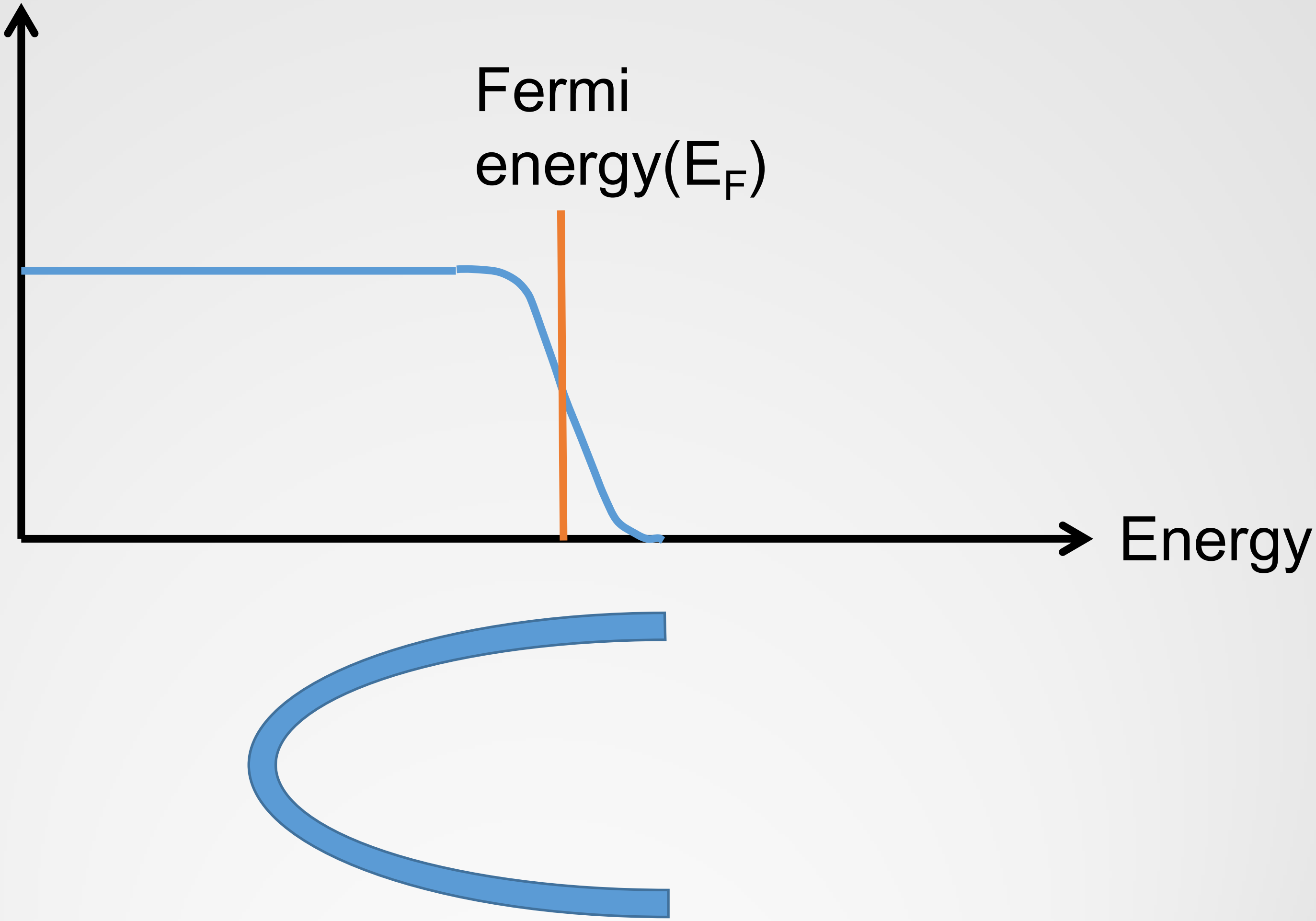


Cultrera, PRSTAB 18, 113401(2015)

[1]Vecchione T, Dowell D, Wan W, et al. Quantum efficiency and transverse momentum from metals[C]//Proceedings of FEL. 2013, 13: 25-30.
[2] Feng J, Nasiatka J, Wan W, et al. Thermal limit to the intrinsic emittance from metal photocathodes[J]. Applied Physics Letters, 2015, 107(13): 134101.
[3] Feng J, Karkare S, Nasiatka J, et al. Near atomically smooth alkali antimonide photocathode thin films[J]. Journal of Applied Physics, 2017, 121(4): 044904.

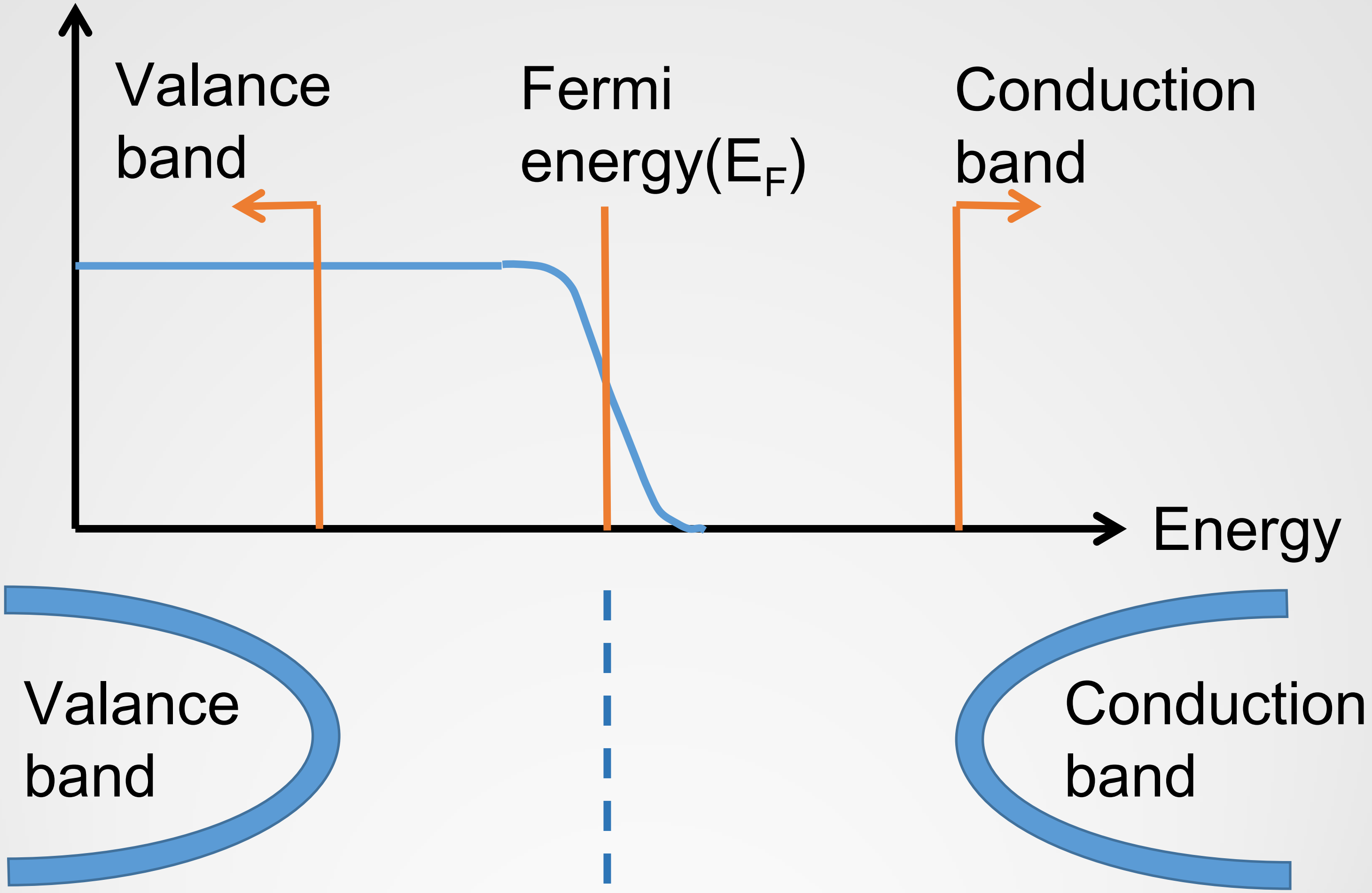
$$F(E) = \frac{1}{\exp(\frac{E - E_F}{kT}) + 1}$$

Metal——Temperature considerably affects the distribution of electrons near the Fermi level.

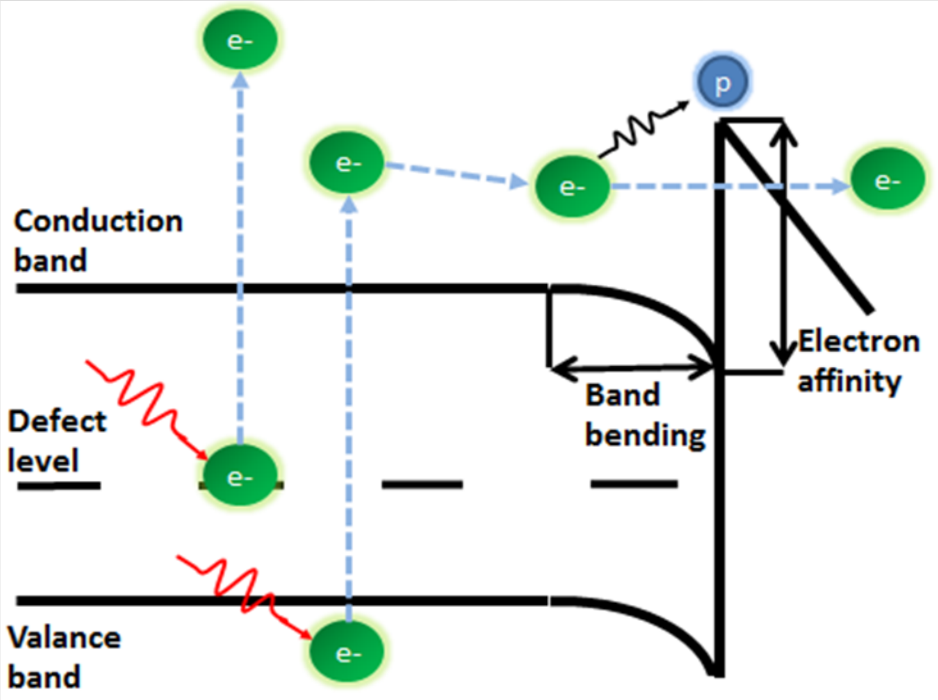


Semiconductor——No electrons at Fermi energy. Temperature do not influence the distribution for large band gap semiconductor.

$$F(E)=\frac{1}{\exp(\frac{E-E_F}{kT})+1}$$

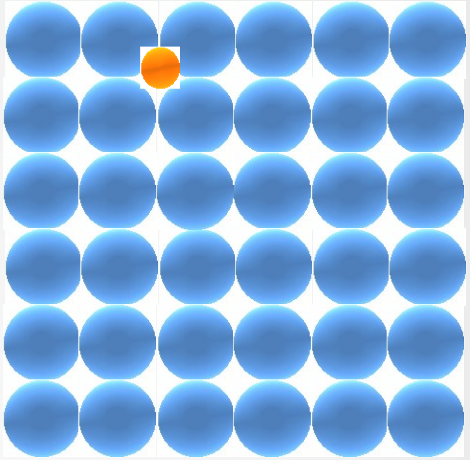


Photoemission model for semiconductor near threshold region



- Electrons from defect level and valance band

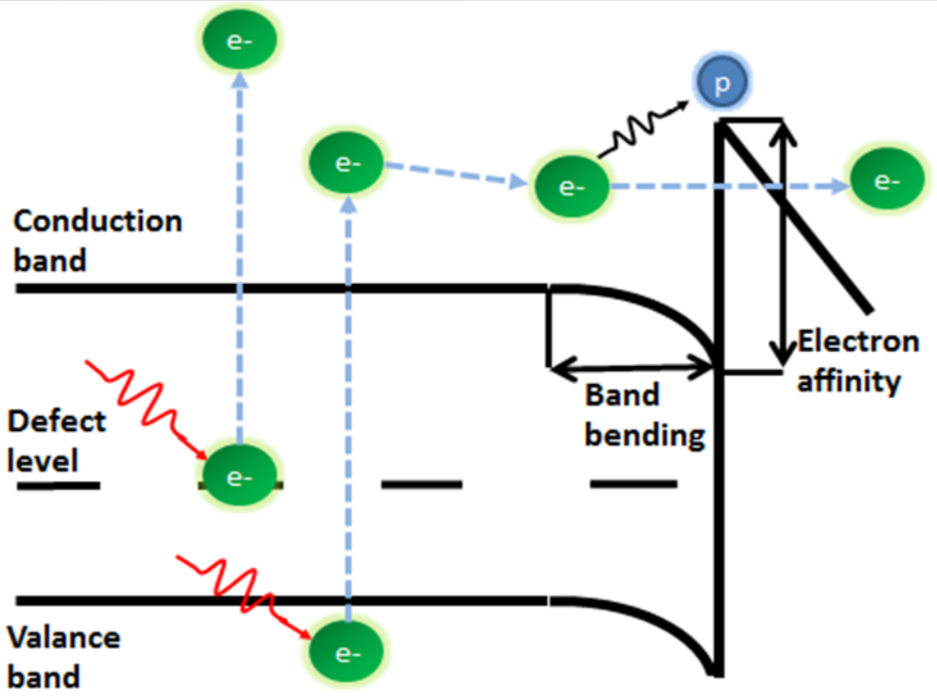
defects ← vacancies



$$
\begin{aligned}
N(E) &= f_v(\hbar\omega - E_g - E)g(\hbar\omega - E_g - E) \times (1 - f_c(E))g(E) \\
&= n_d \sqrt{E}\delta(E - \hbar\omega + E_g - E_A) + \sqrt{E(\hbar\omega - E_g - E)}
\end{aligned}
$$

$$
n_{\mathrm{d}} = \frac{N_A \times f(E_A)}{\frac{1}{2\pi^2}\left(\frac{2m_0}{\hbar^2}\right)^{\frac{3}{2}}}
$$

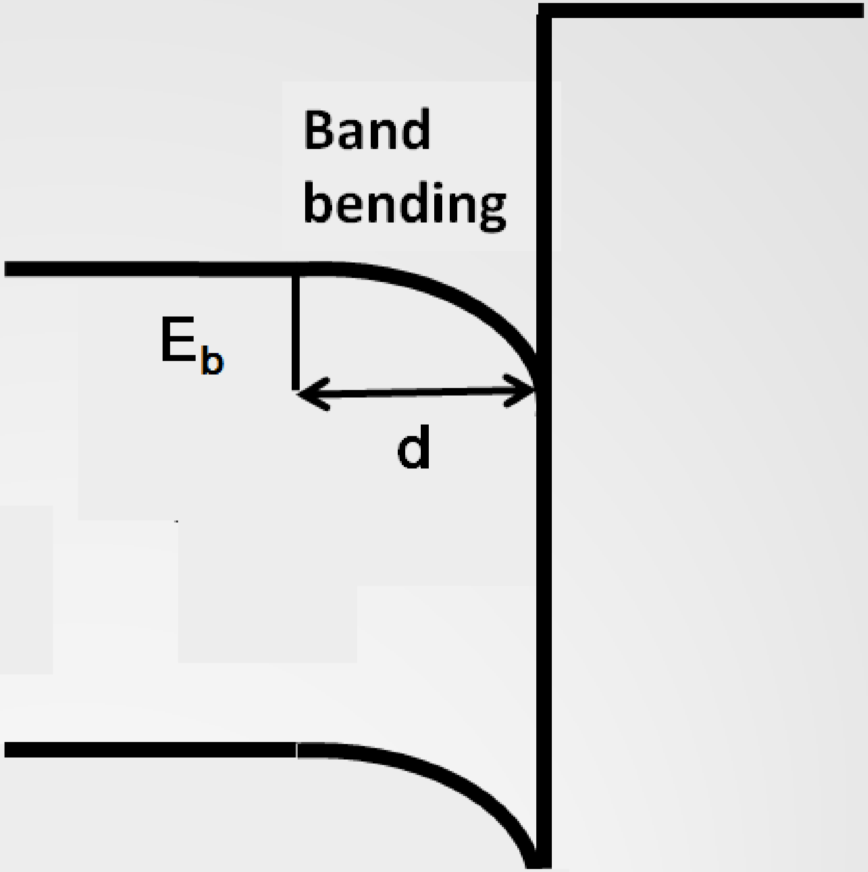
[1]L.Ye, Semiconductor Physics[M]. Beijing; Higher education Press, 2007.



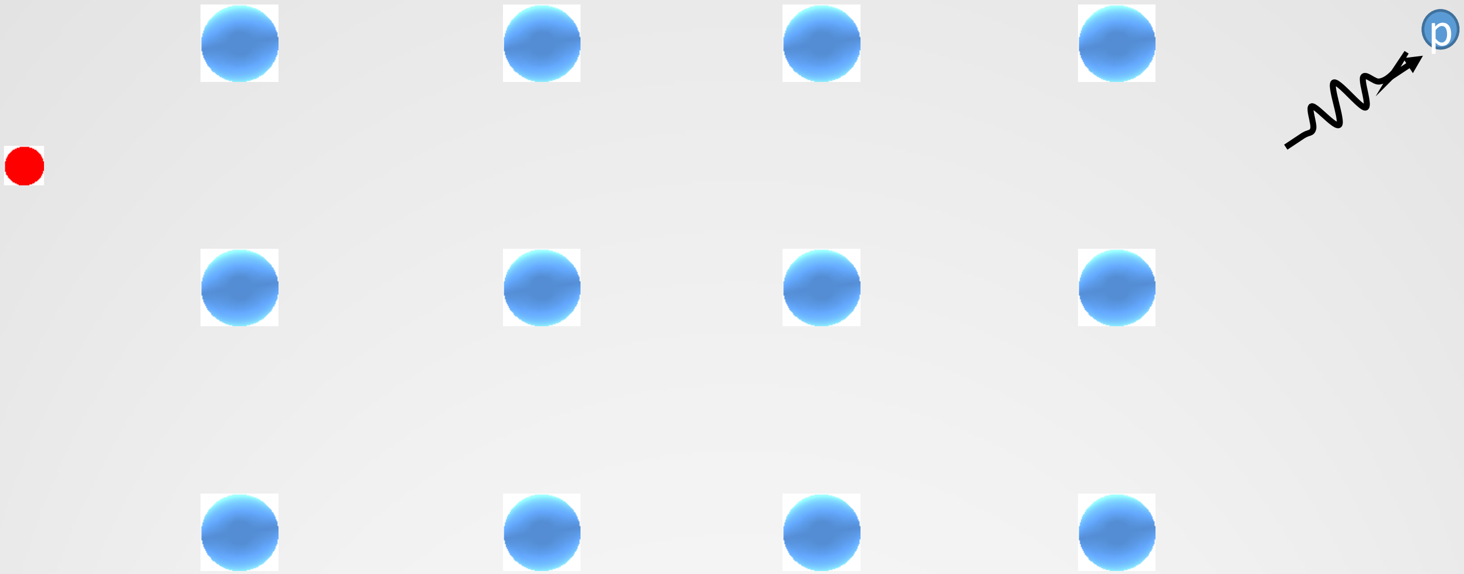
$$E_b = \frac{N_A e d^2}{2\varepsilon\varepsilon_0}$$

- Band bending at the surface

Example:
p-typed bulk; n-typed surface



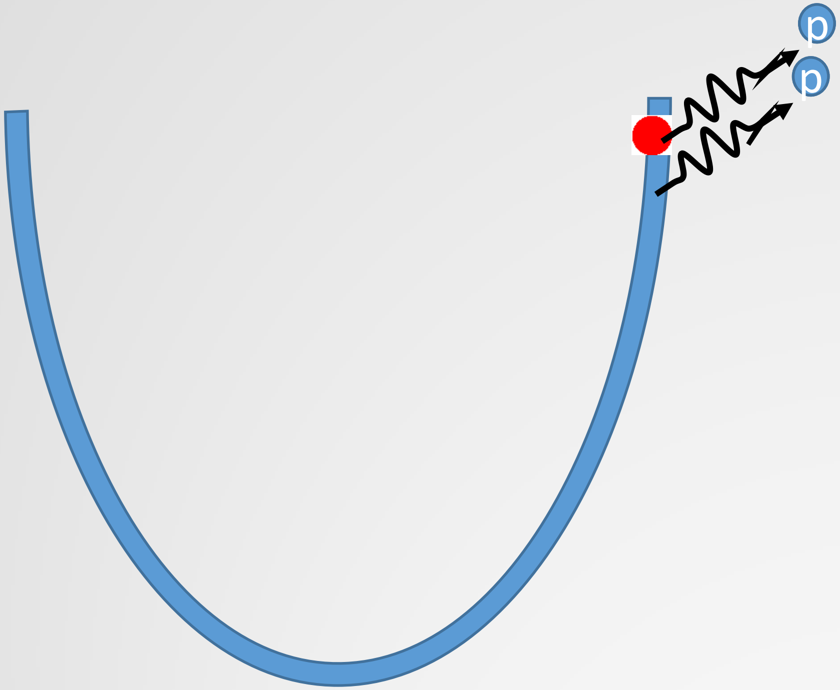
- Energy loss due to the scattering with lattice during the transportation process



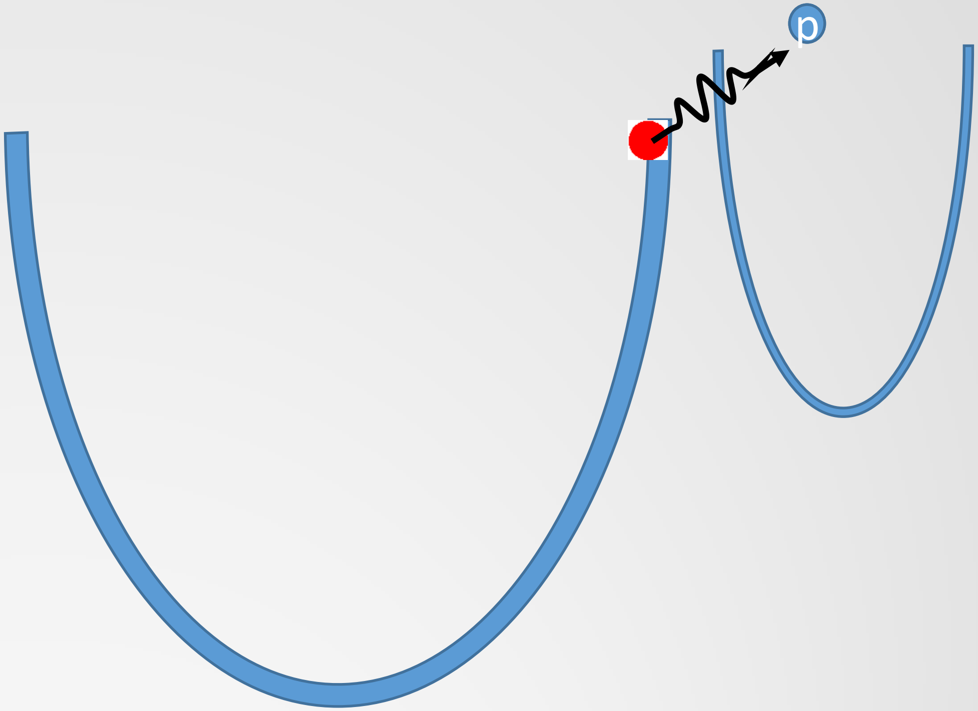
Energy loss: $$\Delta E = t \times \lambda(E) \times E_{ph}$$

t – traversing time $\lambda(E)$ – scattering rate E_{ph} – phonon energy

- Energy loss due to the scattering with lattice during the transportation process

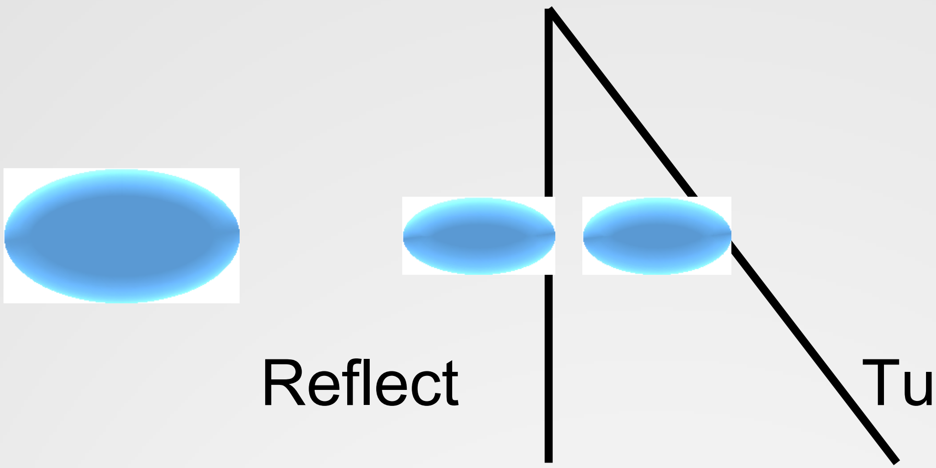


Optical phonon scattering
(For all electrons)
With low scattering rate



Inter valley scattering
(For high energy electrons)
With high scattering rate

- Electron tunnel through the vacuum barrier



Semiconductor

Vacuum

Reflect

Tunnel

Jensen et al. J. Appl. Phys. 104, 044907 (2008)

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

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

$$H(E) = \sqrt{(E-E_a)^2 + (p_0^2\hbar^2(e\beta\xi)^2/2m)^{\frac{2}{3}}}$$

We derive the expression of QE and MTE.

$$\mathrm{QE} = (1 - R(\omega)) \frac{\iiint N(E)F(s)T(E,s,x,\lambda(E))dEdsdx}{\int N(E)dE\int_{-1}^{1}dx}$$

$$\mathrm{MTE} = \frac{\iiint N(E)F(s)T(E,s,x,\lambda(E))(1-x^2)EdEdsdx}{\iiint N(E)F(s)T(E,s,x,\lambda(E))dEdsdx}$$

$$T(E,s,x,\lambda(E)) = D((E - \frac{s}{x\sqrt{2E/m}} \times \lambda(E) \times E_{ph})x^2 + E_{bend})$$

The sampling in Monte Carlo simulation is based on the distribution described in the former slides. The scattering process is more realistic in the simulation. The real scattering rate is able to obtain considering the energy change due to scattering or applied electric field. The phonon absorption and emission can be evaluated. The change of the momentum after scattering , including both magnitude (energy gain or loss) but also direction, can be considered.

Analytical calculation for scattering rate (energy loss rate)

'-' refers to phonon emission.

'+' refers to phonon absorption.

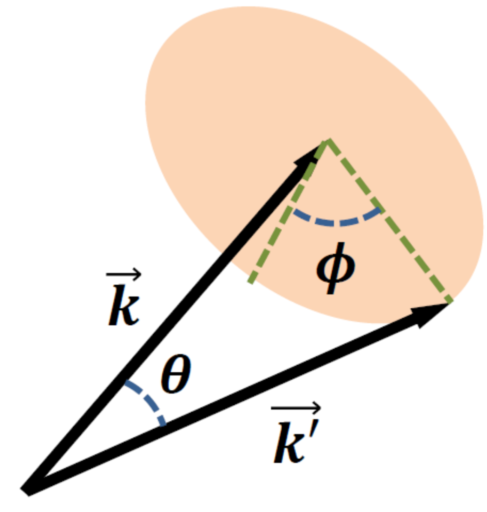
$$\lambda(E) = \lambda_{o-} - \lambda_{o+}$$

$$\lambda(E) = \lambda_{o-} - \lambda_{o+} + \lambda_{i-} - \lambda_{i+}$$

Simulation calculation for scattering rate

$$\lambda = \lambda_{o-} + \lambda_{o+}$$

$$\lambda = \lambda_{o-} + \lambda_{o+} + \lambda_{i-} + \lambda_{i+}$$

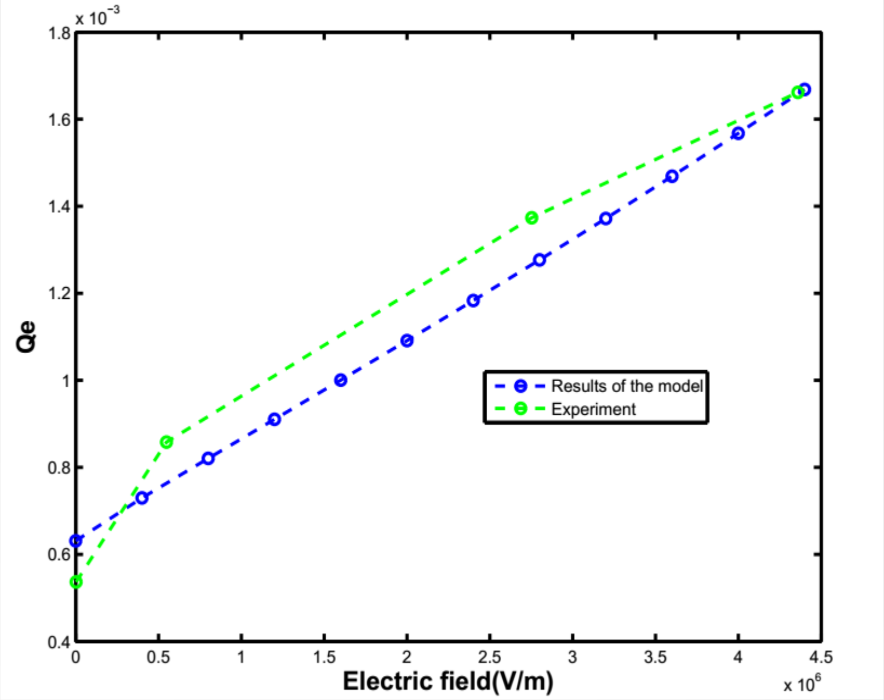


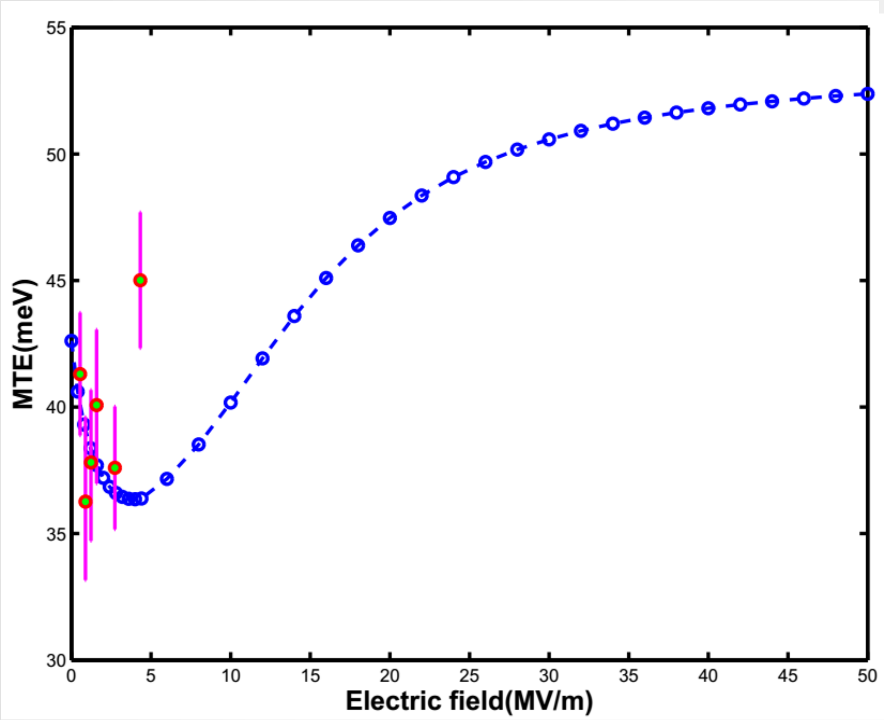
$$g_1(\theta) \propto \frac{\sin\theta}{E + (E \pm E_{ph}) - 2\sqrt{E(E \pm E_{ph})}\cos\theta}$$

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

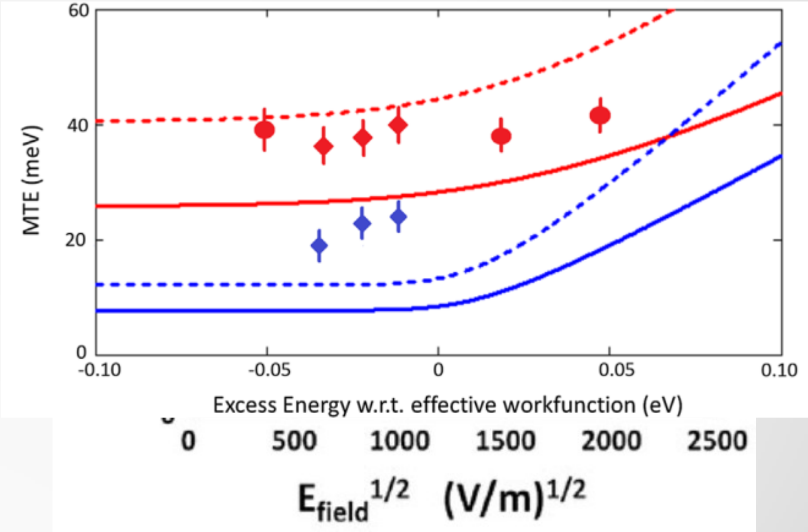
Results

1. Succeed to explain the performance of the cathode when the incident photon energy is lower than the threshold. (e.g. Cs_3Sb, 1.8eV[1])





Cultrera, PRSTAB 18, 113401(2015)

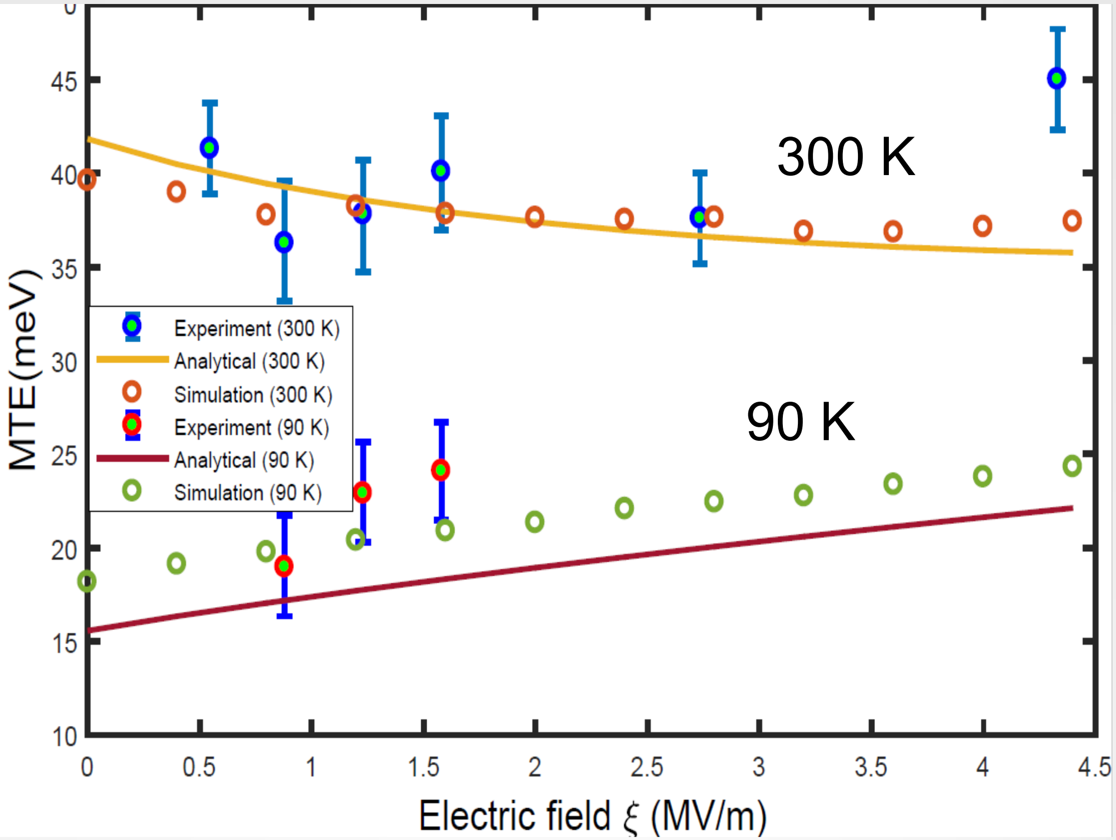


[1]Cultrera L, Karkare S, Lee H, et al. Cold electron beams from cryocooled, alkali antimonide photocathodes[J]. Physical Review Special Topics-Accelerators and Beams, 2015, 18(11): 113401.

For the 90 K, the contribution from defect level can be neglected since the occupation possibility at the defect level is 5 orders of magnitude smaller than the room temperature.

$$n_{\mathrm{d}} = \frac{N_A \times f(E_A)}{\frac{1}{2\pi^2}\left(\frac{2m_0}{\hbar^2}\right)^{\frac{3}{2}}}$$

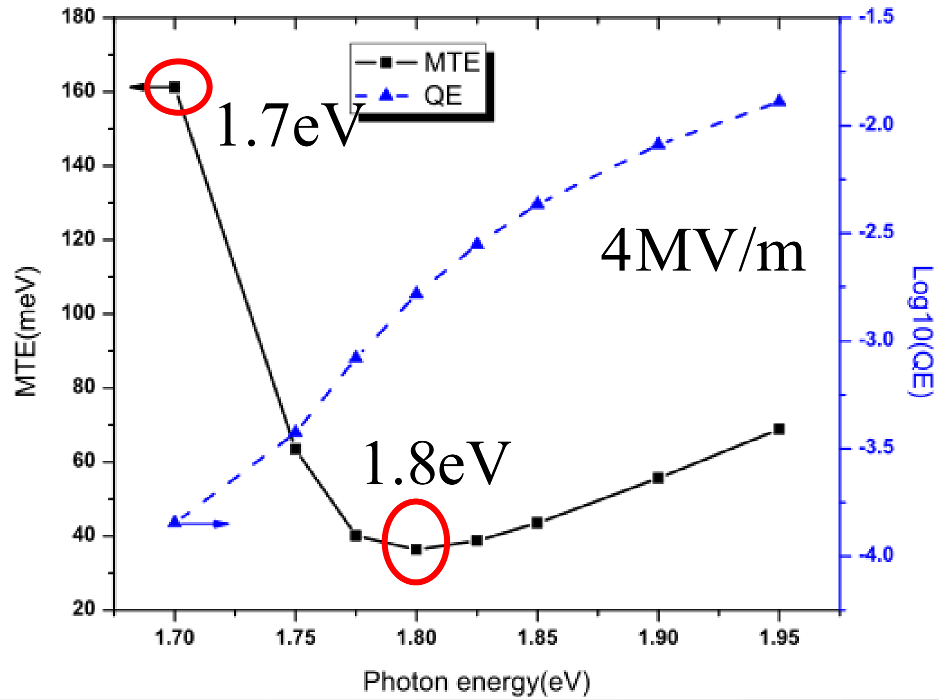
$$N(E,\omega) = n_d \cdot \sqrt{E} \cdot \delta(E - \hbar\omega + E_g - E_A) + \sqrt{E(\hbar\omega - E_g - E)} \cdot H(\hbar\omega - E_g - E),$$

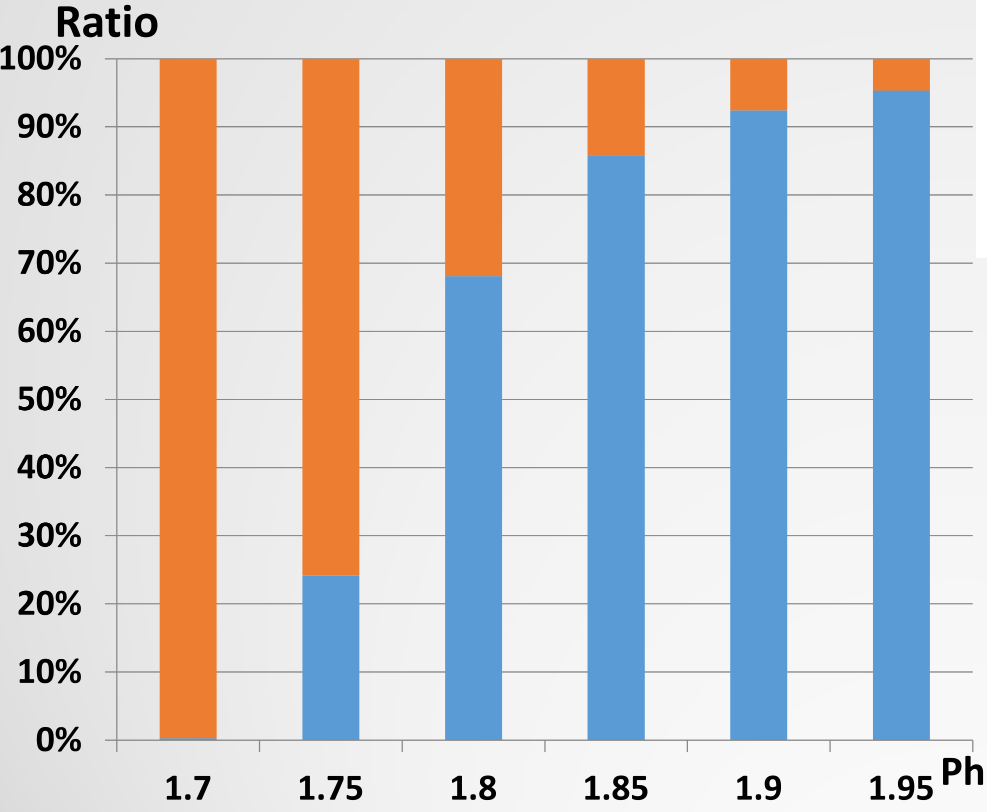


Cultrera, PRSTAB 18, 113401(2015)

Results

2. Due to the defect level, the thermal emittance exists a minimum point regard to the photon energy.





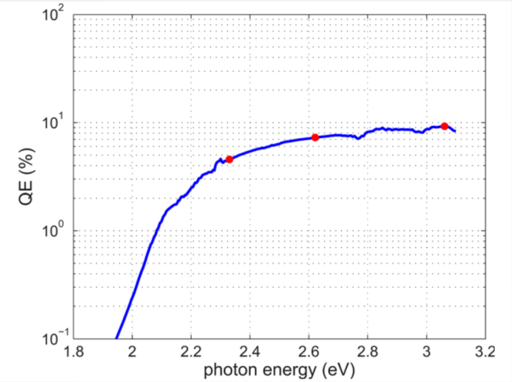
Results

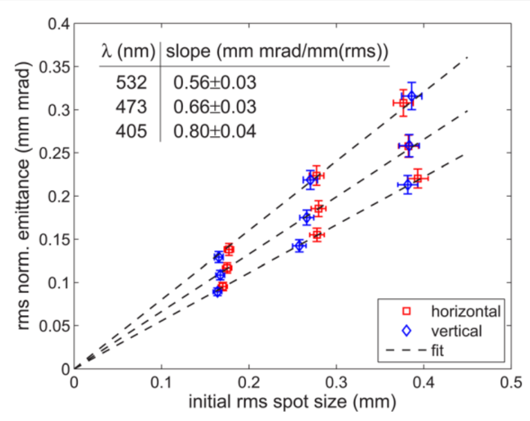
3. The model still applies when the photon energy is higher than the threshold(taking Cs_3Sb as an example).

E-experiment M-model

$\hbar\omega$(eV)	3.06	2.62	2.33
Qe(E)	9.32%	7.29%	4.62%
Qe(M)	9.74%	7.18%	5.01%
ϵ_n(E)(μm/mm)	0.80±0.04	0.66±0.03	0.56±0.03
ϵ_n(M)(μm/mm)	0.8086	0.6600	0.5515

Cultrera, Appl. Phys. Lett. 99, 152110 (2011)





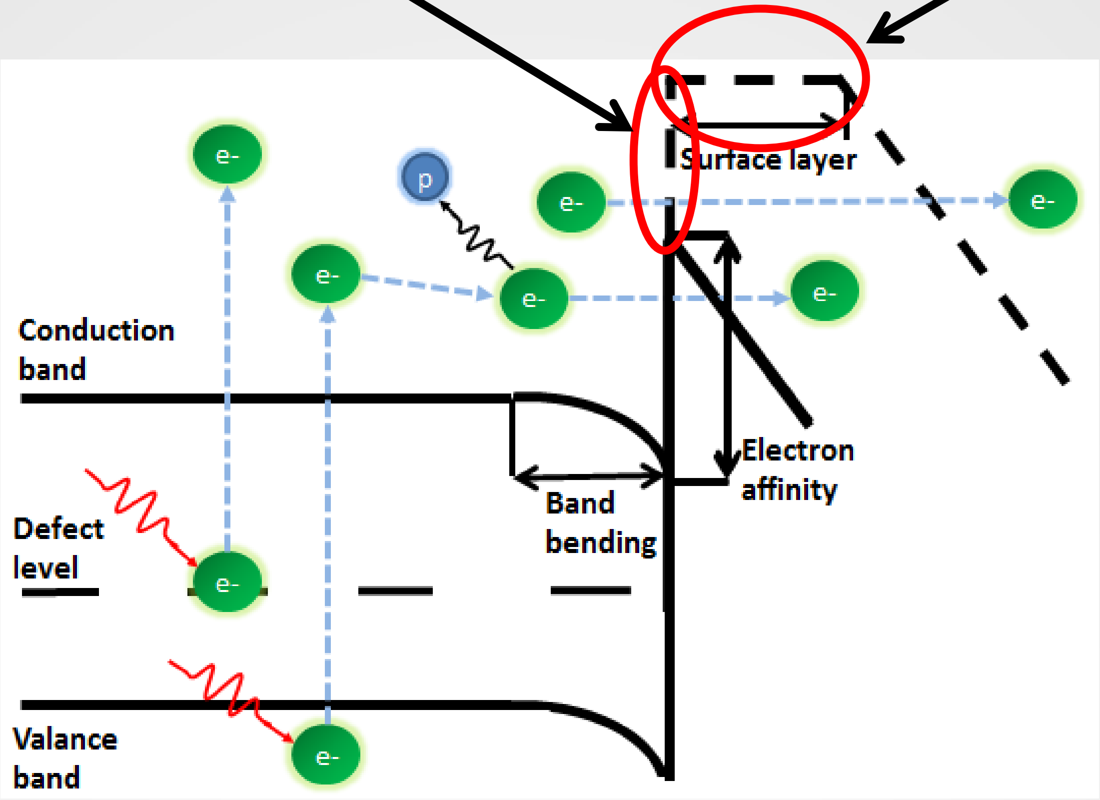
λ (nm)	slope (mm mrad/mm(rms))
532	0.56±0.03
473	0.66±0.03
405	0.80±0.04

[1]Cultrera L, Bazarov I, Bartnik A, et al. Thermal emittance and response time of a cesium antimonide photocathode[J]. Applied Physics Letters, 2011, 99(15): 152110.

The physical picture of degradation due to residue gases

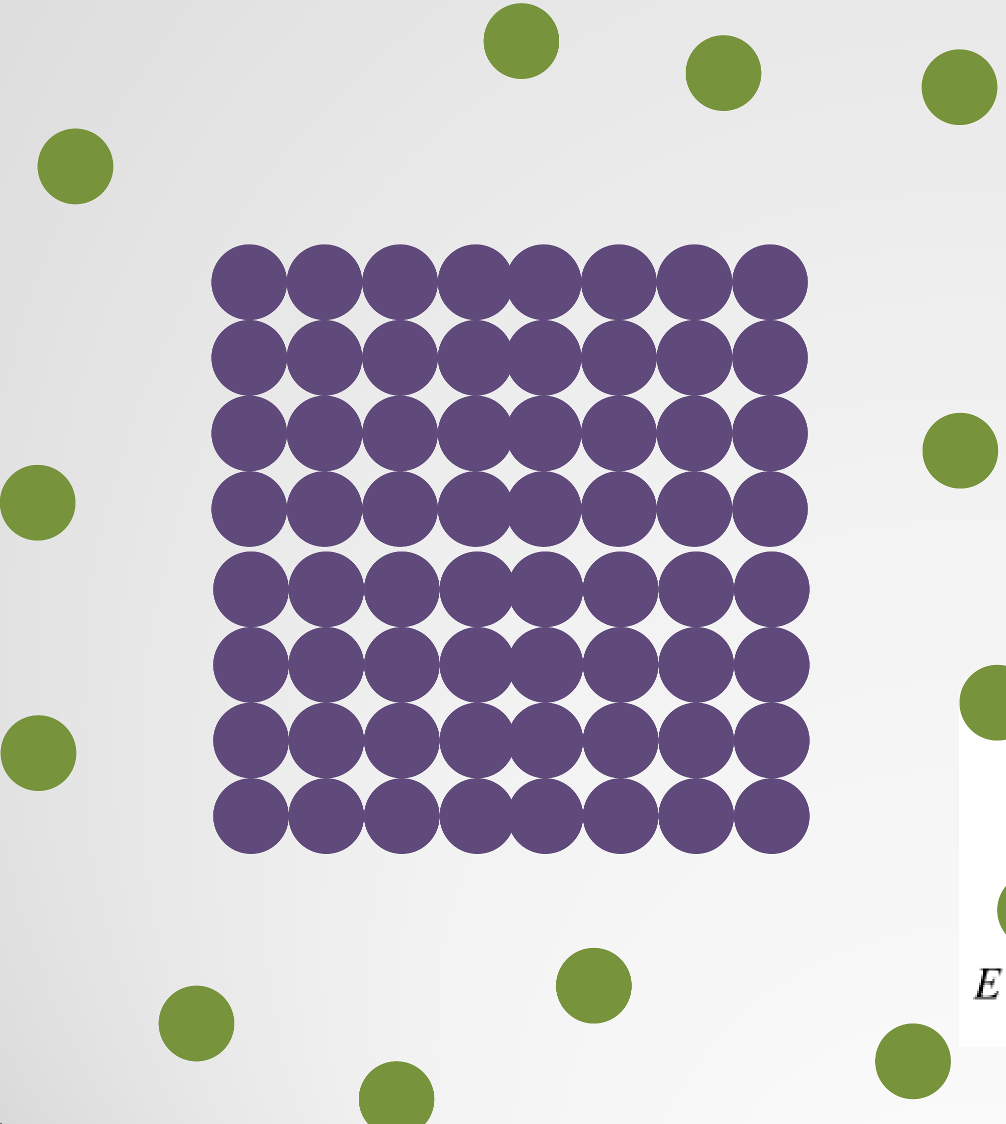
The electron affinity increase with time.

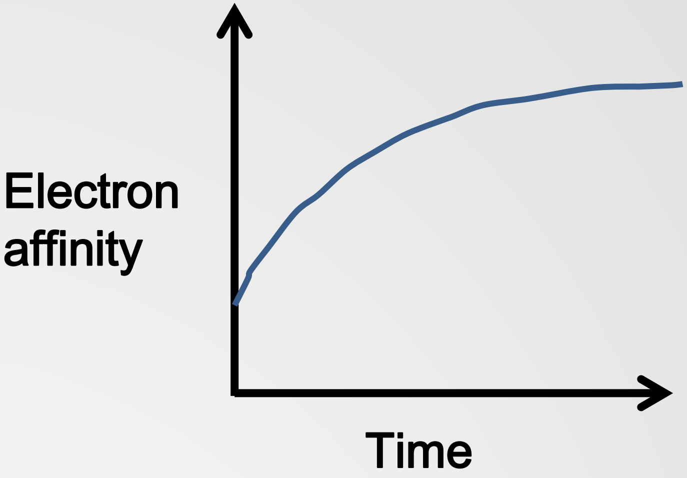
The surface layer become thicker, leading to the reduction of the emission probability.



1、The electron affinity increases with time

- The time relationship of the change of electron affinity $(1-e^{-\frac{t}{\tau}})$





Mean field approximation

$$N_1 + N_2 = N_0,$$

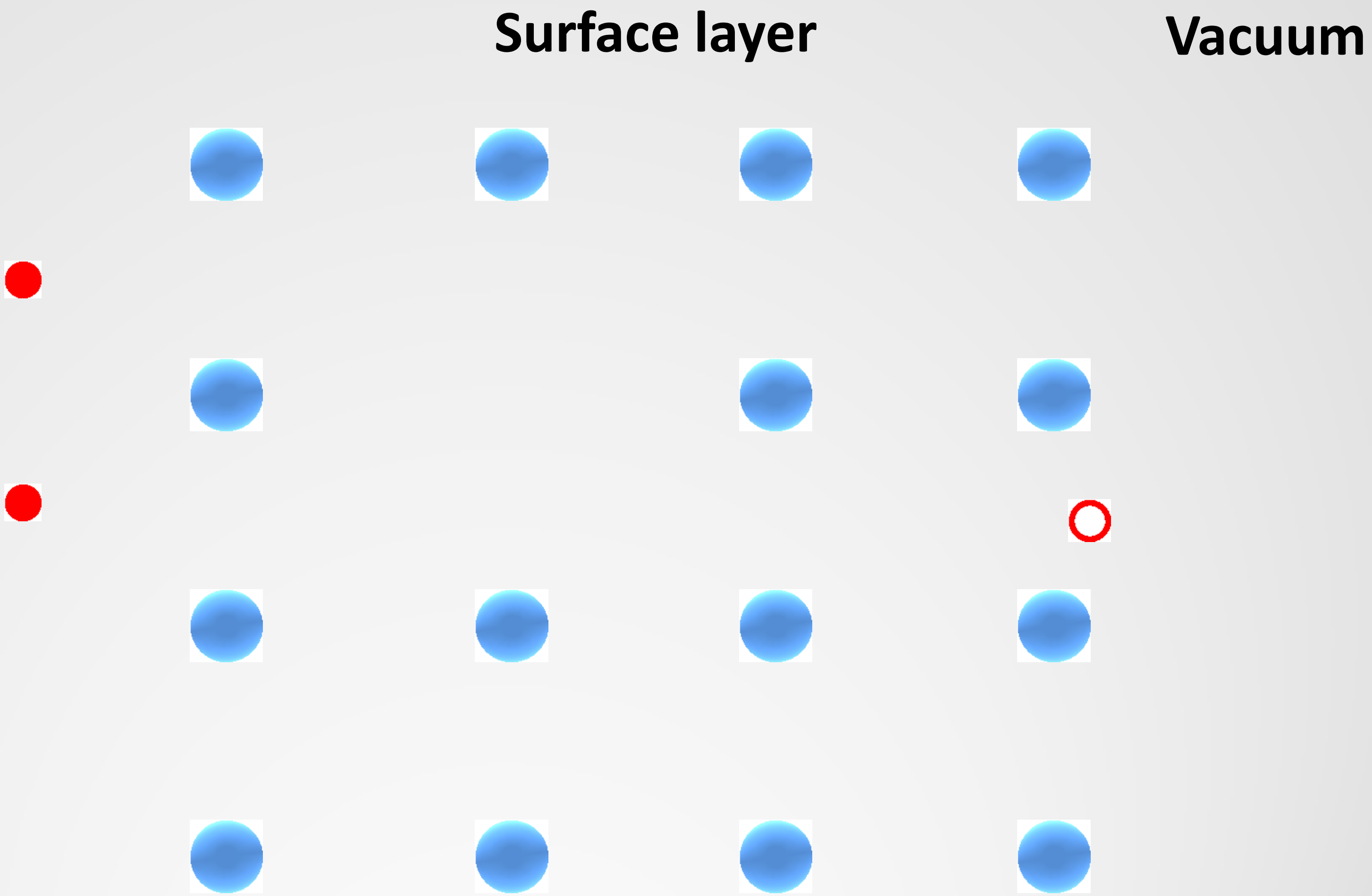
$$\frac{\mathrm{d}N_1}{\mathrm{d}t} = -N_1/\tau \Longrightarrow N_1 = N_0 \exp(-t/\tau),$$

$$N_2 = N_0 - N_1 = (1-\exp(-t/\tau))N_0,$$

$$E = \frac{N_1E_1 + N_2E_2}{N_1 + N_2} = E_1 + (1-\exp(-t/\tau))(E_2 - E_1).$$

2、The reduction rate of emission possibility due to the formation of the surface layer

$$P = \exp(-\frac{v_1 t}{L_d})$$



Surface layer

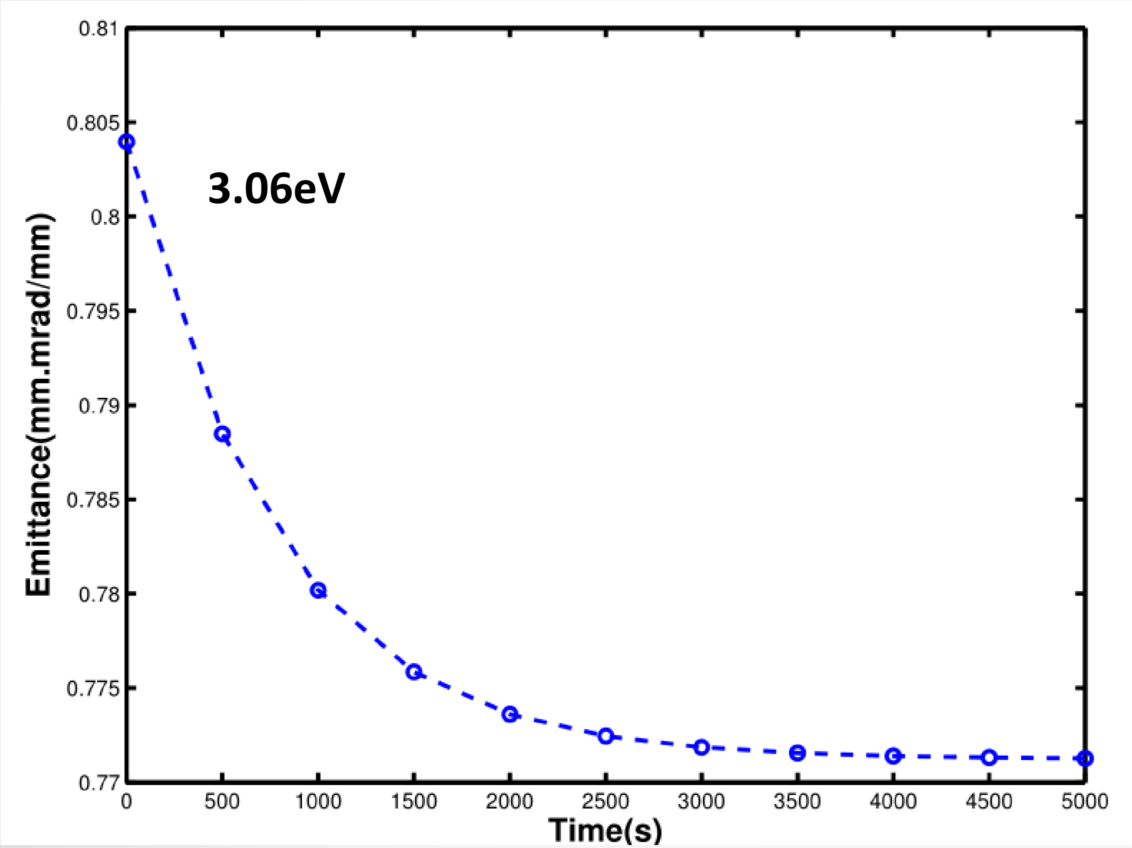
Vacuum

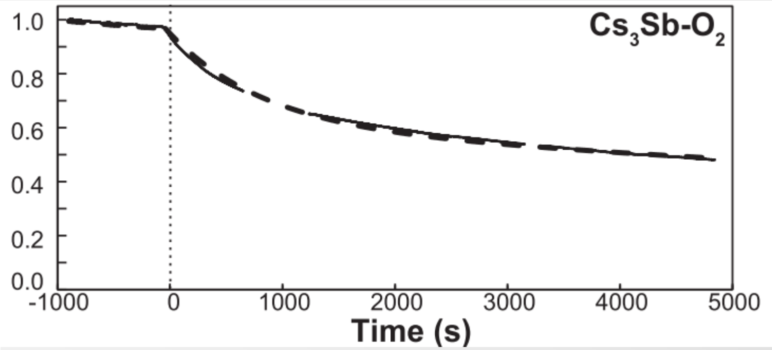
Scatter with defects

Recombine with holes

The application of the kinetics model

Cs_3Sb-O_2(10^{-9}Torr), photon energy 3.06eV.



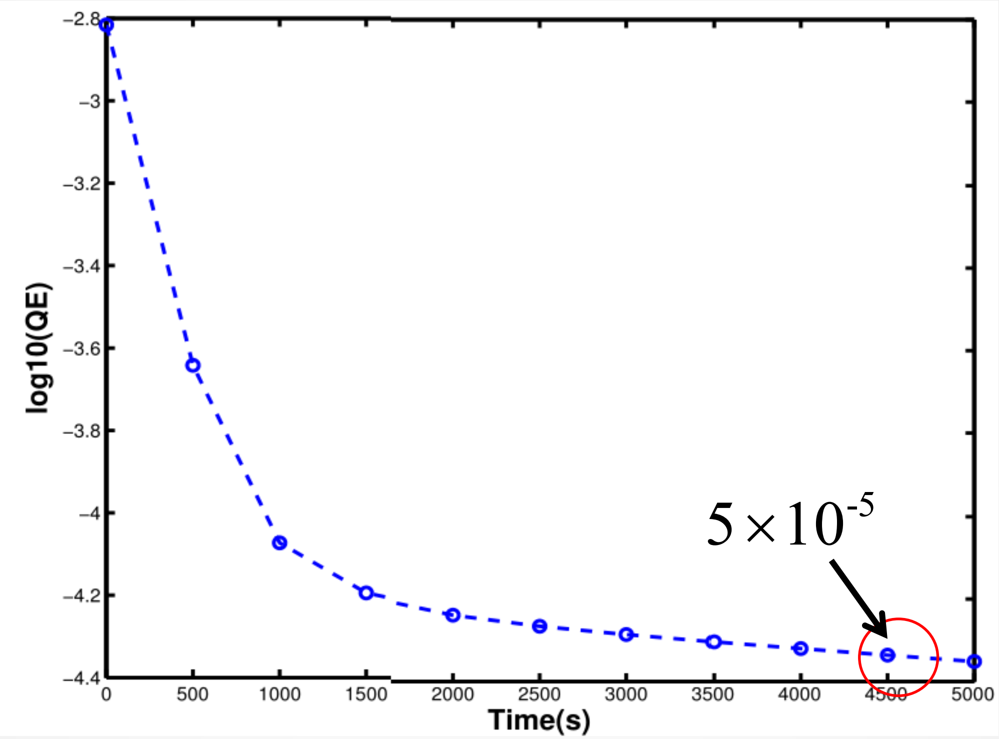


Pavlenko, AIP Advances 6, 115008 (2016)

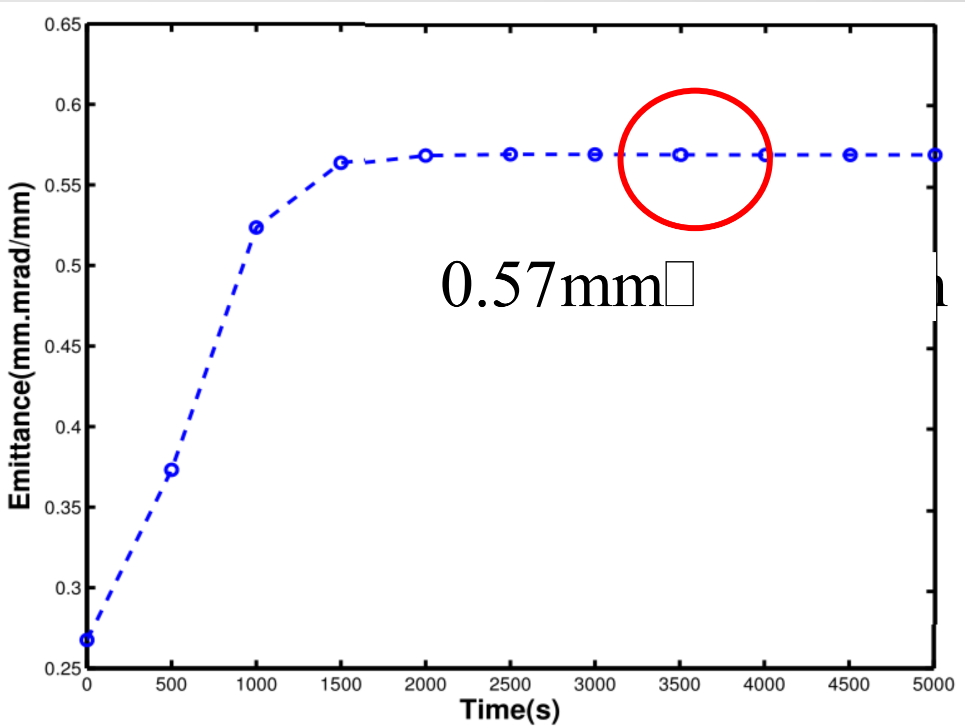
Our kinetics model can show the evolution of thermal emittance with time during the degradation process.

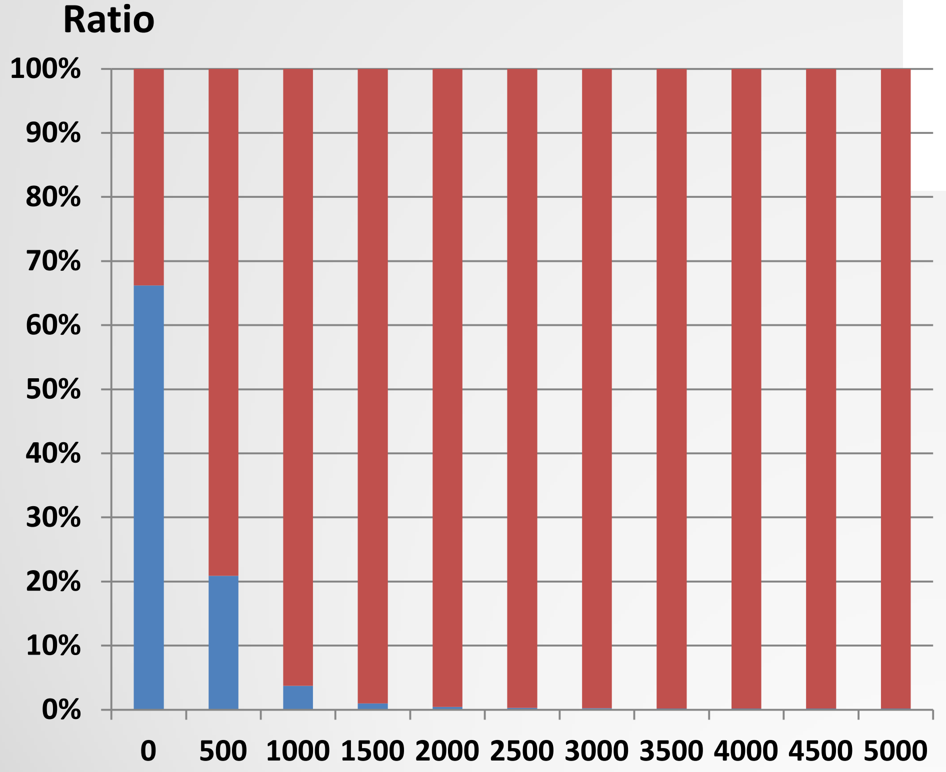
The application of the kinetics model

- Poor vacuum condition (10^{-9}Torr O_2)
- 1.8eV for Cs_3Sb
- 4MV/m——DC gun.



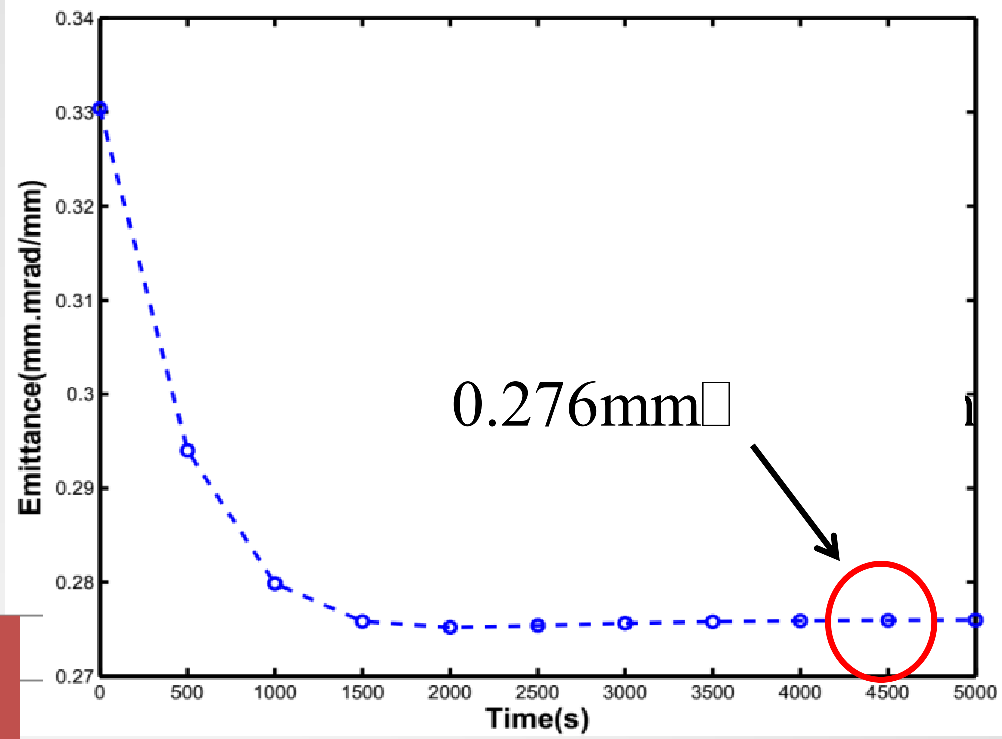
Thermal emittance increase due to the contribution of defect level.

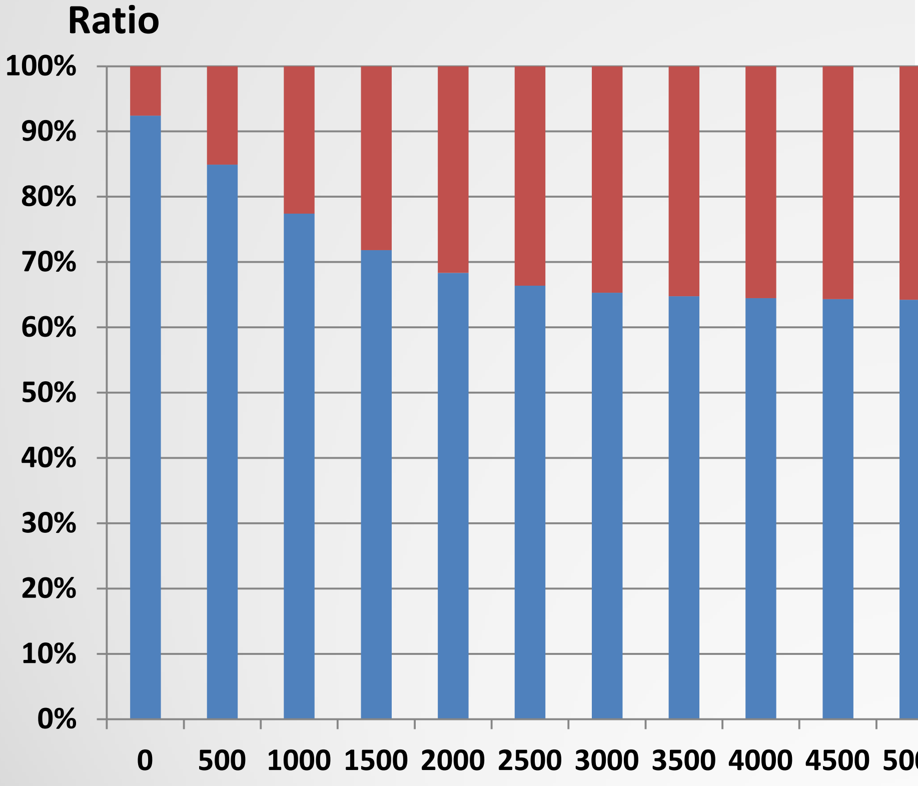




Increase the incident photon energy to 1.9eV

$$QE = 6.5 \times 10^{-4}$$



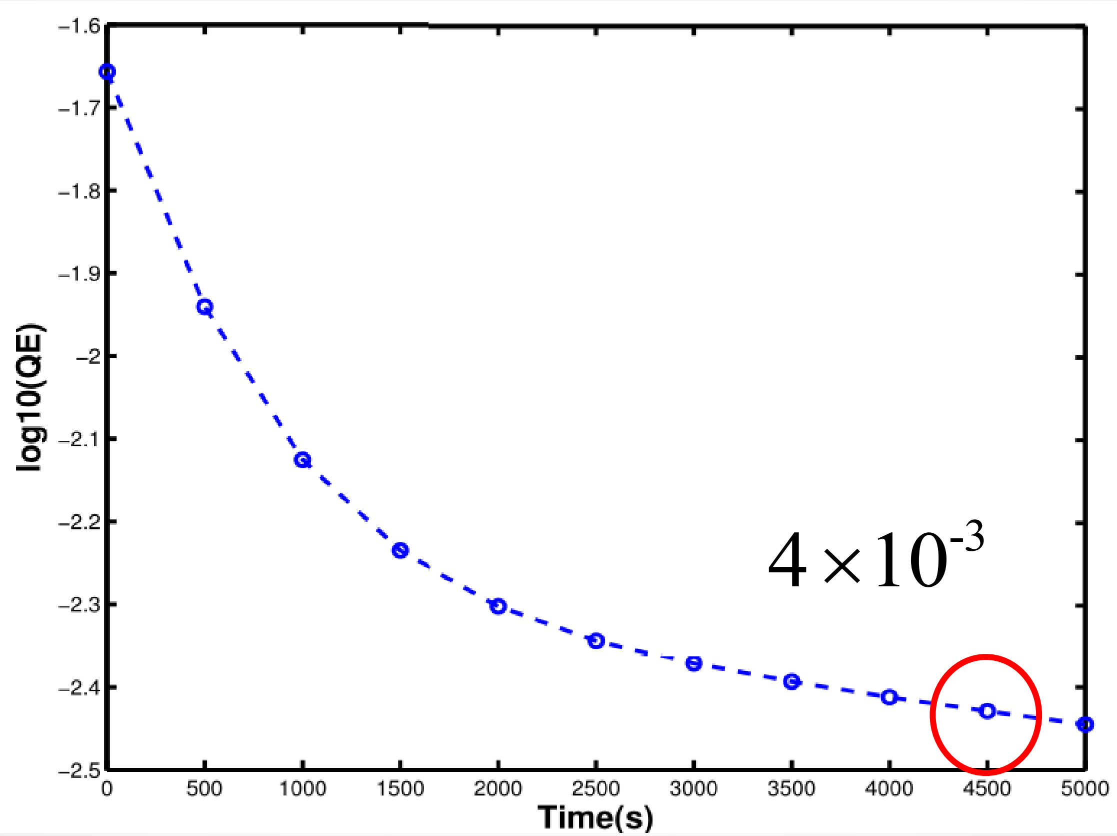


ratio

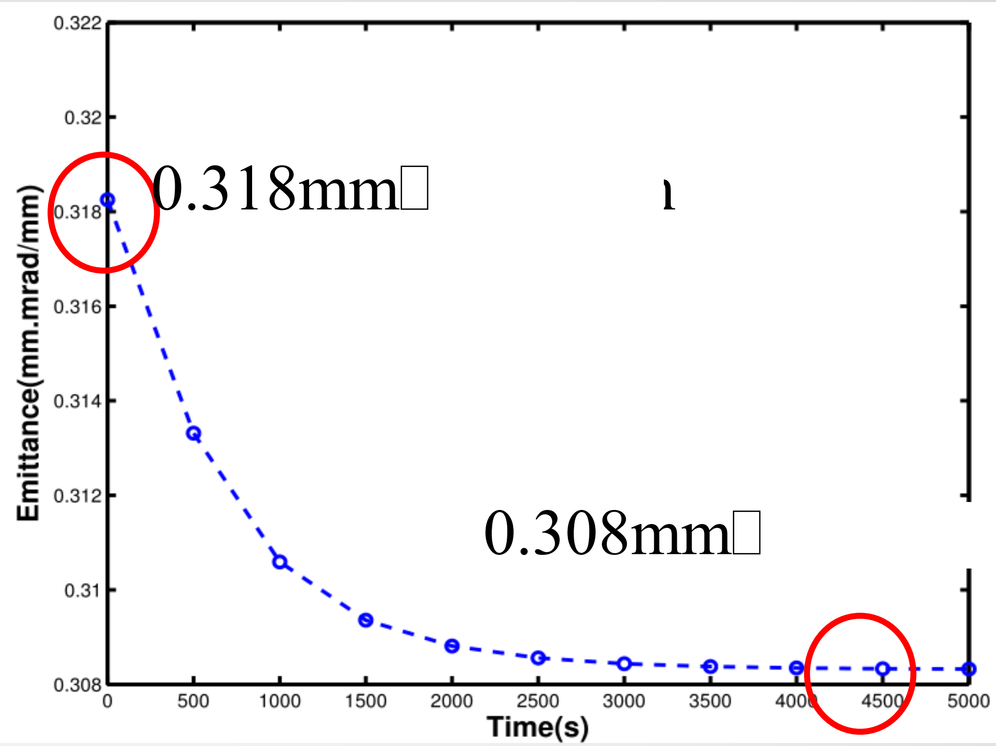
excess energy

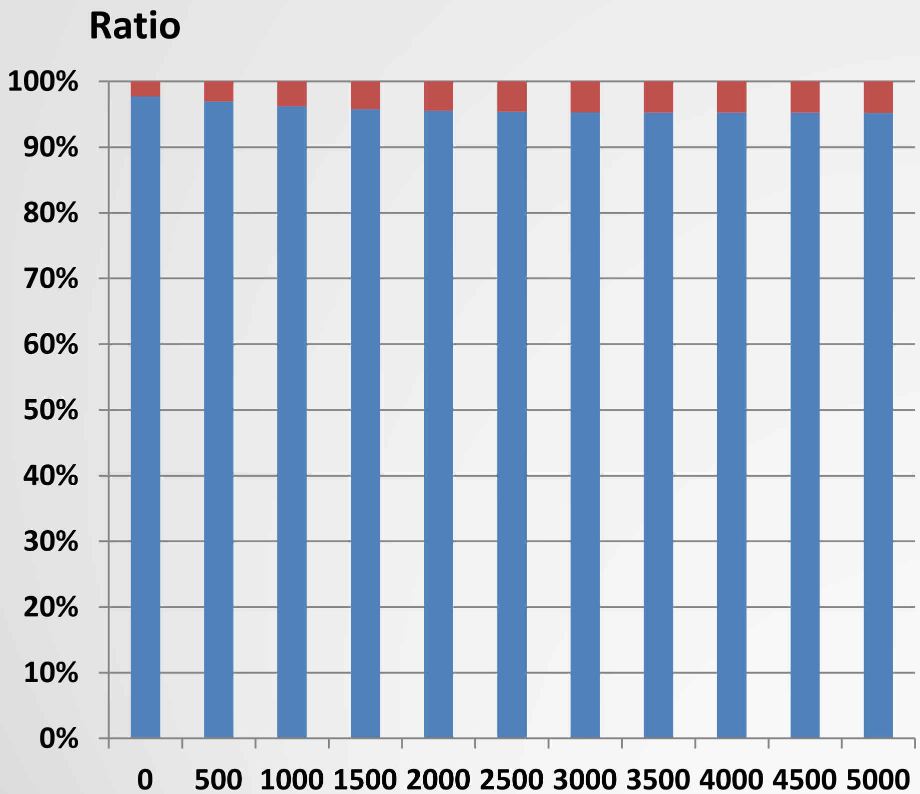
The application of the kinetics model

- Poor vacuum condition (10^{-9}Torr O_2)
- 1.8eV for Cs_3Sb
- 50MV/m——RF gun.



Thermal emittance decrease a little





🟥 **defect level**

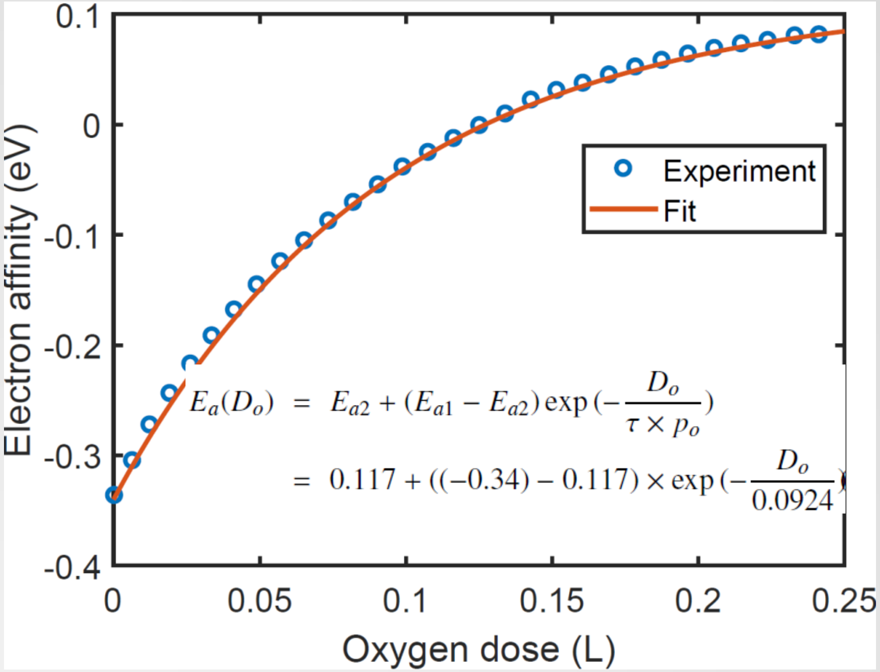
🟦 **valance band**

Time(s)

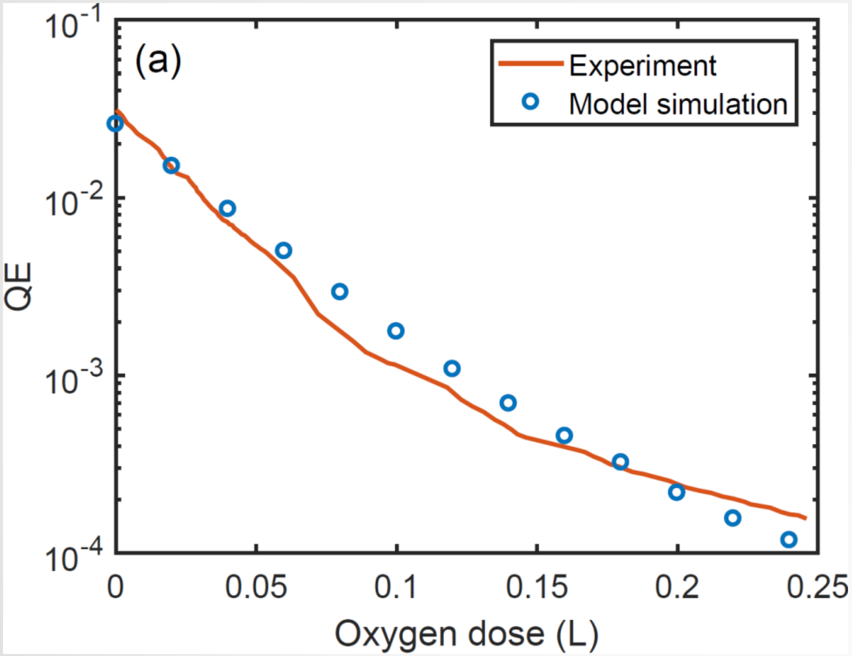
The ratio almost remain unchanged

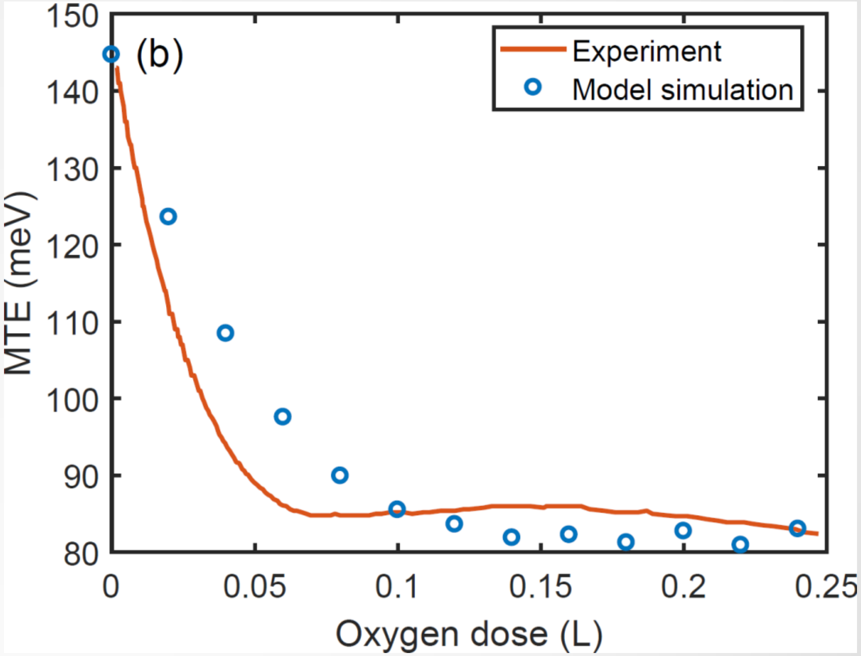
Examples for the degradation of GaAsP. The experiment data comes from J. Appl. Phys. 121, 225703 (2017) .

- Laser wavelength : 532 nm (2.33 eV)
- Threshold of GaAsP : 1.4 eV to 1.8 eV for the whole degradation process.
- There is a significant band bending near the surface (the width and the magnitude)



$$
\begin{aligned}
E_a(D_o) &= E_{a2} + (E_{a1} - E_{a2})\exp\left(-\frac{D_o}{\tau \times p_o}\right) \\
&= 0.117 + ((-0.34) - 0.117) \times \exp\left(-\frac{D_o}{0.0924}\right.
\end{aligned}
$$





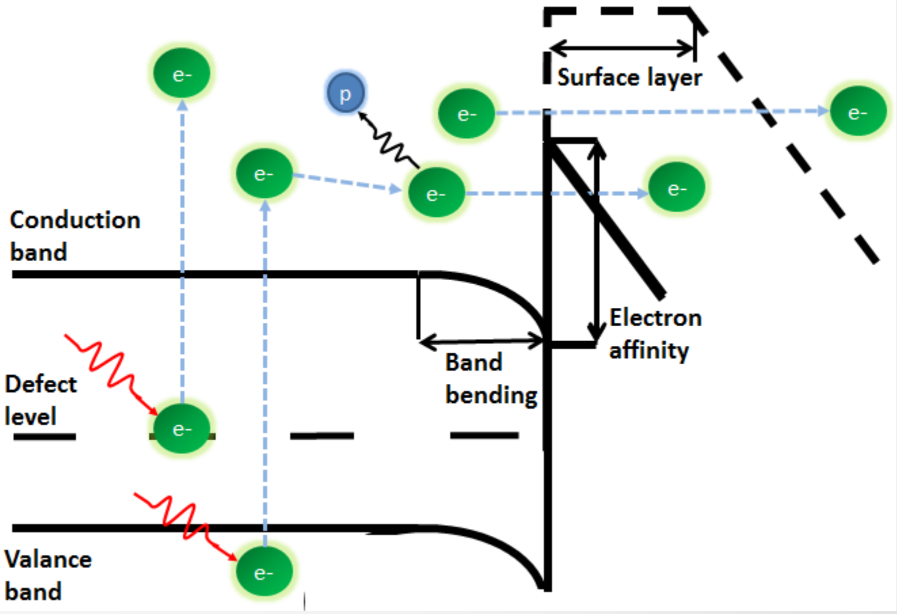
Summary

1. Static model for the photoemission of semiconductors.

- ➢ Explain the performance of semiconductors with varied laser wavelength and electric field
- ➢ Thermal emittance may reach a minimum value with varied photon energy due to the defect level.

2. Kinetics model to explain the degradation due to residue gases.

- ➢ Evaluate the evolution of thermal emittance and QE
- ➢ The possible performance of semiconductor photocathode under poor vacuum condition.
- ➢ Explain the experiment data of Cs3Sb and GaAsP.



Thanks for your attention