1st Workshop on Photo-cathodes: 300nm-500nm

July 20-21, 2009 at the University of Chicago

http://psec.uchicago.edu/photocathodeConference/photocathodeIndex.html

# The Fundamental Processes (Photon & Electron Level)

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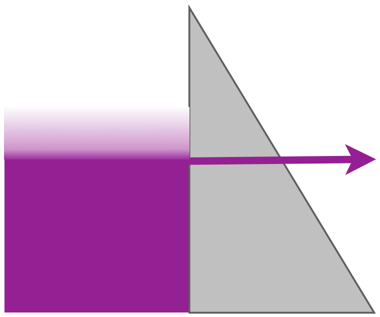
# OUTLINE

**We Shall Discuss Electron Emission (Principally Photoemission) With A Focus On:**

1. The Canonical Equations
2. Photoemission From Metals & Semiconductors: How Terms Are Calculated, Typical Values And Estimates, Comparison Of Models
   - Absorption & Reflection,
   - Transport To Surface
   - Emission
3. Complications: Emittance, Diffusion, Evaporation
4. Other Issues: Geometry, Dark Current, Space Charge

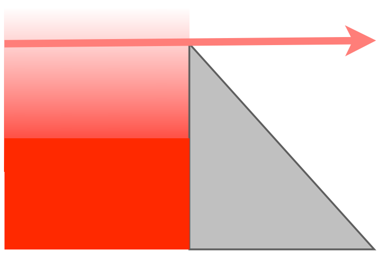
# THE CANONICAL EMISSION EQUATIONS

| Equation | Formula |
|---|---|



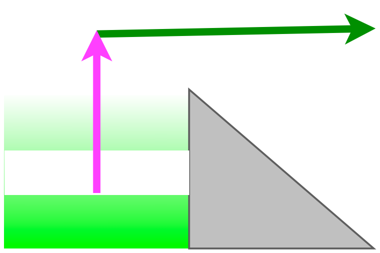
- **Field Emission**
  Fowler Nordheim
  E.L. Murphy, And R.H. Good,
  Physical Review 102, 1464 (1956).

$$J_{FN}(F) = A_{FN} F^2 \exp\left(-\frac{B\Phi^{3/2}}{F}\right)$$



- **Thermal Emission**
  Richardson-Laue-Dushman
  C. Herring, And M. Nichols,
  Reviews Of Modern Physics 21, 185 (1949).

$$J_{RLD}(T) = A_{RLD} T^2 \exp\left(-\frac{\Phi}{k_B T}\right)$$



- **Photoemission**
  Fowler-Dubridge
  L.A. DuBridge
  Physical Review 43, 0727 (1933).

$$J_{FD}(F) \propto (\hbar\omega - \Phi)^2$$

# PHOTOCURRENT AND QUANTUM EFFICIENCY

Simple Restatement of Obvious:

- QE = # of electrons emitted / # of photons absorbed    (proportional to charge emitted ΔQ) / (proportional to energy absorbed ΔE)

$$QE = \frac{\Delta Q / q}{\Delta E / \hbar\omega} \approx \frac{J / q}{I_o / \hbar\omega}$$

If Emission Is Prompt, Then Emitted Current Has Same Temporal Shape As Absorbed Laser Power:

Common Factors Of Pulse Duration (Δt) Drop Out

Left Discussing CURRENT DENSITY And LASER INTENSITY

- RULE OF THUMB: $QE[\%] = 123.98 \frac{J\left[\mathrm{A/cm^2}\right]}{I_o\left[\mathrm{W/cm^2}\right] \times \lambda[\mu\mathrm{m}]}$

| CURRENT DENSITY | LASER INTENSITY |
|---|---|
| Electrons Transport To Surface Subject To Collisions (Look At Scattering) | # Of Photons Absorbed Depends On Reflectivity Of Surface (Look At Reflectivity) |
| # That Escape Depends On Impact Of Surface Barrier If Present (Look At Emission Probability) | Photo-excitation Depth Depends On How Deeply Photon Penetrated (Look At Dielectric Constant) |

# MODELS OF QUANTUM EFFICIENCY

- Fowler-Dubridge Model For Metals
  - L.A. DuBridge. "Theory of the Energy Distribution of Photoelectrons." Physical Review 43, 0727 (1933).
  - K.L. Jensen, D.W. Feldman, N.A. Moody, and P.G. O'Shea. "A Photoemission Model for Low Work Function Coated Metal Surfaces and Its Experimental Validation." J. Appl. Phys. 99, 124905 (2006).

$$QE \propto P_{FD}(\hbar\omega) \propto (\hbar\omega - \phi)^2 + \frac{(\pi k_B T)^2}{6}$$

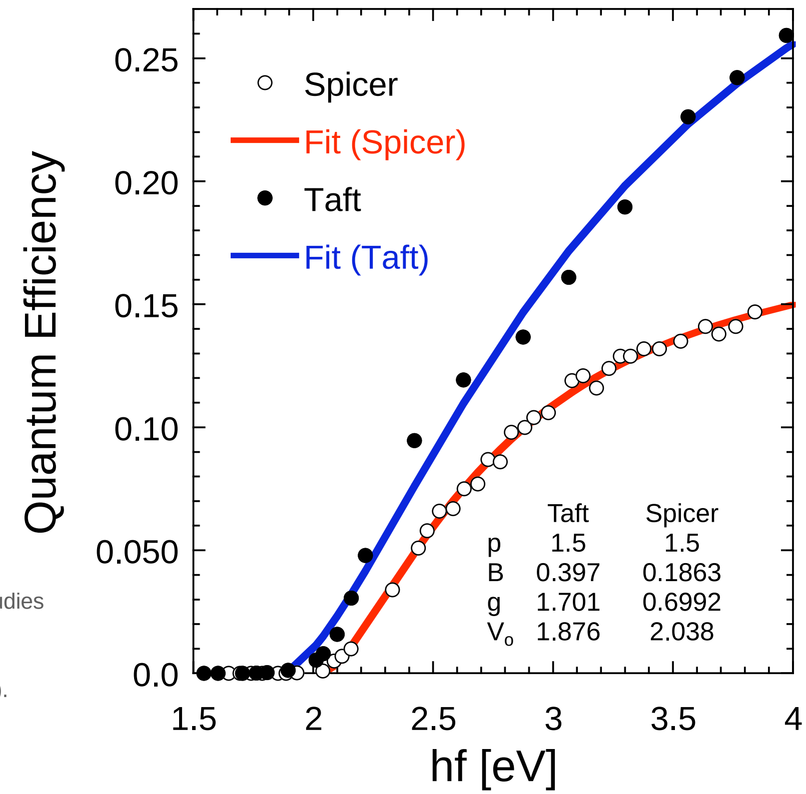
T  Temperature
Φ  Work Function

- (Modified)

$$QE = \frac{q}{\hbar\omega}\underbrace{(1 - R(\omega))}_{\text{absorption}}\underbrace{F_\lambda(\delta,\tau)}_{\text{scattering losses}}\underbrace{P_{FD}(\hbar\omega)}_{\text{transmission}}$$

- Spicer's Model For Semiconductors
  (This Version Looks Different From Spicer, But Is Same)
  - p: quasi-empirical, argued to be 3/2
  - B: (Escape)x(Transport) = B exp(-βx)
  - g: absorption factor
    "over" + "under" barrier terms
  - $V_o$: Band gap $E_g$ + Electron Affinity $E_a$

$$QE \approx \frac{B}{1 + g(E - V_o)^{-p}}$$




Originals: W.E. Spicer. "Photoemissive, Photoconductive, and Optical Absorption Studies of Alkali-antimony Compounds." Physical Review 112, 114 (1958).

E.A. Taft, and H.R. Philipp. "Structure in the Energy Distribution of Photoelectrons From $K_3Sb$ and $Cs_3Sb$." Physical Review 115, 1583 (1959).

For Metals: C.N. Berglund, and W.E. Spicer. "I - Photoemission Studies of Copper and Silver: Theory." Physical Review 136, A1030 (1964).

Modern Usage: D.H. Dowell, F.K. King, R.E. Kirby, J.F. Schmerge, J.M. Smedley. "In Situ Cleaning of Metal Cathodes Using a Hydrogen Ion Beam." Physical Review Special Topics Accelerators and Beams 9, 063502 (2006).

# COMPONENTS OF QE EQUATION

## THREE STEP MODEL OF PHOTOEMISSION

ABSORPTION of light in bulk material and photo-excitation of electrons

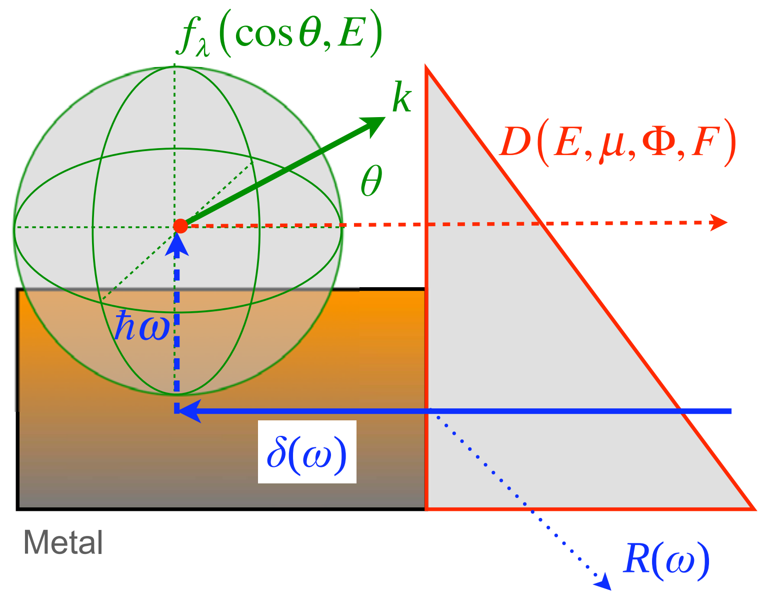
- reflectivity $R(\omega)$
- laser penetration depth $\delta(\omega)$

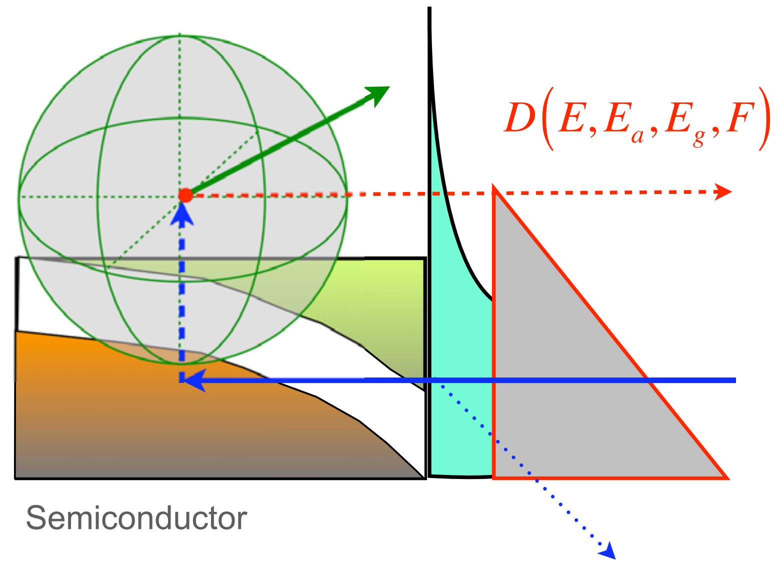
TRANSPORT of photo-excited electrons to surface subject to scattering $f_\lambda(\cos\theta,E)$

- electron energy
- scattering rates (relaxation times)

EMISSION probability $D(E)$

- Metal:
  Chemical Potential μ, Work Function $\Phi$
  (work function measured from Fermi level)
- Semiconductor:
  barrier height $E_a$, band gap $E_g$
  (Electron affinity measured from conduction band minimum)



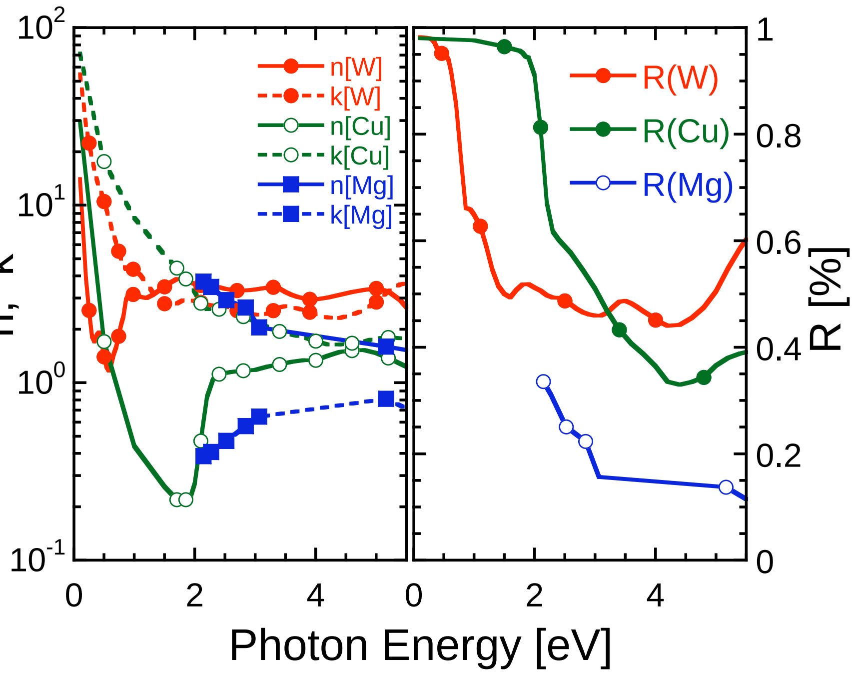



# REFLECTIVITY AND PENETRATION

For **METALS**, spline fitting of readily available n, k data works well

- k = extinction coefficient
- n = index of refraction
- Off-normal reflectivity related to normal values

$$\frac{\varepsilon}{\varepsilon_0} = (n - ik)^2 \Rightarrow \begin{cases} R(\omega) = \dfrac{(n-1)^2 + k^2}{(n+1)^2 + k^2} \\ \delta(\omega) = \dfrac{\lambda}{4\pi k} = \dfrac{c}{2k\omega} \end{cases}$$

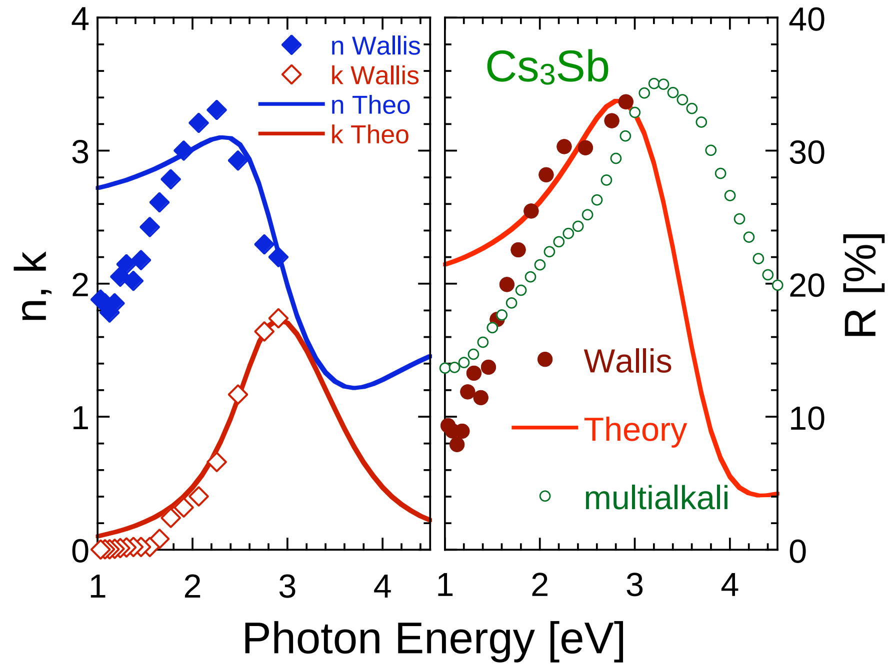



For **SEMICONDUCTORS**... A Drude-Lorentz model makes up for incomplete n,k data

- $K_o$, $K_\infty$ = static & high freq. dielectric const
- $\gamma_o$ = damping term
- $\omega_T$ = transverse optical phonon
- Some semiconductors may require multiple $\omega_T$

$$n^2 - k^2 \Rightarrow K_\infty + (K_o - K_\infty)\frac{\omega_T^2(\omega_T^2 - \omega^2)}{(\omega^2 - \omega_T^2)^2 + (\gamma_o \omega_T \omega)^2}$$

$$2nk \Rightarrow (K_o - K_\infty)\frac{\gamma_o \omega \omega_T^3}{(\omega^2 - \omega_T^2)^2 + (\gamma_o \omega_T \omega)^2}$$



# SCATTERING PROCESSES

## After Photon Absorption, Electrons Migrate And Scatter...

- ... Off Of Each Other (metals; Semiconductors If E > "magic Window" (Off Of Valence Electron If Final State Allowed)
- ... Off Of Lattice Vibrations (Phonons - Primarily Acoustic For Single Atom Material, Polar Optical If Multicomponent)

## Metals: Primary Mechanism Is Electron-Electron, But Acoustic Phonon Can Contribute

$$\tau_{ee} = \frac{4\hbar K_s^2 (\beta E)^2}{\alpha_{fs}^2 \pi m c^2}\left[\left(1+\left(\frac{\beta}{\pi}(E-\mu)\right)^2\right)\gamma\left(\frac{2k_F}{q_o}\right)\right]^{-1}$$

$$= 2.61\,fs \qquad (\mathrm{Cu}, E = \mu + \hbar\omega, \lambda = 266\mathrm{nm}, T = 300\mathrm{K})$$

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

$$= 13.1\text{ fs} \qquad (\mathrm{Cu}, E = \mu + \hbar\omega, \lambda = 266\mathrm{nm}, T = 300\mathrm{K})$$

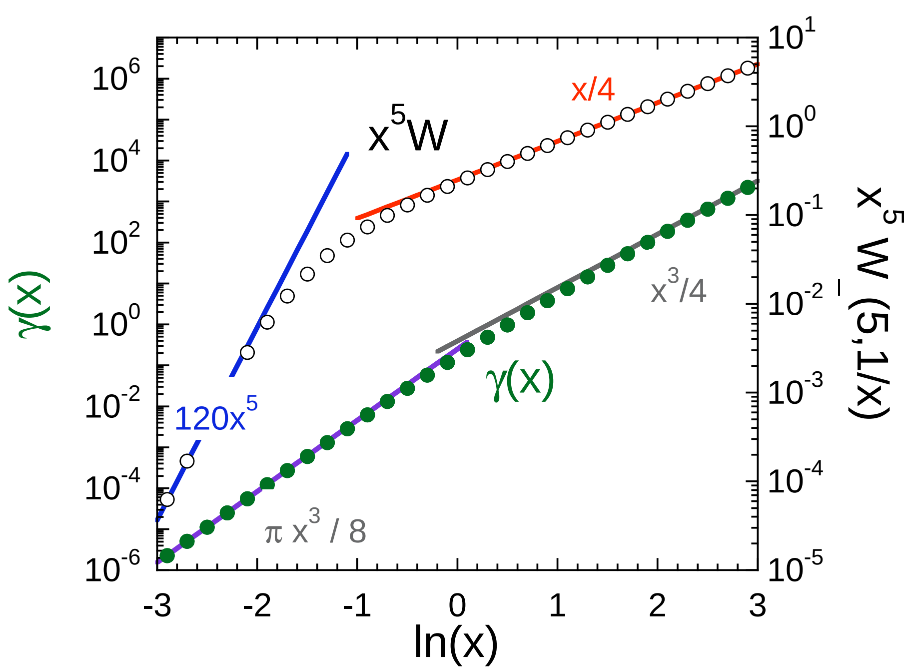
$$\gamma(x) = \frac{x^3}{4}\left(\arctan(x) + \frac{x}{1+x^2} - \frac{\arctan\left(x\sqrt{2+x^2}\right)}{\sqrt{2+x^2}}\right); \qquad q_o^2 = \frac{4k_F}{\pi K_s a_o}$$

General
- $\beta$ = $1/k_BT$ ($T_o$ = RT)
- $k_B$ = Boltzmann's constant
- $a_o$ = Bohr Radius
- $\alpha_{fs}$ = Fine structure constant
- m = e– mass (eff. or rest)
- E = Electron energy

Metal-Specific
- $\mu$ = Fermi level
- $q_o$ = Thomas Fermi Screening
- $K_s$ = Dielectric constant

Semiconductor-Specific
- $\theta$ = Debye Temperature
- $\Xi$ = Deformation Potential
- $\rho$ = Mass density
- $v_s$ = sound velocity
- hk = Momentum $2\pi(2mE)^{1/2}$

Fermi Level for Cu
- $1/\tau_{ee} = AT^2$
- $1/\tau_{ac} = AT$



# GENERIC, OR "ALPHA" SEMICONDUCTOR, MODEL

An Alpha - Semiconductor Model Can Provide Needed Parameters (e.g., Electron Effective Mass) If Such Quantities Are Unknown / Ill-defined... And Even If They're Not...

Also, Gives Forms Of Polar Optical And Ionized Impurity Scattering That Are Related To, But Different Than, Small Electron Energy Representations Found In Transport / Scattering Tomes

Alpha Semiconductor Model Restricts Upper Limit On Electron Velocity In Semiconductor To Half Of Product Of Fine Structure Constant With Speed Of Light; Implies Relationship Between Band Gap Energy And Electron Effective Mass Of:

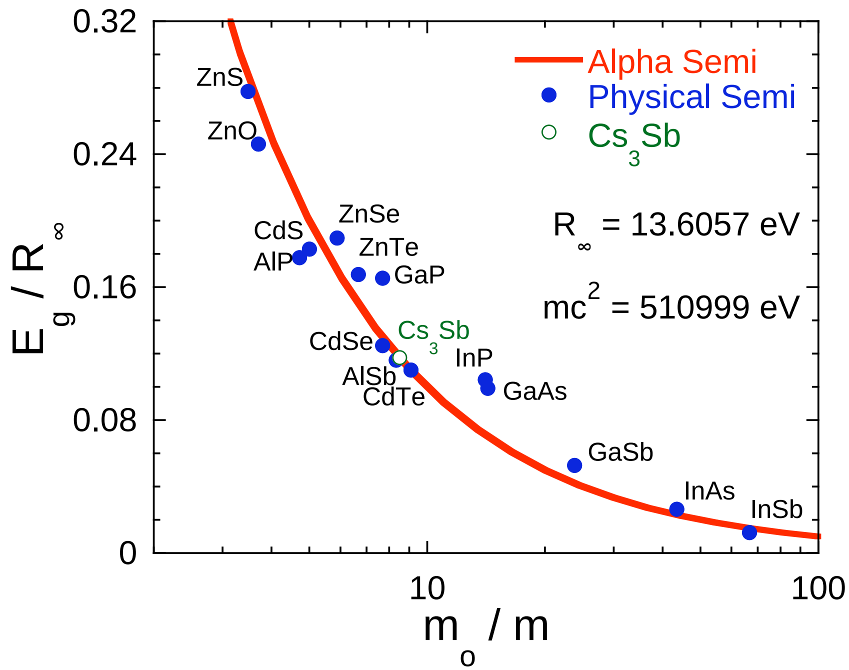
$$\frac{E_g}{R_\infty} = \frac{m}{m_o}$$

$$\frac{1}{\tau_{pop}(\hbar\omega_q, E)} = 2\omega_q\left(\frac{1}{K_o} - \frac{1}{K_\infty}\right)\left(2n(\beta\hbar\omega_q)+1\right)\eta\left(\frac{E}{E_g}\right)$$

$$\eta(u) = \frac{16u^2 + 18u + 3}{3(1+2u)\sqrt{u(u+1)}}$$

For u small, $\eta(u) \approx 1/u^{1/2}$

$$\frac{1}{\tau_{ii}(E)} \approx \frac{4\pi\hbar^2}{\alpha_{fs} m^2 c}\left(\frac{N_i}{K_o^2}\right)\frac{\ln(2)}{k_B T}\frac{E_g^2}{\sqrt{E(E+E_g)}}$$




General

- $\beta$ = $1/k_BT$ ($T_o$ = Room T)
- $k_B$ = Boltzmann's constant
- $K_o, K_\infty$ = Static & High Freq. Dielectric Const.
- $\alpha_{fs}$ = Fine structure constant
- m = electron mass (eff.)
- E = Electron energy
- $N_i$ = ionized impurity concentration
- n(x) = Bose-Einstein Distribution $1/[e^x - 1]$

Scattering for $Cs_3Sb$: Typical Values at RT in fs

- Polar Optical on the order of 26.6
- Ionized Impurity on the order of 4395.0
- Acoustic Phonon on the order of 694.0

# SCATTERING AND TRANSPORT FACTOR

In Polar Coordinates, Velocity of e- at angle $\theta$ to normal

Assume Any Scattering Event Is Fatal To Emission

Matthiessen's Rule: $\tau_{total}^{-1} = \sum_j \tau_j^{-1}$

Ratio of penetration depth to distance between events

$$p(E) = \frac{\delta(\hbar\omega)}{l(E)} = \frac{m\delta(\hbar\omega)}{\hbar k(E)\tau(E)}$$

Fraction Of Surviving Electrons

$$f_\lambda(\cos\theta, p) = \frac{\int_0^\infty \exp\left(-\frac{x}{\delta} - \frac{x}{l(E)\cos\theta}\right)dx}{\int_0^\infty \exp\left(-\frac{x}{\delta}\right)dx} = \frac{\cos\theta}{\cos\theta + p(y)}$$

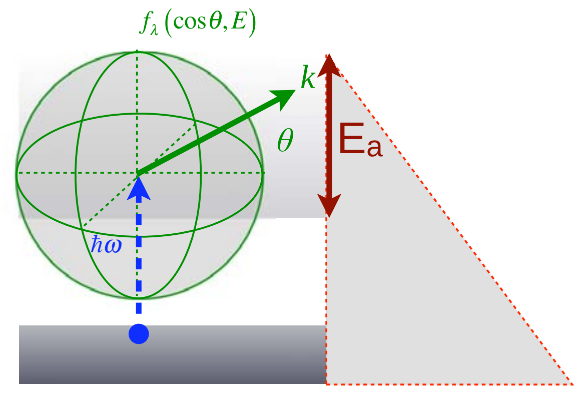
Weighted Scattering Fraction (e.g. MFD Eq.)

(1/y Acts As Cosine Of **Escape Cone Angle**)

$$F_\lambda = \int_{1/y}^{1} x f_\lambda(x,p)dx$$
$$= p^2 \ln\left[\frac{y(1+p)}{1+yp}\right] + \frac{1}{2y^2}(1-y)(2yp - y - 1)$$

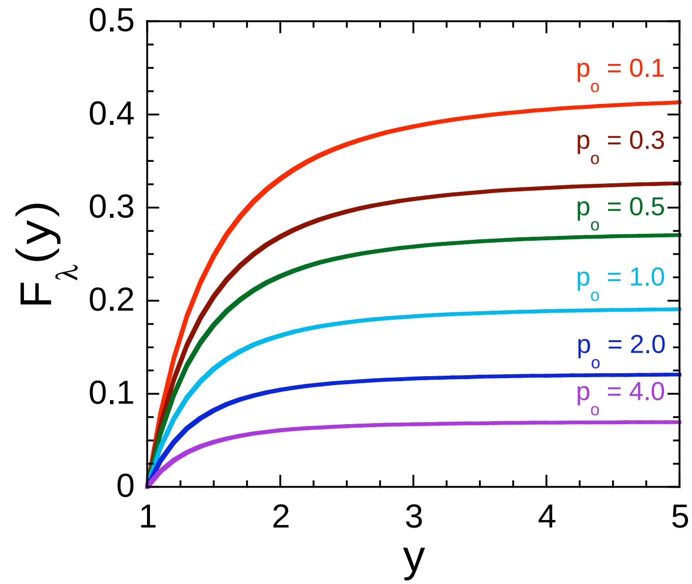
- for semiconductors, measure E w.r.t. $E_a$
- **IF** $\tau$ scales as 1/k, then p is constant

$$E \equiv E_a y^2$$
$$p \approx p_o$$




Example: Cs3Sb-like
- $\delta$ = 27 nm
- v/c = 0.8%
- $\tau$ = 31 fs
- ➡ p ≈ 0.36

Example: Cu-like
- $\delta$ = 12.6 nm
- v/c = 0.675%
- $\tau$ = 2.6 fs
- ➡ p ≈ 2.38



# TRANSMISSION AND CURRENT

## "Moments" Method Of Calculating QE Is Via Solutions To Schrödinger's Eq.

- CLASSICAL: f(x,k,t) Is Distribution Function Where x & k Are Conjugate Coordinates => Boltzmann's Eq.
- Integration Of $k^n$ • f(x,k) = Moments: Continuity Eq. Relates 1st (Density) & 2nd (Current Density) Moment:

velocity acceleration

$$\frac{f(x+dx,k+dk,t+dt)-f(x,k,t)}{dt} \Rightarrow \left\{\frac{\partial}{\partial t}+\frac{\hbar k}{m}\frac{\partial}{\partial x}+\frac{F}{\hbar}\frac{\partial}{\partial k}\right\} f(x,k,t)=0$$

$$\frac{\partial}{\partial t}\rho(x,t)=\frac{\partial}{\partial t}\left[\frac{1}{2\pi}\int_{-\infty}^{\infty} f(x,k,t)\,dk\right]=\frac{\partial}{\partial x}\left[\frac{1}{2\pi}\int_{-\infty}^{\infty}\left(\frac{\hbar k}{m}\right)f(x,k,t)\,dk\right]=-\frac{\partial}{\partial x}J(x,t)$$

- QUANTUM MECHANICS

"pure state" form

$$\partial_t\hat{\rho}(t)=\frac{i}{\hbar}\left[\hat{H},\hat{\rho}(t)\right]=-\frac{\hbar}{2m}\frac{\partial}{\partial\hat{x}}\left\{\hat{k},\hat{\rho}(t)\right\}=-\frac{\partial}{\partial\hat{x}}\hat{j}(t)\Rightarrow j(x,t)=\frac{\hbar}{2m}\left\langle x\left|\left\{\hat{\rho}(t),\hat{k}\right\}\right|x\right\rangle=\frac{\hbar}{2mi}\left\{\psi^{\dagger}\partial_x\psi-\psi\partial_x\psi^{\dagger}\right\}$$

Mixed state form

$$\hat{\rho}(t)=\sum f_{FD}(E_k)\left|\psi_k(t)\right\rangle\left\langle\psi_k(t)\right|\Rightarrow\rho(x)=(2\pi)^{-3}\int dk\int d\mathbf{k}_{\perp}\,f_{FD}(E(\mathbf{k}))\left|\psi_k(x)\right|^2$$

f(x,k) Approximated By Product Of Supply Function *f(k)* X Probability Of Transmission *D(k)* Past Barrier

---

Transmission Probability = ratio of transmitted to incident current density for given k

$$D(k)\equiv\frac{j_{trans}(k)}{j_{inc}(k)}$$

Commonly assumed that energy is parabolic in momentum k

$$E(k)\equiv\frac{\hbar^2}{2m}\left(k^2+k_{\perp}^2\right)$$

Supply Function

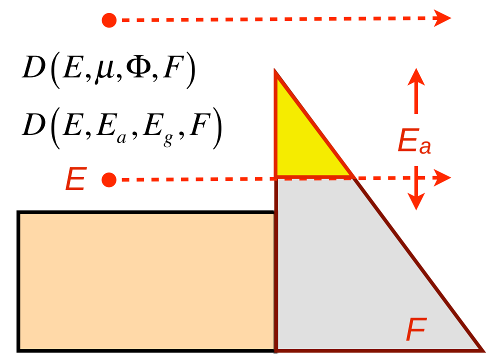
$$f(k)=(2\pi)^{-2}\int f_{FD}\left(E(k,\mathbf{k}_{\perp})\right)d\mathbf{k}_{\perp}$$

Tsu-Esaki-like formula

$$J(F,T)=\frac{q}{2\pi}\int_0^{\infty}\frac{\hbar k}{m}D(k)\,f(k)\,dk$$

- Velocity
- Transmission Probability
- Supply Function

# EMISSION PROBABILITY AND BARRIER

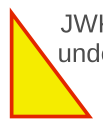



Surface Barrier Subject To Applied Field Does Not Entail That D(E) Is A Step Function

- Triangular Barrier (Fowler-Nordheim Potential)
  Reasonable If No Image Charge Modification
- Exact Solution: Airy Functions
- Approximation: JWKB Method (As Commonly Used)
  D(E) Calculation Requires Auxiliary Terms
  Observe Definitions Work For E > $E_a$ Too

$$\left|E-E_a\right|_+ \approx \left[\left(E-E_a\right)^2+\frac{4}{25}\left(\frac{\hbar^2F^2}{2m}\right)^{2/3}\right]^{1/2}$$

$$\theta\left(E<E_a\right)=2\int k(x)\,dx=\frac{2\hbar^2}{3mF}\left[\frac{2m}{\hbar^2}\left(E_a-E\right)\right]^{3/2} \leftrightarrow$$



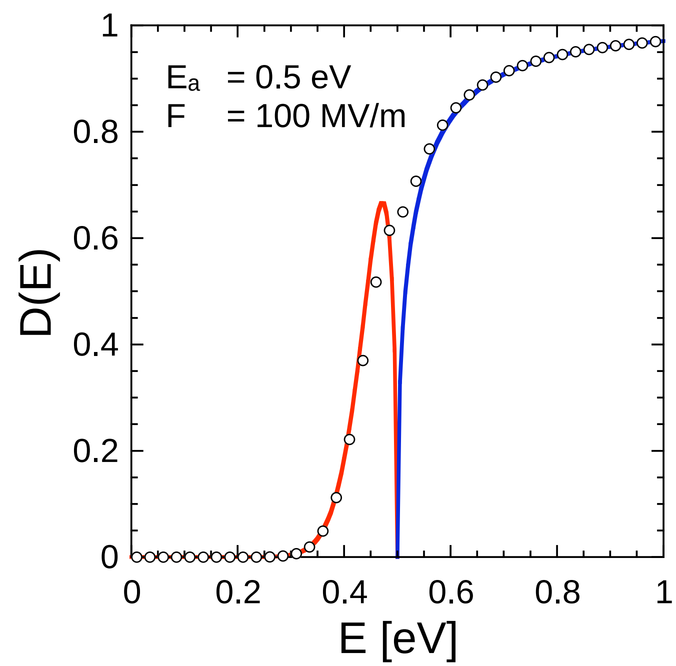
JWKB "area under curve"

$$D_\Delta\left(E\right)=\frac{4\sqrt{E\left|E-E_a\right|_+}}{2\sqrt{E\left|E-E_a\right|_+}+\left(\left|E-E_a\right|_++E\right)e^{\theta(E)}}$$

- Even For Small $E_a$, D(E) Is NOT A Step Function
- To Extend To Metals ( Image Charge ), Append $v(y)$ to $\theta(E)$

$$D_>\left(E\right)\approx\frac{4\sqrt{E\left(E-E_a\right)}}{\left[\left(E-E_a\right)^{1/2}+E^{1/2}\right]^2}$$

$$D_<\left(E\right)=\frac{4}{E_a}\sqrt{E\left(E_a-E\right)}e^{-\theta(E)}$$



# THERMAL-FIELD-PHOTO-EMISSION EQUATION

## Common Forms Of Emission Equations Obtained From One Formulation Using Energy Slope Terms (field) $\beta_F$, (temperature) $\beta_T$ & Expansion Point $E_o$

1D Approach To Evaluation (E Is "forward" Energy)

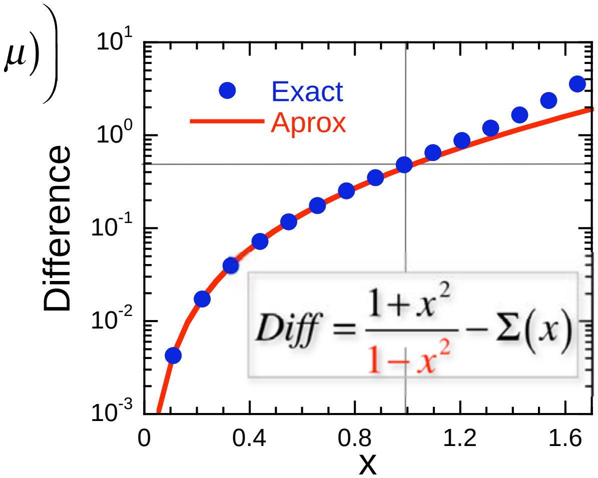
$$J(F,T) = \frac{e}{2\pi\hbar}\left(\frac{m}{\pi\beta_T\hbar^2}\right)\int_0^\infty \frac{\ln\left\{1+\exp\left[\beta_T(\mu-E)\right]\right\}}{\left\{1+\exp\left[\beta_F(E_o-E)\right]\right\}}dE = A_{RLD}T^2 N\left(\frac{\beta_T}{\beta_F},\beta_F(E_o-\mu)\right)$$

- Numerator: Supply Function With $\beta_T = 1/k_B T$
- Denominator: Kemble Form Of D(k) With $\theta(E) = \beta_F(E_o - E)$

$$N(n,s) = n^2\Sigma\left(\frac{1}{n}\right)e^{-s} + \Sigma(n)e^{-ns} = \frac{1}{2}n^2 s^2 + \zeta(2)\left[n^2+1\right] - N(n,-s)$$

$$\Sigma(x) \equiv 1 + \sum_{j=1}^{\infty}\left(1-2^{1-2j}\right)\zeta(2j)\,x^{2j}$$

When $\beta_F$ & $\beta_T$ Become Comparable, Σ Can Be Large




$\zeta(x)$ = Riemann zeta function

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$$J_T \equiv A_{RLD}(k_B\beta_T)^{-2}\,\Sigma\left(\frac{\beta_T}{\beta_F}\right)\exp\left[-\beta_T(E_o-\mu)\right]$$

Limit (n = 0)
Richardson (Thermal) Eq

$$A_{RLD}T^2\exp\left[-\beta_T\phi\right]$$

$$J_F \equiv A_{RLD}(k_B\beta_F)^{-2}\,\Sigma\left(\frac{\beta_F}{\beta_T}\right)\exp\left[-\beta_F(E_o-\mu)\right]$$

Limit (n = ∞)
Fowler-Nordheim (Field) Eq

$$A_{FN}F^2\exp\left[-\frac{B_{FN}}{F}\right]$$

$$QE_{MFD} = (1-R(\omega))F_\lambda\left\{\frac{(\hbar\omega-\phi)^2 + 2\zeta(2)\left(\beta_T^{-2}+\beta_F^{-2}\right)}{2\hbar\omega(2\mu-\hbar\omega)}\right\}$$

Energy Augmented By Photon (s<0)
Fowler-Dubridge Equation

$$\propto (\hbar\omega-\phi)^2$$

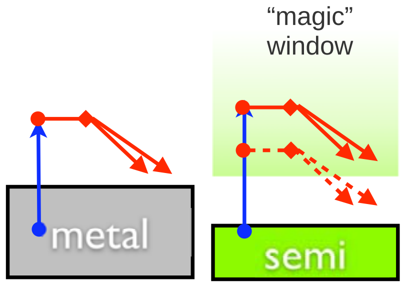
# MOMENTS-BASED EVALUATIONS REDUX

## DEFINE the “Moments” function $M_n$ by generalizing distribution function approach

metals - final state may be occupied (blue)

semiconductors - final state unoccupied & in conduction band (creates “magic” window)

To Calculate Emittance, Swap Forward Momentum With Transverse:




$$M_n = (2\pi)^{-3}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty E^{1/2}\,dE\int_0^{\pi/2}\sin\theta\,d\theta\left(\frac{2m}{\hbar^2}E\cos^2\theta\right)^{n/2}\times$$
$$D\left\{(E+\hbar\omega)\cos^2\theta\right\} f_\lambda\left[\cos\theta, p(\hbar\omega)\right] f_{FD}(E)\left\{1-f_{FD}(E+\hbar\omega)\right\}$$

QE = Ratio Of Emitted $M_1$ To Possible $M_1$ (3D: E Is Total Energy; Semiconductor Shown)

$$QE = (1-R(\omega))\frac{\int_{E_a}^{\hbar\omega-E_g} E\left[\int_{\sqrt{E_a/E}}^{1} x f_\lambda(x,E)\,D_\Delta\left[(E+\hbar\omega)x^2\right]dx\right]dE}{2\int_0^{\hbar\omega-E_g} E\left[\int_0^1 x\,dx\right]dE}$$

Leading Order (FD) Approximation: Ignore cosθ Dependence In D (i.e., take x = 1)

This form will lead to the comparison with the Spicer Model form

$$QE_0 = \frac{(1-R(\omega))}{2(\hbar\omega-E_g)^2}\int_{E_a}^{\hbar\omega-E_g} E D_\Delta(E+\hbar\omega)\left[\int_{\sqrt{E_a/E}}^{1} x f_\lambda(x,E)\,dx\right]dE$$

This Term Is Same As Scattering Factor In MFD

# THE PIC MODEL & SPICER COMPARISON

## Most Adaptable Model For Particle-In-Cell (PIC) Codes Modeling Beams Is $QE_0$

- How Does $QE_0$ Compare To QE?
- How Does $QE_0$ Compare To Spicer 3-Step Model?

Recall:

Define:

$$F_\lambda(x) = \int_{1/x}^{1} s f_\lambda\left(s, E_a x^2\right) ds \Rightarrow G_\lambda(y) = \frac{8}{y^4}\int_1^y x^3 F_\lambda(x)\,dx$$

Define:

$$\chi = \hbar\omega - \left(E_g + E_a\right)$$

## PIC - Ready Formulation

$$QE_0 = \frac{1}{2}\left(1 - R(\omega)\right) G_\lambda\left(\sqrt{1 + \frac{\chi}{E_a}}\right)$$

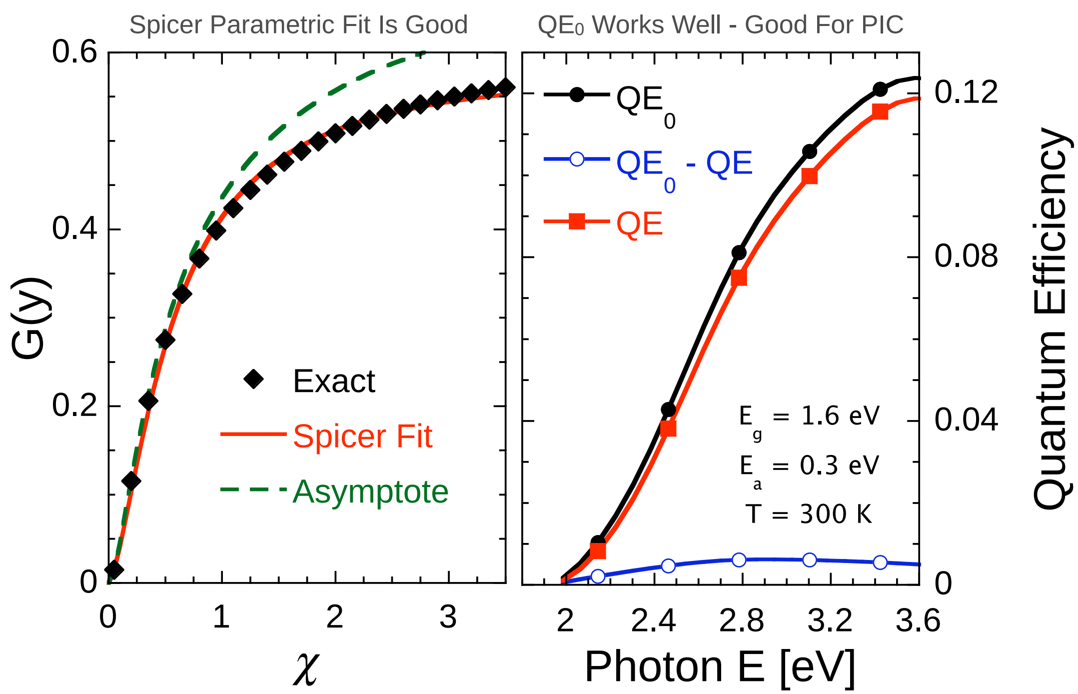
In The Limit Of Small $\chi$ (asymptote)

$$\lim_{\chi \to 0} G_\lambda(y) \approx \frac{1}{\left(p_o + 1\right)\left(1 + \frac{E_a}{\chi}\right)^2}$$

Comparison To Spicer 3-Step Model

- Interpretation Of B, g Altered
- Power Of $\chi$ And Dependence Changed

$$QE_{spicer} \approx \frac{B}{1 + g\chi^{-3/2}}$$

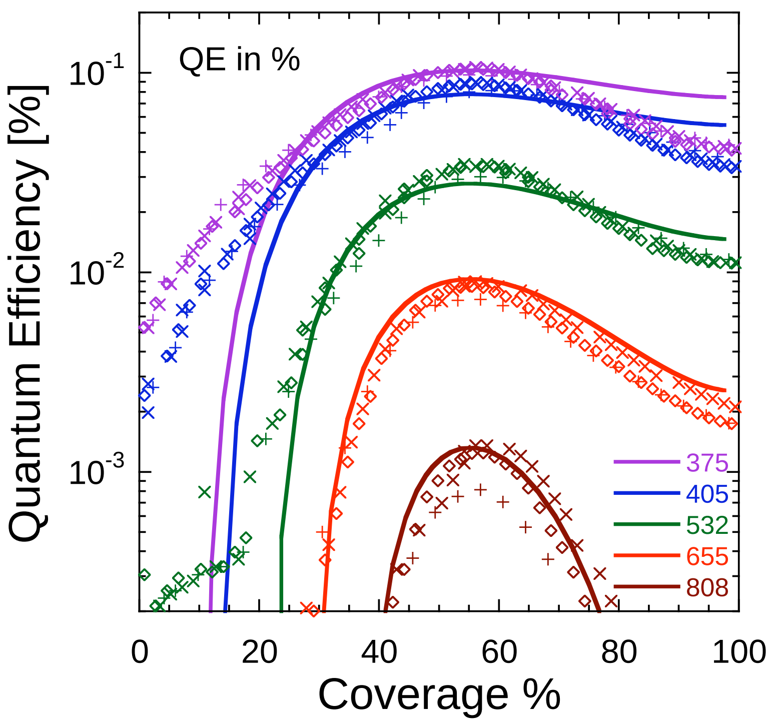


### Photoemission From Metals And Cesiated Surfaces

Kevin L. Jensen, N. A. Moody, D. W. Feldman,
E. J. Montgomery, and P. G. O'Shea

J. Appl. Phys. 102, 074902 (2007); DOI:10.1063/1.2786028

A model of photoemission from coated surfaces is significantly modified by first providing a better account of the electron scattering relaxation time that is used throughout the theory, and second by implementing a distribution function based approach ("Moments") to the emission probability. The latter allows for the evaluation of the emittance and brightness of the electron beam at the photocathode surface. Differences with the Fowler-Dubridge model are discussed. The impact of the scattering model and the Moments approach on the estimation of quantum efficiency from metal surfaces, either bare or partially covered with cesium, are compared to experiment. The estimation of emittance and brightness is made for typical conditions, and the derivation of their asymptotic limits is given. The adaptation of the models for beam simulation codes is briefly discussed.

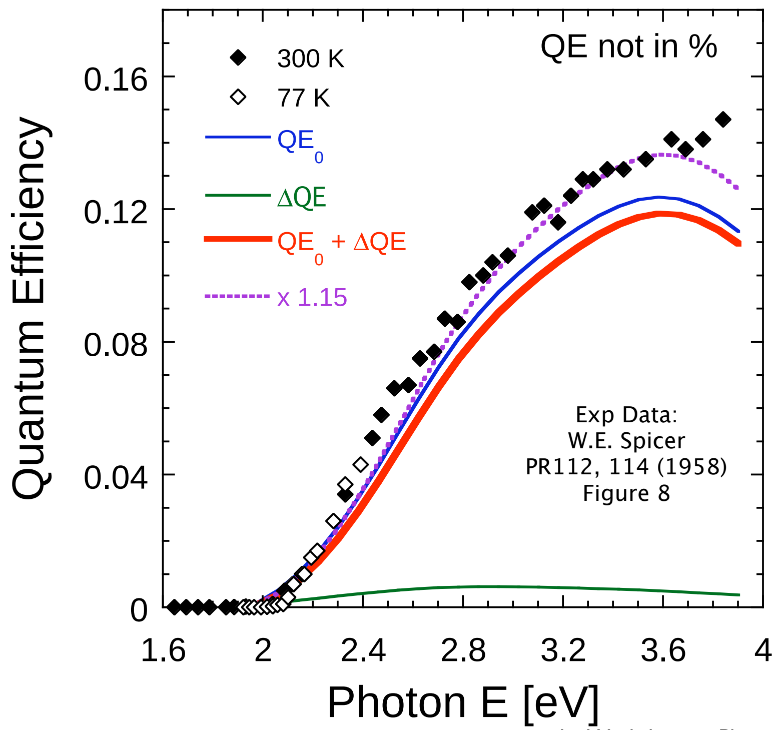



### Theory Of Photoemission From Cesium Antimonide Using An Alpha-semiconductor Model

Kevin L. Jensen, Barbara L. Jensen, Eric J. Montgomery,
Donald W. Feldman, Patrick G. O'Shea, and Nathan Moody

J. Appl. Phys. 104, 044907 (2008); DOI:10.1063/1.2967826

A model of photoemission from cesium antimonide (Cs3Sb) that does not rely on adjustable parameters is proposed and compared to the experimental data of Spicer [Phys. Rev. 112, 114 (1958)] and Taft and Philipp [Phys. Rev. 115, 1583 (1959)]. It relies on the following components for the evaluation of all relevant parameters: (i) a multidimensional evaluation of the escape probability from a step-function surface barrier, (ii) scattering rates determined using a recently developed alpha-semiconductor model, and (iii) evaluation of the complex refractive index using a harmonic oscillator model for the evaluation of reflectivity and extinction coefficient.



# EMITTANCE

## Transverse Moments (metal & semiconductors)

$$M_n = (2\pi)^{-3}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty E^{1/2}\,dE\int_0^{\pi/2}\sin\theta\,d\theta\left\{\frac{2m}{\hbar^2}(E+\hbar\omega)\sin^2\theta\right\}^{n/2} D\{(E+\hbar\omega)\cos^2\theta\}\, f_\lambda\left[\cos\theta, p(\hbar\omega)\right]\begin{cases} f_{FD}(E)\left(1-f_{FD}(E+\hbar\omega)\right) \\ \Theta\left(\hbar\omega+E-E_g\right)\end{cases}$$

Explanation of addition of photon energy to E for $k^n$ term:

- Schrödinger's Eq.: E of e- in vacuum measured wrt conduction band min decreased by barrier height BUT
- Continuity of $\psi$ & $\partial x\, \psi$ means $k_\rho$ is conserved*

THEREFORE:

$$k_\rho^{vacuum} = k_\rho^{semiconductor} = \left(\frac{2m}{\hbar^2}(E+\hbar\omega)\right)^{1/2}\sin\theta$$

* See also: D.H. Dowell, J.F. Schmerge, SLAC-PUB-13535 (2009) they show ε eq. (klj) didn't include hf in $k_\rho$ so ε small by $[\mu/(\mu+hf)]^{1/2}$

### THERMAL EMISSION

| | |
|---|---|
| No photons | $\hbar\omega = 0$ |
| Uniform emission | $2\langle x^2\rangle = \langle\rho^2\rangle = \rho_c^2$ |
| Richardson Approx. | $D(k) = \Theta(E(k)-\mu-\phi)$ |
| No Scattering | $f_\lambda(x,p) = 1$ |
| Maxwell-Boltzmann f(x,k) | $D(k)f(k) \propto \exp\{-\beta_T(E(k)-\mu)\}$ |
| No "final state" issues | $1-f_{FD}(E) \Rightarrow 1$ |

$$\varepsilon_{n,rms}(thermal) = \frac{\hbar}{mc}\sqrt{\langle x^2\rangle\langle k_x^2\rangle} = \frac{\hbar}{mc}\left(\frac{\rho_c}{2}\right)\left(\frac{M_2}{2M_0}\right)^{1/2} = \frac{\rho_c}{2}\left(\frac{k_B T}{mc^2}\right)^{1/2}$$

### PHOTO-EMISSION

| | |
|---|---|
| Photons | $\hbar\omega > 0$ |
| Uniform emission | $2\langle x^2\rangle = \langle\rho^2\rangle = \rho_c^2$ |
| JWKB Approx. | $D(k) = D_{JWKB}(E,F)$ |
| Scattering | $f_\lambda(x,p) = x/\left(x+p(E)\right)$ |
| Schottky Lowering | $\phi = \Phi - \sqrt{q^2F/4\pi\varepsilon_0}$ |

leading order (metal)

$$\varepsilon_{n,rms}(photo) = \frac{\hbar}{mc}\left(\frac{\rho_c}{2}\right)\left(\frac{M_2}{2M_0}\right)^{1/2} \approx \frac{\rho_c}{2}\left[\frac{(\hbar\omega-\phi)}{3mc^2}\right]^{1/2}$$

Note: for metals, p large & $f_\lambda \approx \cos\theta/p$: therefore, emittance indep. of p. Semiconductors larger ε due to p small, but D behavior also has impact

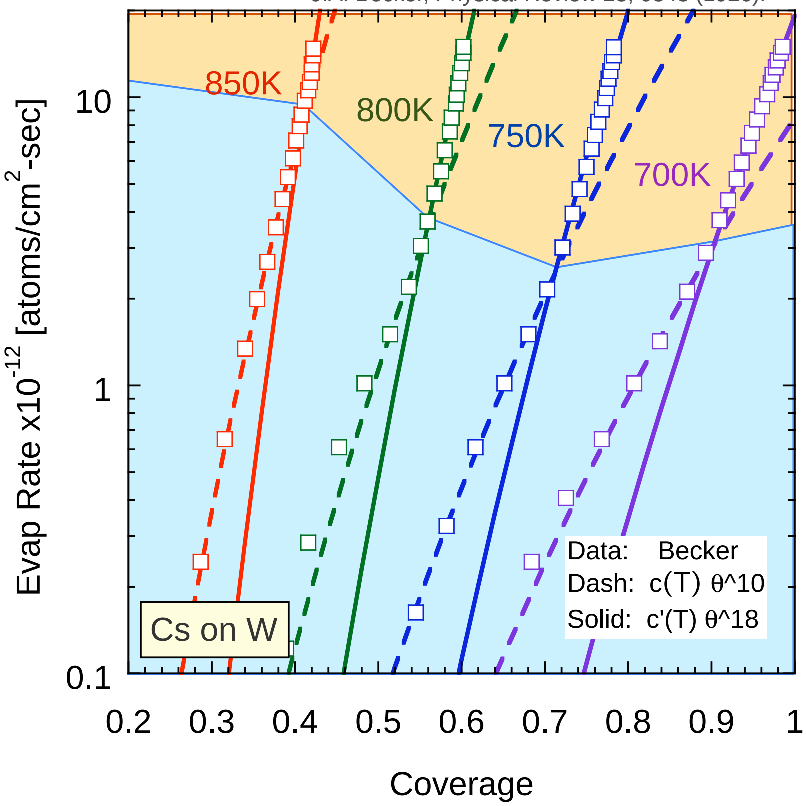
# COVERAGE, EVAPORATION, WORK FUNCTION

Evap of Cs on W shows power-law dependence on coverage θ of form c(T) x $\theta^n$

BUT c & n change depending on θ

- Yellow: $c \approx \exp(-68.1 + 5.19/k_B T)$ n = 18
- Blue: $c \approx \exp(-39.6 + 3.04/k_B T)$ n = 10

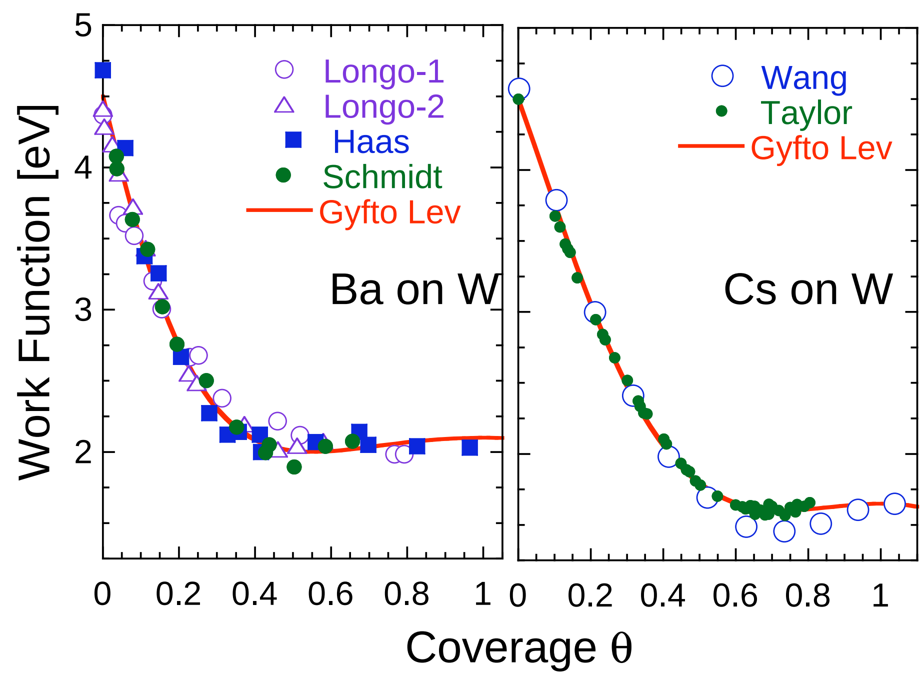
J.A. Becker, Physical Review 28, 0343 (1926).




## θ related to Φ of surface via Gyftopoulos-Levine Theory

Experiments at UMD to understand relation of QE to coating & rejuvenation methods

- Work function depends on crystal face, bulk material, and alkali (or alkali earth) coating
- Work function minimizes at sub-monolayer θ
- Coatings on metals simplest - increasingly more complex semiconductor surfaces under study
- With evap/diff, possibility of uniform coverage at desired factor (e.g., dispenser photocathode)

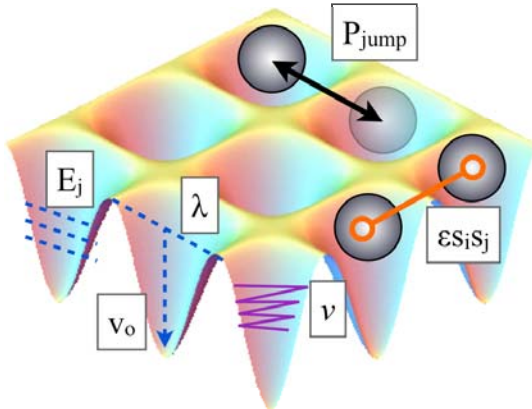


# COATINGS - DIFFUSION & EVAPORATION

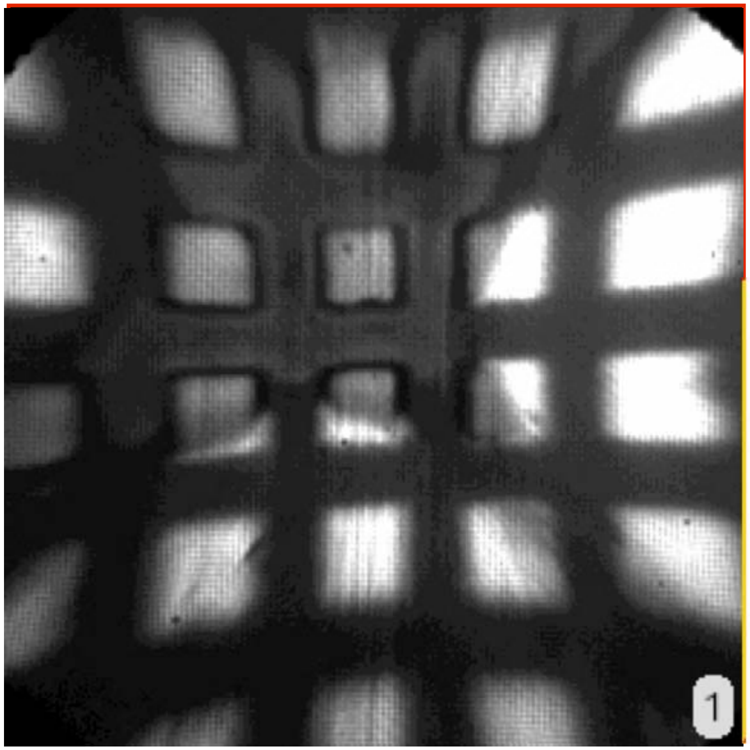
$$E = -v_o \sum_{j=1}^{\gamma} s_j - \varepsilon \sum_{j=1}^{\gamma} s_0 s_j$$

Energy of coating atoms:

- $v_o$ = depth of well
- $\varepsilon$ = interaction energy
- $\gamma$ = # of nearest neighbors
- $s_j$ = 0,1 occupation factor
- $\nu$ = osc. frequency
- $\lambda$ = hopping distance
- $\Gamma(\theta)$ = hopping prob.
- $P(E>v_o)$ = Prob. evap




10 nm Cs on 200 nm Sb on SILICON
365 nm Hg, Heated by lamp, T~320-330K




What's happening:

These are PEEM images of squares of Cs (25 μm on a side) laid down on Sb, & heated. QE images: frames taken about 10 seconds apart; intensity adjusted for image (not held fixed)

Diffusion and evaporation of coatings: atoms as harmonic oscillators $\partial_t \theta \approx D_o \nabla^2 \theta$

- Diffusion $D(\theta)$ = product of oscillation freq $\nu$, jump length $\lambda^2$, and jump probability $P_{jump}$
- Both Jump prob & evap rate proportional to $\exp(-\beta v_o)$

- **Question:** If atom only sees four ($\gamma$) nearest neighbors (microscopic view), how does it "know" what local coverage is (macroscopic view)?
- **Answer:** can be shown value of $v_o$ is related to coverage, and therefore affects evaporation (through $c(T)$) & diffusion (through $P_{jump}$)

$$D(\theta) = \Gamma(\theta)\lambda^2\left(\frac{1}{1-\theta} + \gamma\varepsilon\beta\theta\right) \Leftrightarrow D_o = \frac{3}{\pi R_o}\left(\frac{v_o}{M}\right)^{1/2}\exp(-\beta v_o)$$

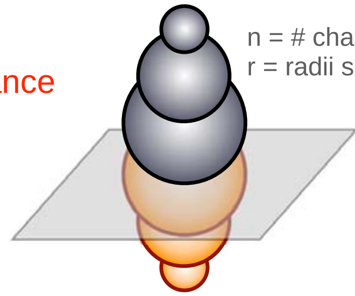
$$\frac{\theta}{1-\theta} = e^{-\beta v_o}\frac{\left(1+e^{\beta v_o - \beta\varepsilon}\right)}{\left(1+e^{-\beta v_o}\right)} \Leftrightarrow \Gamma(\theta) = \Gamma(0)\frac{\left(1+e^{-\beta v_o}\right)^3}{\left(1+e^{-\beta v_o - \beta\varepsilon}\right)^4}$$

**Questions:** Can QE of coated surface be related to how evaporation & diffusion rates change coverage for surface w/ supply pores; Can predictions be made of optimal rejuvenation protocol for dispenser photocathodes? (joint UMD/NRL program)

# DARK CURRENT

## POINT CHARGE MODEL

- Goal: Impact of surface features on emittance
- Serendipity: Dark current model (field emission if enhancement β is high, Φ low, or both) is analytically tractable
- 3D, get trajectories, estimate emittance




tip height factor z

$$z_n = \sum_{j=0}^{n} a_j = \sum_{j=0}^{n} r^{j-1} a_0$$

Field Enhancement

$$\beta_n(r) = -\partial_z V_n(0,z)\Big|_{z=z_{n+1}}$$

Apex Radius

$$a_n(r) = -\frac{\partial_\rho V_n(\rho,z)}{\partial_\rho^2 V_n(\rho,z)}\Bigg|_{\rho=0,z=z_{n+1}}$$

β & $a_n$ all that is needed for analytical model of current from an apex: well-tested against real conical emitters

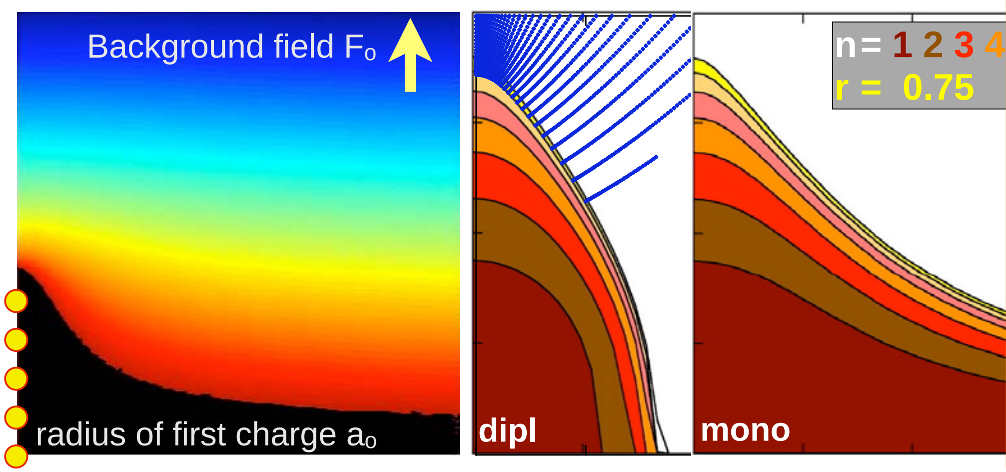
$$V(\rho,z) \equiv F_o a_0 V_n\left(\frac{\rho}{a_0}, \frac{z}{a_0}\right)$$

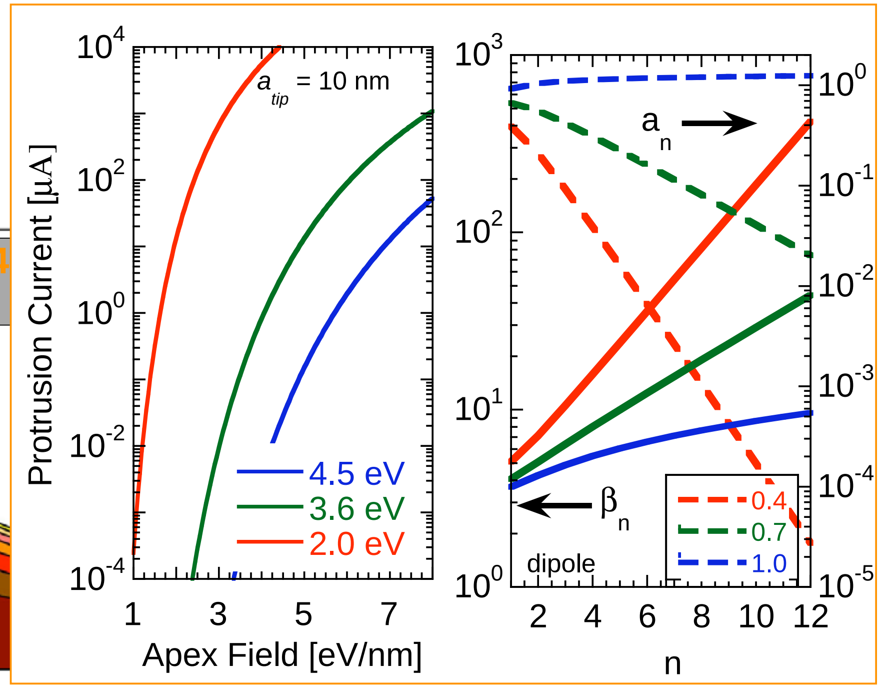
PCM is dimensionless, scalable analytical method to get tip radii, field enhancement, total current

$$V_n(\rho,z) \equiv -z + \left(\rho^2 + z^2\right)^{-1/2}$$ (monopole term)

$$+\left\{\sum_{j=1}^{n} \lambda_j \left(\left(\rho^2 + (z - z_j)^2\right)^{-1/2} - \left(\rho^2 + (z + z_j)^2\right)^{-1/2}\right)\right\}$$ (dipole term)

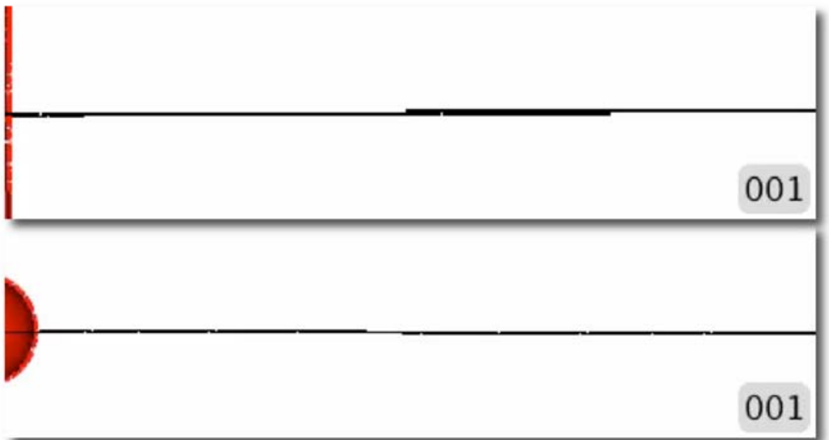
$$V_n(0, z_{n+1}) \equiv 0$$ (boundary conditions)



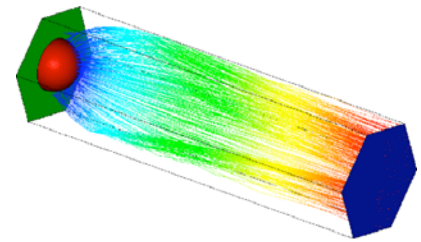
# SPACE CHARGE INDUCED OSCILLATIONS

Emitted Charge Changes Fields On Surface That Affects Subsequent Emissions - Oscillations Induced By A Sudden Influx Of Charge Can Persist. Demonstration For Metal (Cu) And Semiconductor ($Cs_3Sb$) Using Particle-in-Cell (PIC) Code MICHELLE



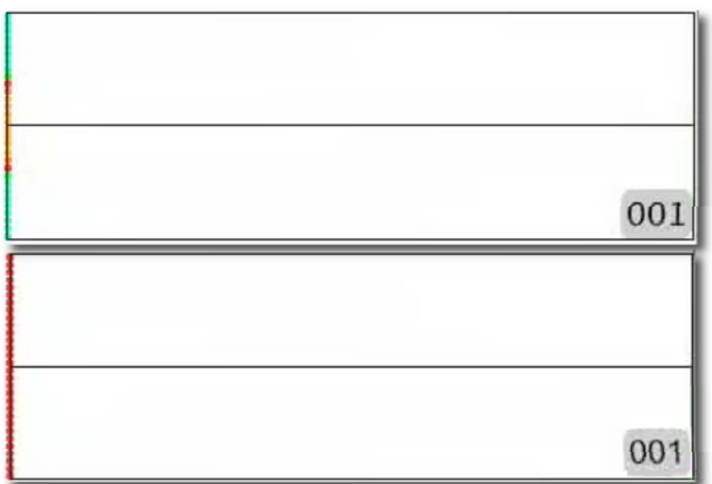

Flat metal copper surface without & with hemispherical bump

- Copper Photoemission from Boss
- Bulk Temp = 300 Kelvin
- Wavelength = 266 nm
- Field = 100 MV/m
- Laser Intens = 160 MW/cm2
- 45 µm length (cath-anode)
- 12 µm center to center spacing



MICHELLE in action:

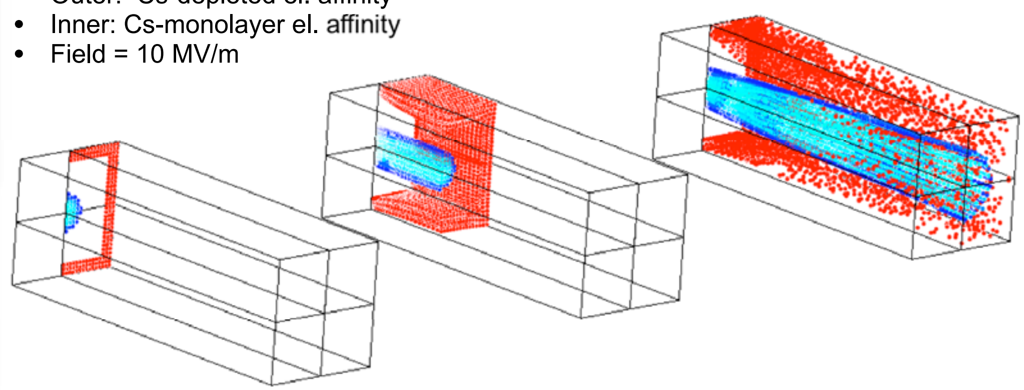
- J.J. Petillo, E.M. Nelson, J.F. Deford, N.J. Dionne, and B. Levush, IEEE Trans. Electron Devices 52, 742 (2005).
- K.L. Jensen, J.J. Petillo, E.J. Montgomery, Z. Pan, D.W. Feldman, et al. J. Vac. Sci. Technol. B 26(2), 831 (2008).




Flat Sb surface with an inner square coated with Cs monolayer & depleted

Cs3Sb:

- Outer: Cs-depleted el. affinity
- Inner: Cs-monolayer el. affinity
- Field = 10 MV/m



# CONCLUSION

What We Attempted

- Treatment Of Photoemission
  - Spicer Model, Fowler-Dubridge, Moments-based Approach, And Their Relation
    - Absorption - Dielectric Constant And Drude-Lorentz Model
    - Transport - Scattering Mechanisms (electron-electron, Acoustic, Polar Optical, Ionized Impurity)
    - Emission - Transmission Probability Through The Fowler-Nordheim Barrier
  - General Thermal-Field-Photoemission Equation
- Comparison Of Theory To Experiments (UMD & NRL)
- Related Matters
  - Emittance
  - Evaporation And Desorption
  - Dark Current Via Point Charge Model
  - Space-Charge Induced Current Oscillations

What We Did