Lecture 2: Cathode Theory

- Yesterday, we discussed the properties we care about quantum efficiency, emittance and brightness. Today we'll begin to see what we can theoretically expect.
- We'll discuss the basic electronic structure of materials, the origin of the surface barrier and the electron emission statistics.
- We'll derive the cathode emission current and emittance for thermal, photo-electric and field emission. For photoemission, we'll discuss the three types of cathodes.
- We'll look at the effect of surface roughness on emittance
- We'll derive the expressions for the space charge limited current
- ...and come up with the ultimate brightness!

Modern Theory and Applications of Photocathodes W.E. Spicer & A. Herrera-Gómez SAC-PUB-6306 (1993)

Much of this lecture is courtesy of Dave Dowell

http://www.philiphofmann.net/surflec3/index.html

Electronic structure of Materials

- In an atom, electrons are bound in states of defined energy
- In a molecule, these states are split into rotation and vibration levels, allowing the valence electrons to have a range of discrete values
- In a solid, these levels merge, forming bands of allowed energies, with gaps between them. In general these bands confine both the energy and linear momentum of the electrons. These bands have an Electron Density of States (EDoS) that governs the probability of electron transitions.
- For now, we will be concerned with the energy DoS, and not worry about momentum. For single crystal cathodes (GaAs, Diamond), the momentum states are also important.
- Calculated using a number of methods: Tight binding, Density functional theory. Measured using photoemission spectroscopy.

DOS Examples

 For a free electron gas in 3 dimensions, with the "particle in a box" problem gives:

 $E = \hbar^2 k^2 / 2m = (\hbar^2 / 2m) (k_x^2 + k_y^2 + k_z^2)$

• For periodic boundary conditions:

 $k_x = (2\pi/L) n_x; n_x = 0, \pm 1, \pm 2, \pm 3, \dots$

- The number of states in a sphere in k-space goes as V $\propto k^3$
- The Density of States (states/eV) is then \propto V/E \propto E^{1/2}
- This is good for simple metals, but fails for transition metals





E = p²/2m <u>http://mits.nims.go.jp/matnavi/</u>

Nb Density of States



NRL Electronic Structures Database

Occupancy: the Fermi-Dirac Distribution

 As fermions, electrons obey the Pauli exclusion principle. Thus the energy distribution of occupied states (DOS) is given by the Fermi-Dirac (F-D) function,

$$f_{FD} = \frac{1}{1 + e^{(E - E_F)/k_B T}}$$

- The temperature dependence of this distribution is typically not important for field emission and photoemission, but is critical for thermionic emission
- For T=0, this leads to full occupancy of all states below E_F and zero occupancy for all states above E_F

Surface Barrier

- As discussed yesterday, the workfunction is the energy required to extract an electron from the surface
- This has two parts, the electrostatic potential binding the electrons in the bulk, and the surface dipole which occurs due to "spill-out" electrons



http://www.philiphofmann.net/surflec3/surflec015.html#toc36

Surface Barrier

- This surface dipole portion can be modified by adsorbates
- We use alkali metals to reduce the workfunction of cathodes
 - Cs on Ag
 - Cs on W
 - Cs-O on GaAs
- Adsorbates can also raise $\boldsymbol{\varphi}$
 - This is the motivation behind laser cleaning of metal cathodes
- Note that different faces of a crystal can have different surface dipoles, and therefore different workfunctions



Workfunction change upon the adsorption of K on W(110) R. Blaszczyszyn et al, Surf. Sci. **51**, 396 (1975).

Workfunctions of metals have values between about 1.5 eV and 5.5 eV.

Fields Near the Cathode



Electron Emission Equations and Emittance

Now that we have a idea of how the electrons are confine to the surface, let's focus on helping them escape

We develop the emission equations, and estimate the emittance of each method. This ultimate emittance is often called the thermal emittance, due to the Maxwell-Boltzmann (MB) distribution of thermionic emitters. Strictly speaking, the term 'thermal emittance' should only be applied to thermionic emission, but the concept of thermal emittance or the intrinsic emittance of the cathode can be applied to the three forms of electron emission:

- 1. thermionic emission
- 2. field emission
- 3. photo-electric emission

Thermionic Emission(1)

In order for an electron to escape a metal it needs to have sufficient kinetic energy in the direction of the barrier to overcome the work function,



Since only the high energy tail of the F-D distribution will matter, we can neglect the material density of states

Thermionic Emission(2)

 Assume that the cathode has an applied electric field large enough to remove all electrons from the surface, so there are no space charge effect, but low enough to not affect the barrier height. Then the thermionic current density for a cathode at temperature,

$$j_{thermionic} = n_0 e \langle v_x \rangle = n_0 e \int_{v_x > \sqrt{\frac{2e\phi_{work}}{m}}} v_x f_{FD} d\vec{v}$$



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Comparison of M-B and F-D Distributions



• If we are only considering the high energy tail, we can use the Maxwell-Boltzmann distrubtion

Thermionic Emission (3)

The interactions involving the high energy electrons in the tail of the Fermi-Dirac density of states allows it's replacement with the classical, Maxwell-Boltzmann distribution,

$$j_{thermionic} = n_0 e \int_{v_x > \sqrt{\frac{2e\phi_{work}}{m}}} v_x f_{MB} d\vec{v} = n_0 e \int_{v_x > \sqrt{2e\phi_{work}/m}} v_x e^{-\frac{m(v_x^2 + v_y^2 + v_z^2)}{2k_B T}} d\vec{v}$$

Performing these simple integrals gives the thermionic current density,

$$j_{thermionic} = 2n_0 e \left(\frac{2k_B T}{m}\right)^2 e^{-\phi_{work}/k_B T}$$

Thermionic Emission(4)

• Or with a small change in the leading constants, gives the Richardson-Dushman equation for thermionic emission,

$$j_{thermionic} = A(1-r)T^2 e^{-\phi_{work}/k_B T}$$

 Here A is 120 amp/cm²/degK², and (1-r) accounts for the reflection of electrons at the metal surface. The reflection and refraction of electrons as they transit the surface is discussed in a later section. In terms of fundamental quantities, the universal constant A is ["Solid State Physics", by Ashcroft and Mermin, p. 363]

$$A = -\frac{em}{2\pi^2\hbar^3}$$

Thermionic Emittance (1)

• The velocity distribution for thermally emitted electrons is obtained from the derivative of Maxwell-Boltzmann particle distribution,

$$\frac{1}{n_e} \frac{dn(v_x)}{dv_x} = \frac{m}{k_B T} v_x e^{\frac{-mv_x^2}{2k_B T}}$$



Maxwell-Boltzmann electron energy distributions at 300 degK where the rms electron energy spread is 0.049 eV, and at 2500 degK corresponding to an rms energy spread of 0.41 eV. The initial spread in transverse velocity due to the electron temperature gives the beam angular divergence and hence its thermionic emittance.

Thermionic Emittance (2)

 Following Lawson [Lawson, p. 209], we assume the normalized emittance is evaluated close to the cathode surface where the electron flow is still laminar (no crossing of trajectories) and any correlation between position and angle can be ignored. In this case, normalized cathode emittance is given by,

$$\epsilon_N = \beta \gamma \sigma_x \sigma_{x'}$$

 The root-mean-square (rms) beam size, σ_x, is given by the transverse beam distribution which for a uniform radial distribution with radius R is R/2. The rms divergence is given by

$$\sigma_{x'} = \frac{\langle p_x \rangle}{p_{total}} = \frac{1}{\beta \gamma} \frac{\sqrt{\langle v_x^2 \rangle}}{c}$$

• The normalized, rms thermal emittance is then

$$\epsilon_n = \sigma_x \frac{\sqrt{\langle v_x^2 \rangle}}{c}$$

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Thermionic Emittance (3)

• The mean squared transverse velocity for a M-B velocity distribution is,

$$\langle v_x^2 \rangle = \frac{\int_0^\infty v_x^2 e^{-\frac{mv_x^2}{2k_B T}} dv_x}{\int_0^\infty e^{-\frac{mv_x^2}{2k_B T}} dv_x} = \frac{k_B T}{m}$$

• Therefore the thermionic emittance of a Maxwell-Boltzmann distribution at temperature, T, is

$$\epsilon_{thermionic} = \sigma_x \sqrt{\frac{k_B T}{mc^2}}$$

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Thermionic Emittance (4)

 The divergence part of the cathode emittance contains all the physics of both the emission process and the cathode material properties and as such summarizes much of the interesting physics of the emission process. The beam size in coordinate space simply traces out the angular distribution to form the transverse phase space distribution as illustrated.



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Thermionic Emission (5)

Given that σ_x depends upon the particular transverse distribution being used, there is often a serious ambiguity which arises when expressing the thermal emittance in terms of "microns/mm". The confusion results in not knowing whether rms or flat top radii are used for the transverse radius. Therefore we suggest quoting a quantity called the normalized divergence, which for thermionic

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Field Emission



Field Emission (1)

 Field emission occurs when electrons tunnel through the barrier potential under the influence of very high fields of 10⁹ V/m or more. Since emission is by tunneling the effect is purely quantum mechanical and requires an extremely high electric field to lower the barrier enough for useful emission.

$$j = \int n(E_x, T) D(E_x, E_0) dE_x$$

- where the supply function, $n(E_x,T)$, is the flux of electrons incident upon the barrier with energies between E_x and $E_x + dE_x$. The barrier is same as that shown earlier and is determined by the work function, the image charge and the applied electric field, E_0 . The transmission of electrons through this barrier is given by the transparency function, $D(E_x, E_0)$.
- The tunneling probability is significant only for electrons very close to $\rm E_{\rm F},$ so the material DoS is generally not important

Field Emission (2)

• The transparency function was solved by Nordheim for the barrier produced by the image charge and the applied field (Schottky potential),

$$\phi_{Schottky}(x) = -\frac{e^2}{16\pi\epsilon_0 x} - eE_0 x$$

• The result is

$$D(E_x, E_0) = \exp\left[\frac{-8\pi\sqrt{2m}}{3he}\frac{E_x^{3/2}}{E_0}\theta\left(\frac{\sqrt{e^3E_0}}{\phi_{work}}\right)\right]$$

• $\theta(y)$ is the Nordheim function which to a good approximation is given by

$$\theta(y) = 1 - 0.142y - 0.855y^2$$

Field Emission (3)

 The supply function for a Fermi-Dirac electron gas was also derived by Nordheim,

$$n(E_x,T) = \frac{4\pi m k_B T}{h^3} \ln\left(1 + e^{\frac{E_x - E_F}{k_B T}}\right)$$

• Combining the supply and transparency functions gives the electron energy spectrum, $N_{field}(E_x, E_0, T) = n(E_x, T)D(E_x, E_0)$



"Field Emission in Vacuum Microelectronics," G. Fursey, Kluwer Academic/Plenum, 2005

Field Emission (4)

• Electron spectra for field emission electrons for various applied fields. Left: Electron emission spectra plotted with a linear vertical scale and with arbitrarily normalization to illustrate the spectral shapes.

Right: The spectral yields plotted logarithmically to illustrate the strong dependence of yield and shape upon applied field.



Field Emission Emittance

 Armed with the energy spectra the rms energy spread and the field emission emittance are numerically computed for external fields between 10⁹ and 10¹⁰ Volts/m. (Solved numerically.)



Field Enhancement Factor, β

 In field emission the electron yield is exponentially sensitive to the external field and any significant current requires fields in excess of 10⁹ V/m. Such high fields are difficult to achieve but are possible using pulsed high voltages and/or field-enhancing, sharp emitters.





A collated representation of the field enhancement factors β associated with various idealised microprotrusion geometries. (From Rohrbach [31], with permission.)

"High Voltage Vacuum Insulation, Basic Concepts and Technological Practice," HigEd Rod Latham, Academic Press 1995

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Photo-Electric Emission

- Photoelectric emission from a metal can be described by the three steps of the Spicer model:
 - 1. Photon absorption by the electron
 - 2. Electron transport to the surface
 - 3. Escape through the barrier



Direction normal to surface

Three Step Model of Photoemission in Metal



- Excitation of e⁻ in metal Reflection (angle dependence) Energy distribution of excited e⁻
- 2) Transit to the Surface

e⁻-e⁻ scattering Direction of travel

3) Escape surface

Overcome Workfunction Reduction of Φ due to applied field (Schottky Effect)

Integrate product of probabilities over all electron energies capable of escape to obtain Quantum Efficiency

Krolikowski and Spicer, Phys. Rev. **185** 882 (1969) M. Cardona and L. Ley: <u>Photoemission in Solids 1</u>, (Springer-Verlag, 1978)

Step 1: Absorption of Photon



The reflectivity is given by the Fresnel relation in terms of the real part of the index of refraction,

Reflectivity =
$$R(n_1(\omega), n_2(\omega), \theta_i)$$

 $\lambda = \frac{\lambda}{\lambda}$

 $\lambda_{opt} = \frac{1}{4\pi k}$

where k is the imaginary part of the complex index of refraction,

$$\eta = n + ik$$

and λ is the free space photon wavelength.

Step 1 – Absorption and Excitation

Fraction of light absorbed: $I_{ab}/I = (1-R)$

Probability of absorption and electron excitation:

$$P(E,\omega) = \frac{N(E)N(E+\hbar\omega)}{\int\limits_{E_f - \hbar\omega}^{E_f} N(E')N(E'+\hbar\omega)dE'}$$

• N(E) is the Density of states. The above assumes T=0, so N(E) is the density of filled states capable of absorbing, and N(E+ $\hbar\omega$) is the density of empty states for the electron to be excited into.

- Only energy conservation invoked, conservation of k vector is not an important selection rule (phonon scattering and polycrystalline)
- We assume the matrix element connecting the initial and final state is constant (not energy dependent)

Nb Density of States



Copper Density of States



Fong&Cohen, Phy. Rev. Letters, 24, p306 (1970)

Step 2 – Probability of reaching the surface w/o e⁻-e⁻ scattering

$$F_{e-e}(E,\omega,\theta) = \frac{\lambda_e(E+\hbar\omega)/\lambda_{ph}(\omega)}{1+\lambda_e(E+\hbar\omega)/\lambda_{ph}(\omega)}C(E,\omega,\theta)$$
$$\lambda_{ph} = \frac{\lambda}{4\pi k}$$

- e⁻ mean free path can be calculated
 - Extrapolation from measured values
 - From excited electron lifetime (2 photon PE spectroscopy)
 - Comparison to similar materials
- Assumptions
 - Energy loss dominated by e-e scattering
 - Only unscattered electrons can escape
 - Electrons must be incident on the surface at nearly normal incidence => Correction factor $C(E, v, \vartheta) = 1$

Step 2 – Probability of reaching the surface w/o $e^{-}-e^{-}$ scattering

- In the near-threshold regime, an e⁻-e⁻ event is unlikely to leave either electron with energy sufficient to escape
 - Treat scattering as a loss mechanism
 - Can ignore other scattering mechanisms
- Assume the probability, *S*, of an excited electron of energy $E > E_f$ interacting with a valence electron of energy $E_0 < E_f$ and imparting energy ΔE is proportional to:
 - The number of electrons, $N(E_0)$, with energy E_0 .
 - The number of empty states, $N(E_0 + \Delta E)$, with energy $E_0 + \Delta E$.
 - The number of empty states, $N(E \Delta E)$ with energy $E \Delta E$. $S(E, E_0, \Delta E) \propto N(E_0) N(E_0 + \Delta E) N(E - \Delta E)$
- Again, we assume the matrix elements connecting these states are not energy dependent, so that the probability depends only on the DoS

Step 2 – Probability of reaching the surface w/o e⁻-e⁻ scattering

To obtain the total probability of scattering for an electron of energy *E* by an electron of energy E_0 , we must integrate over all possible energy transfers, ΔE :

$$E - E_f$$

S(E,E_0) $\propto \int d(\Delta E) N(E_0) N(E - \Delta E) N(E_0 + \Delta E)$
 $E_f - E_0$

The total scattering probability of an excited electron is obtained by integrating over all possible "valence" electron energies, yielding

$$E_f \qquad E - E_f$$

$$S(E) \propto \int dE_0 \qquad \int d(\Delta E) \ N(E_0) \ N(E - \Delta E) \ N(E_0 + \Delta E)$$

$$2E_f - E \ E_f - E_0$$

The lower limit of integration represents the kinematic limitation that $E + E_0 \ge 2E_f$.

Step 2 – Probability of reaching the surface $w/o e^{-}-e^{-}$ scattering

The lifetime of the excited state, $\tau(E)$, is inversely proportional to this scattering probability: $\tau(E) \propto 1/S(E)$

The scattering length, $\lambda_e(E)$, is related to the lifetime by the velocity. We assume a free electron-like velocity, using E_f as the zero of energy for metals and the bottom of the conduction band for semiconductors:

$$\lambda_e(E) = v(E) \ \tau(E) = \frac{\lambda_0 \sqrt{E - E_f}}{\int dE_0 \quad \int d(\Delta E) \ N(E_0) \ N(E - \Delta E) \ N(E_0 + \Delta E)}$$
$$\frac{2E_f - E \ E_f - E_0}{2E_f - E \ E_f - E_0}$$

 λ_0 is a constant that is chosen so that the e-e scattering length (the length over which the intensity of unscattered electrons is 1/e of the initial intensity) matches a known value of the electron's mean free path at a single energy for a given material.
Step 2: Transport to the Surface



Step 2 – Probability of reaching the surface w/o e⁻-e⁻ scattering

The probability that an electron created at a depth *d* will escape is $e^{-dl\lambda_e}$, and the probability per unit length that a photon is absorbed at depth *d* is $(1/\lambda_{ph}) e^{-dl\lambda_{ph}}$. Integrating the product of these probabilities over all possible values of d, we obtain the fraction of electrons that reach the surface without scattering, $F_{e-e}(E,\omega)$,

$$F_{e-e}(E,\omega) = \frac{\lambda_e(E+\hbar\omega)/\lambda_{ph}(\omega)}{1+\lambda_e(E+\hbar\omega)/\lambda_{ph}(\omega)}$$

Homework: Show this



Step 3: Escape Over the Barrier



While photoemission is regarded quantum mechanical effect due to quantization of photons, emission itself is classical. I.e., electrons do not tunnel through barrier, but classically escape over it.

This is analogous to Snell's law in optics



Step 3 - Escape Probability

• Criteria for escape:

$$\frac{p_{\perp}^2}{2m} = \frac{\hbar^2 k_{\perp}^2}{2m} > \phi$$

• Requires electron trajectory to fall within a cone defined by angle:

$$\cos\theta = \frac{k_{\perp \min}}{\left|\vec{k}\right|} = \left(\frac{\phi}{E + \hbar\omega - E_F}\right)^{\frac{1}{2}}$$

• Fraction of electrons of energy E falling with the cone is given by:

$$D(E) = \frac{1}{4\pi} \int_{0}^{\theta} \sin \theta' d\theta' \int_{0}^{2\pi} d\varphi = \frac{1}{2} (1 - \cos \theta) = \frac{1}{2} (1 - (\frac{\phi}{E + \hbar \omega - E_F})^{\frac{1}{2}})$$

 For small values of E-E_τ, this is the dominant factor in determining the emission. For these cases:

$$QE(\nu) \propto \int_{\phi+E_f-\hbar\omega}^{E_f} D(E) dE$$

• This gives:

$$QE(\nu) \propto (h\nu - \phi)^2$$



EDC and QE

At this point, we have N(E, $\hbar\omega$) - the Energy Distribution Curve of the emitted electrons:

 $EDC(E,\hbar\omega)=(1-R(\omega))P(E,\omega)F_{e-e}(E,\omega)D(E)$

To obtain the QE, integrate over all electron energies capable of escape:

$$QE(\omega) = (1 - R(\omega)) \int_{\phi + E_f - \hbar\omega}^{E_f} P(E, \omega) F_{e-e}(E, \omega) D(E) dE$$

More Generally, including temperature:

$$QE(\omega) = (1 - R(\omega)) \quad \frac{\int_{E_F + \phi - \hbar\omega}^{\infty} dE \quad N(E + \hbar\omega)(1 - F(E + \hbar\omega))N(E)F(E) \int_{\cos\theta_{\max}(E)}^{1} d(\cos\theta)F_{e-e}(E,\omega,\theta) \int_{0}^{2\pi} d\Phi}{\int_{0}^{\infty} dE \quad N(E + \hbar\omega)(1 - F(E + \hbar\omega))N(E)F(E) \int_{-1}^{1} d(\cos\theta) \int_{0}^{2\pi} d\Phi}$$

D. H. Dowell et al., Phys. Rev. ST-AB **9**, 063502 (2006)

Photo-Electric Emission

Elements of the Three-Step Photoemission Model



Derivation of QE





If we assume N(E)=constant, and a approximate F-D with step function since $k_BT << E_F$:

$$QE(\omega) = (1 - R(\omega))F_{e-e}(\omega) \frac{\int_{E_F + \phi_{eff} - \hbar\omega}^{E_F + \phi_{eff}} \int_{0}^{1} d(\cos\theta) \int_{0}^{2\pi} d\Phi}{\int_{E_F - \hbar\omega}^{E_F - \hbar\omega} \int_{-1}^{1} d(\cos\theta) \int_{0}^{2\pi} d\Phi}$$

The QE is then given by:

$$QE(\omega) = \frac{1 - R(\omega)}{1 + \frac{\lambda_{opt}(\omega)}{2\lambda_{e-e}(E_m)} \frac{\hbar\omega\sqrt{\phi_{eff}}}{E_m^{3/2}} \left(1 + \sqrt{\frac{\phi_{eff}}{\hbar\omega}}\right)} \frac{\left(E_F + \hbar\omega\right)}{2\hbar\omega} \left[1 - 2\sqrt{\frac{E_F + \phi_{eff}}{E_F + \hbar\omega}}\right]^2$$

D. H. Dowell, K.K. King, R.E Kirby, J.F. Schmerge and J. Smedley, "In situ cleaning of metal cathodes using a hydrogen beam," PRST-AB 9, 063502 (2006)

QE for a metal

Step 3: Escape over the barrier



"Prompt"

Metals have very low quantum efficiency, but they are prompt emitters, with fs response times for near-threshold photons:

To escape, an electron must be excited with a momentum vector directed toward the surface, as it must have

$$\frac{\hbar^2 k_{\perp}^2}{2m} > \phi$$

The "escape" length verses electron-electron scattering is typically under 10 nm in the near threshold case. Assuming a typical hot electron velocity of 10⁶ m/s, the escape time is 10 fs.

(this is why the LCLS has a Cu photocathode)

W.F. Krolikowski and W.E. Spicer, Phys. Rev. 185, 882 (1969)
D. H. Dowell *et al.*, Phys. Rev. ST Accel. Beams 9, 063502 (2006)
T. Srinivasan-Rao *et al.*, PAC97, 2790

Schottky Effect and Field Enhancement

• Schottky effect reduces work function

$$\Delta \phi_{schottkey}[eV] = \alpha \sqrt{\mathsf{E}}[\frac{V}{m}]$$
$$\alpha = e \sqrt{\frac{e}{4\pi\varepsilon_0}} = 3.7947 \times 10^{-5} [e\sqrt{Vm}]$$

• Field enhancement

Typically, β_{eff} is given as a value for a surface. In this case, the QE near threshold can be expressed as:

$$QE = B(h\nu - \phi_0 + \alpha \sqrt{\beta_{eff}E})^2$$

Field Enhancement

Let us consider instead a field map across the surface, such that $E(x,y) = \beta(x,y)E_0$

For "infinite parallel plate" cathode, Gauss's Law gives:

$$\frac{1}{A} \int_{A} \beta(x, y) dx dy = 1$$

In this case, the QE varies point-to-point. The integrated QE, assuming uniform illumination and reflectivity, is:

$$QE = \frac{B\int_{emission} (hv - \phi_0 + \alpha \sqrt{\beta(x, y)E})^2 dxdy}{A}$$

Relating these expressions for the QE:

$$\int (h\nu - \phi_0 + \alpha \sqrt{\beta_{eff}E})^2 = \frac{\int (h\nu - \phi_0 + \alpha \sqrt{\beta(x, y)E})^2 dxdy}{A}$$

Field Enhancement

Solving for effective field enhancement factor:

$$\beta_{eff} = \frac{1}{\alpha^2 E_0} \left(\left(\frac{\int (h\nu - \phi_0 + \alpha \sqrt{\beta(x, y)E_0})^2 dx dy}{A} \right)^{1/2} - (h\nu - \phi_0) \right)^2$$

Not Good – the field enhancement "factor" depends on wavelength

In the case where
$$hv = \phi_0$$
, we obtain $\beta_{eff} = \frac{1}{A} \int_{emission} \beta(x, y) dx dy = 1$

Local variation of reflectivity, and non-uniform illumination, could lead to an increase in beta

Clearly, the field enhancement concept is very different for photoemission (as compared to field emission). Perhaps we should use a different symbol?

Sqrt QE vs Sqrt F, KrF on Cu





Implementation of Model

- Material parameters needed
 - Density of States
 - Workfunction (preferably measured)
 - Complex index of refraction
 - e mfp at one energy, or hot electron lifetime
 - Optional surface profile to calculate beta
- Numerical methods
 - First two steps are computationally intensive, but do not depend on phi only need o be done once per wavelength (Mathematica)
 - Last step and QE in Excel (allows easy access to EDCs, modification of phi)
 - No free parameters (use the measured phi)

Predicted QE for Pb & Nb



Lead QE vs Photon energy



Copper QE vs Photon Energy



Energy Distribution Curves



Calculated EDC for Copper

Energy Distribution Curves - Copper



Improvements

- Consider momentum selection rules
- Take electron heating into account
- Photon energy spread (bandwidth)
- Consider once-scattered electrons (Spicer does this)
- Expand model to allow spatial variation
 - Reflectivity
 - Field
 - Workfuncion?

Photo-Electric Emittance (1)

• The mean square of the transverse momentum is related to the electron distribution function, $g(E, \theta, \phi)$, just inside the cathode surface,

$$\langle p_{tot}^2 \rangle = \frac{\int \int \int g(E,\theta,\varphi) p_x^2 dE d(\cos\theta) d\varphi}{\int \int \int g(E,\theta,\varphi) dE d(\cos\theta) d\varphi}$$

• The *g*-function and the integration limits depend upon the emission processes. We assume for the three-step photo-emission model that *g* depends only on energy, and that we can use the flat DoS,

$$g_{photo} = (1 - f_{FD}(E + \hbar\omega))f_{FD}(E)$$

Derivation of Photo-Electric Intrinsic Emittance



Intrinsic emittance for photoemission from a metal

$$\varepsilon_n = \sigma_x \sqrt{\frac{\hbar\omega - \phi_{eff}}{3mc^2}}$$

Photo-Electric Emittance (3)

1.2 r

50 MV/m 100 MV/m

Normalized divergence vs. photon energy for various applied fields

$$\Delta_{photo} = \beta \gamma \sigma_{x'}^{photo} = \sqrt{\frac{\hbar \omega - \phi_{eff}}{3mc^2}}$$

$$\epsilon_{photo} = \sigma_x \sqrt{\frac{\hbar \omega - \phi_{eff}}{3mc^2}}$$

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Photo-Electric Emittance & QE



QE & Emittance are related via the excess energy

Define the excess energy as:
$$E_{excess} = \hbar \omega - \phi_{eff}$$

$$QE = \frac{(1 - R(\hbar\omega))}{1 + \frac{\lambda_{opt}}{\overline{\lambda_{e-e}}}} \frac{(E_F + \hbar\omega)}{2\hbar\omega} \left(1 - \sqrt{\frac{E_F + \phi_{eff}}{E_F + \hbar\omega}}\right)^2 \approx \frac{(1 - R(\hbar\omega))}{1 + \frac{\lambda_{opt}}{\overline{\lambda_{e-e}}}} \frac{E_{excess}^2}{8\phi_{eff}(E_F + \phi_{eff})}$$

$$\frac{\varepsilon_n}{\sigma_x} = \sqrt{\frac{\hbar\omega - \phi_{eff}}{3mc^2}} = \sqrt{\frac{E_{excess}}{3mc^2}}$$



Three Step Model of Photoemission - Semiconductors



Cs₃Sb (Alkali Antimonides)

Work function 2.05 eV, E_g= 1.6 eV Electron-phonon scattering length ~5 nm

Loss per collision ~0.1 eV

Photon absorption depth

~20-100 nm

Thus for 1 eV above threshold, total path length can be ~500 nm (pessimistic, as many electrons will escape before 100 collisions)

This yields a response time of ~0.6 ps

Alkali Antimonide cathodes have been used in RF guns to produce electron bunches of 10's of ps without difficulty



FIG. 1. Cs₃Sb absorption coefficients obtained by various workers. A coefficient of 10^5 /cm at 3.0 ev was assumed in the present work.



Figure 4. Transport of a photoemitted electron when the electron-phonon scattering is dominant. The integrated path, L_T , is the sum of the distances traveled between collisions.

D. H. Dowell *et al.*, *Appl. Phys. Lett.*, **63**, 2035 (1993) W.E. Spicer, *Phys. Rev.*, **112**, 114 (1958)

Assumptions for K₂CsSb Three Step Model

- 1D Monte Carlo (implemented in Mathematica)
- e⁻-phonon mean free path (mfp) is constant
- Energy transfer in each scattering event is equal to the mean energy transfer
- Every electron scatters after 1 mfp
- Each scattering event randomizes e⁻ direction of travel
- Every electron that reaches the surface with energy sufficient to escape escapes
- Cathode and substrate surfaces are optically smooth
- e⁻-e⁻ scattering is ignored (strictly valid only for E<2E_{gap})
- Field does not penetrate into cathode
- Band bending at the surface can be ignored

Parameters for K₂CsSb Three Step Model

- e⁻-phonon mean free path
- Energy transfer in each scattering event
- Number of particles
- Emission threshold (E_{gap}+E_A)
- Cathode Thickness
- Substrate material

Parameter estimates from:

Spicer and Herrea-Gomez, Modern Theory and Applications of Photocathodes, SLAC-PUB 6306

K₂CsSb DOS



A.R.H.F. Ettema and R.A. de Groot, Phys. Rev. B 66, 115102 (2002)

Spectral Response – Bi-alkali



Laser Propagation and Interference



Monte Carlo for K₂CsSb





Data from Ghosh & Varma, J. Appl. Phys. 48 4549 (1978)

QE vs Mean Free Path



Thickness dependence @ 543 nm


Spatial Variation of QE for a Thin K₂CsSb Cathode

QE in reflection mode



Three Step Model – NEA Semiconductors



 1) Excitation of e⁻ Reflection, Transmission, Interference
2) Transit to the Surface e⁻-lattice scattering thermalization to CBM diffusion length can be 1µm recombination
Random Walk Monte Carlo Response Time (10-100 ps)

3) Escape surface

Direct and Indirect band gap materials



Direct Band Gap

Momentum

Conservation of energy and crystal momentum

Conduction Band Phonon assisted transition Valence Band Momentum

Indirect Band Gap

Conservation of energy, mediated by phonon for conservation of crystal momentum

Deeper absorption depth Longer life time

E-ph scattering is also important Electron decays to bottom of conduction band Surface dipole produces NEA

Effect of Doping GaAs



Triveni Rao, USPAS 2011, Hampton VA

NEA GaAs



Triveni Rao, USPAS 2011, Hampton VA

Intrinsic Emittance: Estimates for metal and semiconductor cathodes



BUT it's not so simple for NEAs: Due to electron-phonon scattering the excited electrons can thermalize with the lattice, giving an NEA like GaAs a thermal-like emission component: $\frac{1}{2} = \frac{1}{2} = \frac{1$

$$\frac{\varepsilon_{GaAs,n}}{\sigma_x} = A_{slow} \sqrt{\frac{k_B T}{mc^2}} + A_{fast} \sqrt{\frac{\hbar\omega - E_G - E_A}{3mc^2}}$$

This gives rise to a slow thermionic-like emission and a fast prompt photoelectric emission which is dependent upon wavelength band gap energy and affinity.

Emittance Summary

- The intrinsic emittance of the source is the ultimate limit for the volume of phase space
- The intrinsic emittance for thermionic emission is approximately 0.3 microns/mm for a cathode temperature of 2500 degK.
- The photo-electric emittance for a copper cathode ranges between 0.5 to 1 micron/mm depending upon the photon wavelength
 - Going to higher photon energy improves QE, but also increases emittance
- The field-emission emittance is found to vary between 0.5 to 2 microns/mm for fields from 10⁹ to 10¹⁰ V/m, and hence has larger emittance for the same source size than the other two processes.
- Now we'll address space charge and calculate the ultimate emittance we can achieve

Space Charge Limit (SCL) is different for DC diode and short pulse photo-emission

Space Charge Field Across a Diode, Child-Langmuir law:

$$J_{CL} = \frac{4}{9} \varepsilon_0 \sqrt{\frac{2e}{m}} \frac{V^{3/2}}{d^2}$$

For more complicated geometries:

$$I = P \cdot V^{3/2}$$

Where P is the perveance of the cathode

Space Charge Field Across a Short Electron Bunch from a Laser-driven Photocathode, parallel plate (capacitor) model:

$$\sigma_{SCL} = \varepsilon_0 E_{applied}$$



Comparison of space charge limits for Child-Langmuir and Short Pulse Geometries/Conditions



LCLS typically operates at approximately half the space charge limit for short pulse emission and a factor of 4 to 5 higher than the space charge limit given by the Child-Langmuir law.

Intrinsic Emittance: The Brightest Beam Possible Starts at the Cathode*

Assume all linear and non-linear space charge effects can be corrected/compensated for, the cathode is perfectly flat and the cathode physics is correct. Then the lower limit on the emittance depends on the intrinsic emittance for the divergence and the space charge limit for the beam size:



*I. Bazarov et al., Phys. Rev. Lett., **102** (2009) 104801

D. H. Dowell -- P3 Workshop

Transverse Electron Beam Shape: The beam core is clipped at the SCL



Derivation of Schottky Scan Function:



Putting this into the QE formula gives,

$$QE = \frac{1-R}{1+\frac{\lambda_{opt}}{\overline{\lambda_{e-e}}}} \frac{E_F + \hbar\omega}{2\hbar\omega} \left(1 - \sqrt{\frac{E_F + \phi_W - e\sqrt{e\beta E_{rf}}\sin\phi_{rf}/(4\pi\varepsilon_0)}{E_F + \hbar\omega}}\right)^2$$

Everything is known except for material work function, ϕ_W , and the field enhancement factor, β . Fit Schottky scan data to find them.

Emitted charge vs. launch phase

Begin with the QE for a metal cathode:

$$QE = \frac{1-R}{1+\frac{\lambda_{opt}}{\overline{\lambda_{e-e}}}} \frac{E_F + \hbar\omega}{2\hbar\omega} \left(1 - \sqrt{\frac{E_F + \phi_{eff}}{E_F + \hbar\omega}}\right)^2$$

where the effective work function is

$$\phi_{eff} = \phi_W - e_{\sqrt{rac{eeta E_{rf}}{4\piarepsilon_0}}}$$

QE Uniformity: Space Charge Emittance Near the Cathode

The emittance due to space charge expansion of an initial modulation with spatial frequency f_s and total beam current, I, is

$$\Delta \varepsilon_{n,sc} = \frac{\sigma_x}{2\pi f_s} \sqrt{\frac{I}{I_o}}$$

emittance for 100% modulation depth

 I_0 is the characteristic current: $I_0 = \frac{ec}{r_e} \approx 17kA$ The spatial frequency, f_s ,

(modulations/radius) is the number of vertical surface modulations or waves across the radius of emission.

This frequency can be quite high as seen in PEEM images at 266 nm:



PEEM measurement compliments of H. Padmore, ALS-LBNL



D. H. DOWEII -- P3 WORKSNOP

Intrinsic Emittance: Expt. and Theory for metals



Expt.-to-theory is ~2, consistent with other experiments

Intrinsic Emittance of GaAs: Response time and emittance depend upon photon wavelength

Due to electron-phonon scattering the delayed-emission electrons can reach thermal equilibrium with the lattice, giving the intrinsic emittance of GaAs a thermal-like emission component (given by kT) as well as prompt emission(given by the excess energy) part.

Several good features: low intrinsic emittance, long photon wavelength, low roughness

But: The slow response time will be problematic for use in high frequency RF guns & Requires excellent vacuum



Intrinsic Emittance: Reducing the cathode emittance What cathode will allow us to achieve 0.01 micron at 20 pC? Intrinsic emittance vs. cathode field



-Achieving 0.01 micron emittance will require higher cathode fields to keep the laser beam size small unless the cathode has a very small intrinsic emittance. -It appears metal cathodes have too high an intrinsic emittance above a couple of pC

-This will also be true for PEA cathodes such as CsTe and CsK₂Sb -NEA cathodes like GaAs can work at 20 pC, and if cooled, produce even lower emittances?

Intrinsic Emittance: Cathode Surface Roughness

AFM measurement

Emittance Growth Due to Non-Uniform Emission & Field Enhancement -Highest cathode field not necessary best emittance-



Concluding Thoughts

- As much as possible, it is best to link models to measured parameters, rather than fitting
 - Ideally, measured from the same cathode
- Whenever possible, QE should be measured as a function of wavelength. Energy Distribution Curves would be *wonderful!*
- Spicer's Three-Step model well describes photoemission from most metals tested so far
- The model provides the QE and EDCs, and a Monte Carlo implementation will provide temporal response
- The Schottky effect describes the field dependence of the QE for metals (up to 0.5 GV/m). Effect on QE strongest near threshold.
- Field enhancement for a "normal" (not needle, grating) cathode should have little effect on average QE, though it may affect a "QE map"
- A program to characterize cathodes is needed, especially for semiconductors (time for Light Sources to help us)

Thank You!