One-step photoemission simulation: Exact triangular barrier solution with bulk and vacuum electronic states

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INTRODUCTION

- One-step photoemission simulation based on the exact quantum solution for transmission through (excess energy, $\Delta E < 0$) and over ($\Delta E > 0$) a triangular barrier evaluated by Forbes and Deane [1].

- The photoemission analysis includes,
  - Transverse momentum conservation in electron emission
  - Bulk electron-like emission bands of spherical symmetry with its effective mass m* (i.e., $E(\mathbf{p}) = \frac{p_z^2+p_T^2}{2m^*}$)
  - The local density of the emitting bulk band states AND the recipient vacuum density of states.
  - Fermi Dirac population distribution at an electron temperature T_e.
  - The surface acceleration field

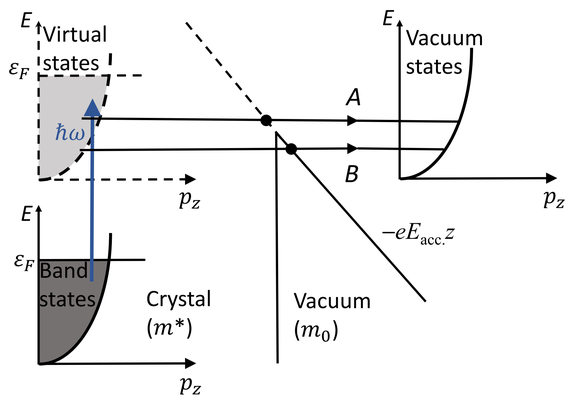

Figure 1: *Schematic of the simulated one-step photoemission process: Photo-excitation of the bulk band states into a set of identical virtual band states from which electrons transmit (with transverse momentum conservation) into the vacuum states either above (photoemission with $\Delta E > 0$; path A) or below (photo-assisted tunneling with $\Delta E < 0$; path B) the triangular barrier generated by the applied acceleration field in an electron gun.*

The transmission coefficient of the triangular barrier for emitted electrons [1],

$$T = \frac{4Cp_z}{\left(2Cp_z+\pi C^2 p_z^2\left(Ai^2(\xi)+Bi^2(\xi)\right)+\pi\left((Ai'(\xi))^2+(Bi'(\xi))^2\right)\right)} \quad (1)$$

The Airy function argument is given by ξ

$$\xi = \sqrt[3]{\frac{2m_0}{(\hbar e E_{acc})^2}}\left(E_{th} - K_z\right) \quad (2)$$

where $C = (2m_0\hbar e E_{acc})^{-1/3}$ with e the free electron charge and $Ai(\xi)$ and $Bi(\xi)$ are the Airy functions of the first and second kind, respectively, with the prime denoting the first derivative. The bulk band threshold energy for above barrier photoemission $E_{th} = \mathcal{E}_F - \Delta E$, where $\mathcal{E}_F$ is the Fermi energy and the z component of bulk band kinetic energy is given by $K_z = E(p) - \frac{p_T^2}{2m^*}$.

Expressions for MTE and QE derived by Vecchione [2] are

$$MTE = k_B T_e \left\{\frac{Li_3[-Exp(\frac{\Delta E}{k_B T_e})]}{Li_2[-Exp(\frac{\Delta E}{k_B T_e})]}\right\} \quad (3)$$

and

$$QE = S_{12}\left\{\frac{Li_2[-Exp(\frac{\Delta E}{k_B T_e})]}{Li_2[-Exp(\frac{E_F}{k_B T_e})]}\right\} \quad (4)$$

where Li_n is the ploy-logarithm function of order n and S_{12} is a constant associated with the matrix element of optical excitation, transmission into the vacuum, etc.

References

[1] R.G. Forbes and J.H.B. Deane, *Proc. R. Soc. A* 467 (2011) 2927

[2] T. Vecchione, et al., 35th Intl. FEL Conf., New York (2013), pp.424-426

[3] D.H. Dowell & J.F. Schmerge, *Phys. Rev. ST – Acc. & Beams* 12 (2009) 074201

[4] G.N. Derry et al., *J. Vac. Sci. & Tech. A* 33 (2015) 060801

SIMULATION RESULTS FOR $m^* = m_0$

Mean transverse energy (MTE) and relative quantum efficiency (QE) of the emitted electrons are presented using a Ag(100) photocathode (work function ϕ = 4.32 eV [4], $\mathcal{E}_F$ = 5.49 eV, and $m^* = m_0$ the free electron mass) in a DC electron gun as a template.

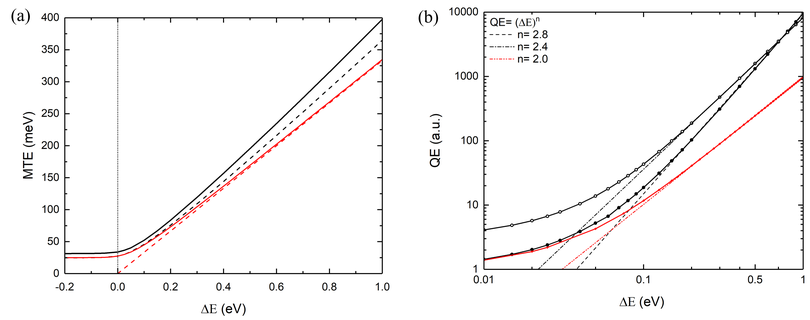

Figure 2: *Emission properties of a Ag(100) photocathode at 300K and $E_{acc.}$= 1MV/m: (a) MTE as a function of the excess photoemission energy ΔE; full one-step simulation (black line), one-step simulation without the vacuum states (black dashed line), equation 3 (red line), and ΔE/3* [3] *(red dashed line). (b) QE as a function of ΔE; full one-step simulation (black circles), one-step simulation without the vacuum states (open circles), and equation 4 (red diamonds), with power law fits for ΔE > 0.25eV shown as dashed lines.*

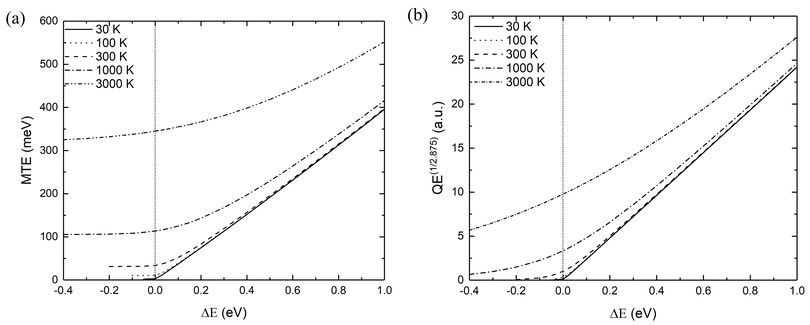

Figure 3: *Emission characteristics of a Ag (100) photocathode for electron temperatures T_e of 30, 100, 300, 1000, and 3000 K: (a) MTE and (b) $QE^{1/2.875}$ as a function of excess photoemission energy.*

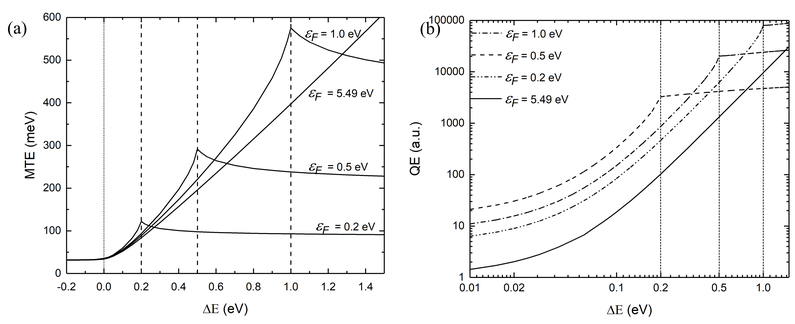

Figure 4: *Simulated dependence of (a) the MTE and (b) the QE on the excess photoemission energy for Fermi energies of 0.2, 0.5, and 1.0eV (T_e = 300K, and $E_{acc.}$ = 1MV/m). The vertical dashed lines indicate were $\Delta E = \mathcal{E}_F$ for the three cases and the dot-dashed line are the results for the the Ag (100) photocathode ($\mathcal{E}_F$ = 5.49eV).*

SIMULATION RESULTS FOR $m^* \neq m_0$

Mean transverse energy (MTE) of the emitted electrons when $m^* \neq m_0$ for Ag(100) photocathode (work function ϕ = 4.32 eV [4], and $\mathcal{E}_F$ = 5.49 eV.

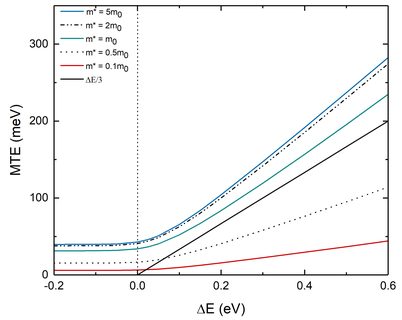

Figure 4: *Simulated dependence of the MTE on the excess photoemission energy for different effective masses; $m^* = 5m_T, 2m_T, m_T, 0.5m_T, 0.1m_T$ together with MTE = ΔE/3* [3].

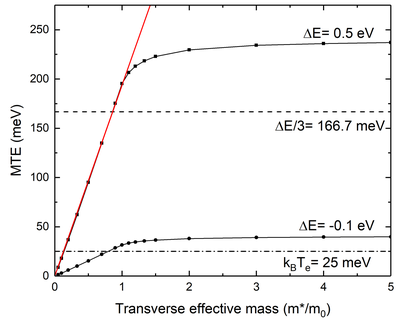

Figure 5: *Simulated dependence of the MTE for different effective masses at -0.1 eV and 0.5 eV excess energies.*

SUMMARY

- Extended the exact one dimensional triangular barrier quantum transmission solution using transverse momentum conservation to evaluate MTE and QE associated with the transition from the emitting bulk bands to the recipient vacuum states.
- The density of vacuum states has a significant effect on both the MTE and QE of photoemission
- MTE below work function ($\Delta E < 0$) is strongly temperature T_e dependent and greater than k_BT_e, for $m^*>0.8m_0$.
- Low effective electron mass is required for low MTE at T_e=300 K.

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