CORRECTIONS TO QUANTUM EFFICIENCY PREDICTIONS FOR LOW WORK FUNCTION ELECTRON SOURCES

K. L Jensen, Naval Research Laboratory, Washington, DC 20735, U.S.A.
E. J. Montgomery, D. W. Feldman, P, G. O'Shea, U. Maryland, College Park, MD 20742 U.S.A.
J. J. Petillo, SAIC, Billerica, MA 01821 U.S.A.

Abstract

The Three-Step Model of Spicer, or the analogous Moments-based models, can be used to predict photoemission from metals and cesiated metals. In either, it is a convenient approximation to neglect electrons that have undergone scattering. Using Monte Carlo to follow scattered electrons, we assess the utility of the approximation particularly for low work function (cesiated) surfaces.

MOTIVATION

For metals, scattering is electron-electron or acoustic phonon: the former reduces the energy of photoexcited electron and changes its direction, whereas the later changes direction (energy loss is negligible). However, particularly when the work function is low, a scattered electron may retain enough energy to still be emitted. In the present work, we seek to quantify the impact on QE predictions from having neglected scattered electrons, and to do so, we make use of Monte Carlo simulations of transport and emission of photoexcited electrons.

By "Fatal Approximation" the following assumptions are made: photoexcited electrons will contribute to QE if their energy after photoexcitation exceeds surface barrier height (E_F + Φ), their energy component directed into surface barrier is greater than surface barrier height, and they do not suffer a scattering event on way to surface. By "Non-Fatal Approximation" it is meant that if electrons do suffer a scattering event then either the photoexcited electron's post-scattering energy is not brought below barrier height *or* the collisionally excited electron's energy is brought above barrier height, as indicated in Figure 1.

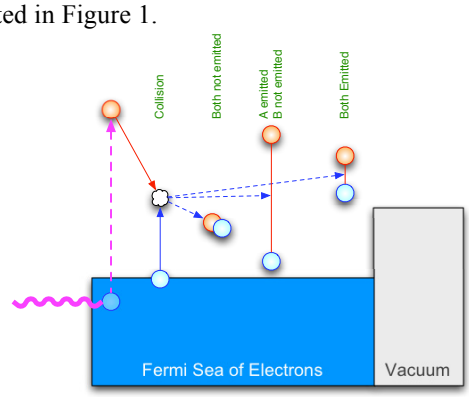

Figure 1: Outcome of scattering of electrons by other electrons and relation to emission.

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MOMENTS & MONTE CARLO

The calculation of QE contains a scattering factor f_λ that relates the penetration depth of photons (δ) to the distance between scattering events $l(E)$ and accounts for how many electrons lost on migration to surface. It is given by

$$f_\lambda\left(\cos\theta,\frac{\delta}{l}\right)=\frac{\cos\theta}{\cos\theta+\left(\delta(\hbar\omega)/l(E)\right)} \qquad (1)$$

The ratio δ/l is of order unity for metals, and l is the product of the velocity of the electron and the scattering time. The energy and temperature dependent scattering times are evaluated from their fundamental definitions. Therefore, the evaluation of relaxation times is already on hand for usage by the Monte Carlo simulations.

The Monte Carlo is implemented as follows. The scattering times are first evaluated as a function of photoexcited electron energy, temperature, and material parameters. A vector is generated of unit magnitude, the elements of which mark off the relative weight of each scattering term in the total relaxation time, and compared to a random number r: where r fits between the vector elements determines which scattering has occurred. If acoustic scattering occurs, the direction of the electron is randomly changed. If *e-e* scattering occurs, the target electron is taken to be at the Fermi level, and the final state velocities are calculated subject to the constraints of energy and momentum conservation as well as final state occupation. The relaxation times are shown in Figure 2.

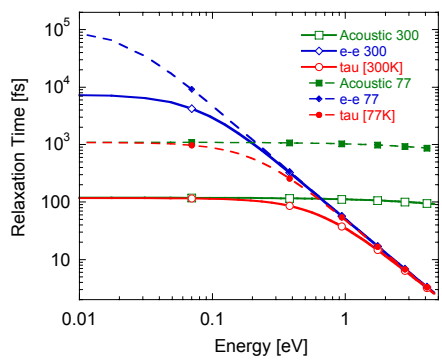

Figure 2: Outcome of scattering of electrons by other electrons and relation to emission.

The *e-e* scattering is dominant in metals like copper, and so the evaluation of final conditions must be carefully done. To do so, the collision is shifted to the rest frame of the target electron, in which the final velocities are

orthogonal. This involves setting up rotation matricies to govern the collision and insuring that final states do not fall below the Fermi level. The process is repeated for N particles ("Synchronous ensemble") and the location, velocity, and time of the event are recorded so as to reconstruct the trajectories. At all times, only those electrons that have an energy sufficient to be emitted (whether or not they are) are tracked. A visualization of the particle trajectories then gives an indication of when the Fatal approximation is good, and when it is not. Bare copper is compared to Cs on copper in Figure 3, from which it is seen that the Fatal Approximation is good in the former, but not in the latter.

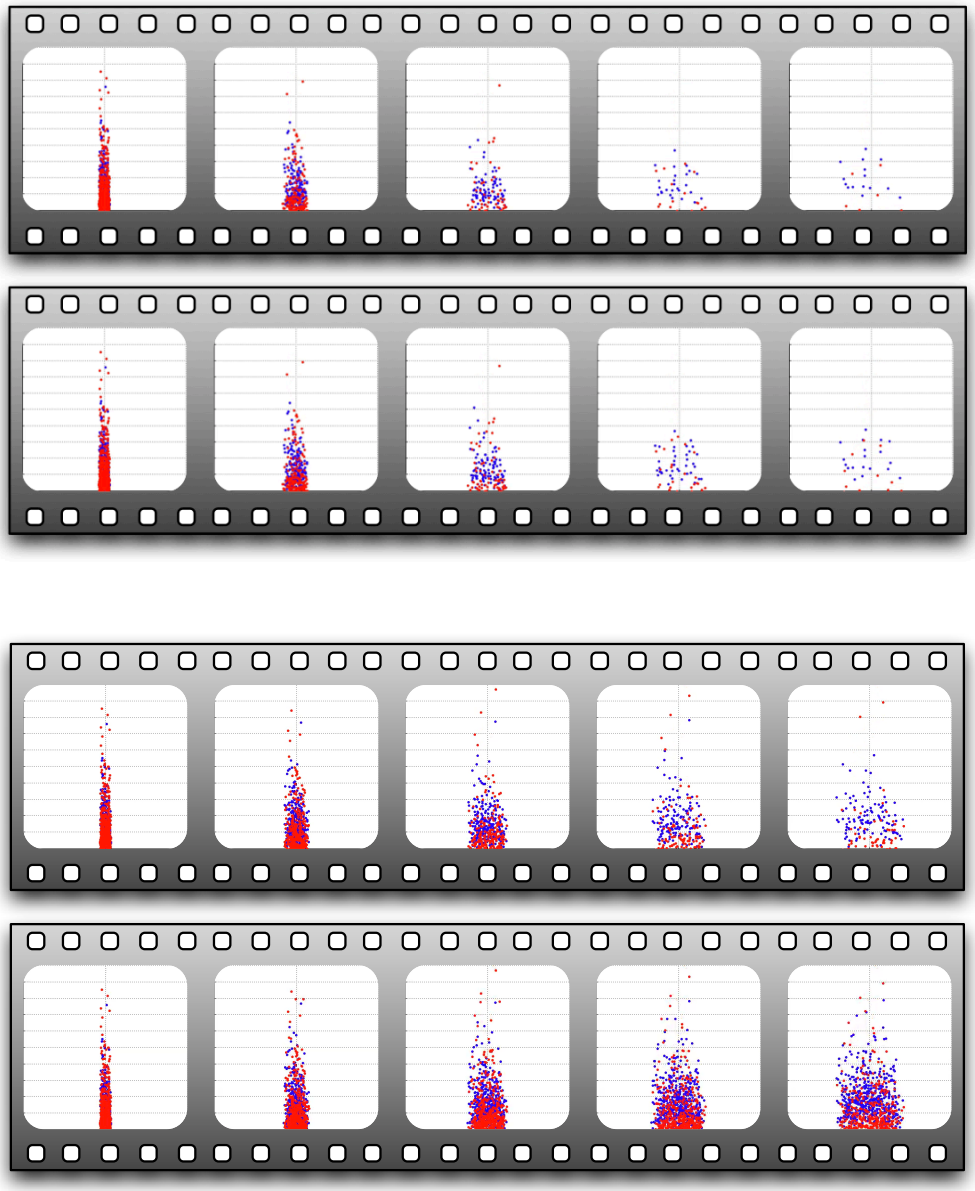

Figure 3: Each frame is 1 fs. The bottom of the square is the copper surface. Red electrons move down, blue electrons move up. First (top) = Copper / Fatal approximation; Second = Copper / Non-Fatal approximation: their close visual similarity indicates the Fatal Approximation is good for bare metal parameters. Third = Cs on Cu / Fatal approximation; Fourth = Cs on Cu / Non-Fatal approximation: their evident differences show that the Fatal approximation is not good when the surface barrier is small.

For a general simulation for which $\lambda = 266$ nm; T = 300 K, F = 10 MV/m, in copper, each "scattering" removes about 90% of the number of electrons eligible to be emitted. In contrast, for cesium on copper, about 5 collisions are necessary to remove about 90% of the electrons, and about 7 to 8 collisions removes about 99% of the electrons eligible to scatter. This is shown in Figure 4, wherein the average energy and standard deviation of the electrons eligible to scatter is shown.

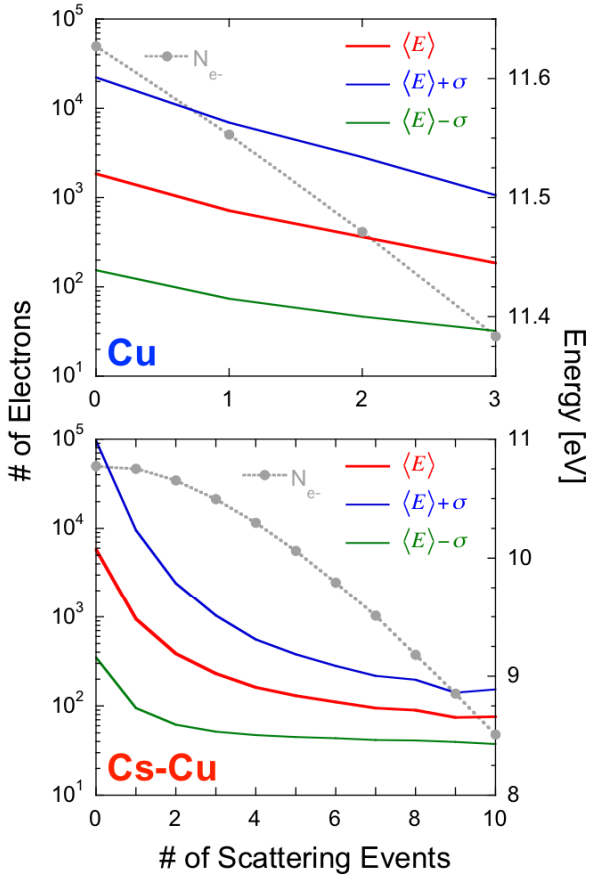

Figure 4: Average energy and number of electrons still eligible to scatter as a function of # of scattering events.

It is clear that for low work function conditions, a portion of the emitted current is made up of electrons that have undergone a number of scattering events and therefore "thermalize" – and this implies that each population of electrons (those that scatter and those that do no) will have a characteristic time behavior. A model of that behavior can be obtained by assuming that unscattered electrons constitute an expanding shell of charge, whereas scattered electrons are an expanding diffusive sphere of charge. In the shell model, the amount of *emitted* charge emitted as a function of time is

$$Q(t) = \frac{Q_r}{4\pi R(t)^2} \times \int_0^{2\pi} R\,d\varphi \int_0^{\cos^{-1}(R(0)/R(t))} R\sin\theta\,d\theta \qquad (2)$$
$$= \frac{1}{2}Q_r\left\{1-\frac{R(0)}{R(t)}\right\} = Q_r\frac{v_o t}{(2v_o t+\delta)}$$

where $R(t)$ is the radius of the shell as a function of time, and v is the velocity at which the shell expands. By comparison, the diffusively expanding sphere of charge gives rise to

$$Q(t) = Q_d \frac{\int_{v_o t}^{\infty} t^{-1/2}\exp\left(-z^2/4Dt\right)dz}{\int_{-\infty}^{\infty} t^{-1/2}\exp\left(-z^2/4Dt\right)dz} \qquad (3)$$
$$\equiv \frac{1}{2}Q_d\left\{1-Erf\left(\sqrt{\tau^*/t}\right)\right\}$$

where it is assumed that D (the diffusion term) is the product of a relaxation time and the square of a velocity, and τ^* is defined by this relation. In fact, the Monte Carlo evaluation of emission current compares with the time derivatives of $Q(t)$ well, as shown in Figure 5.

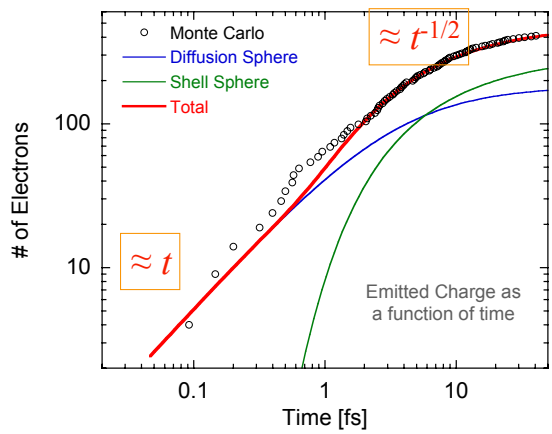

Figure 5: Emitted charge as a function of time for Cs-Cu conditions. The emitted current shows contributions from both an expanding shell of charge and a diffusively expanding sphere of charge.

In conclusion when the work function is low, as it is for cesiated surfaces, the neglect of scattered electrons in the estimation of quantum efficiency or in the temporal characterization of the current is a poor approximation, although it functions well for high work function (bare metal) conditions.

REFERENCES

[1] K.L. Jensen, D.W. Feldman, N.A. Moody, and P.G. O'Shea, J. Appl. Phys. 99, 124905 (2006).