



## Calculation of photofield emission current in tungsten by using transfer Hamiltonian method

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### ABSTRACT

We present here the results of the calculations of photofield emission current. Free electron potential model was used to describe crystal potential to derive wave functions. Transfer Hamiltonian method was applied for calculation of the transition probability. Photofield emission current is calculated from tungsten. Variation of photofield emission current is explained from the result.

**Key words:** Photofield emission; photofield emission current; transfer Hamiltonian; wavefunctions.

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### INTRODUCTION

Photofield emission (PFE) is a technique in which a metal is irradiated by an incident laser radiation of photon energy ( $\hbar\omega$ ). Photon energy is usually less than the work function ( $\phi$ ) of the metal. The incident radiation photoexcites the electrons to states which lie between the Fermi level and the vacuum level, hence these electrons are confined within the metal surface. A strong static electric field ( $\sim 10^{11}$  V/m) when applied to the surface of the metal causes the photoexcited electrons to

tunnel through the surface potential barrier into the vacuum region. These electrons which are now emitted into the vacuum region constitute the measurable current called photofield emission current (PFEC). The transition of electrons from the initial state to the final states can be represented by matrix element,

$$M_{fi} = \langle f | \mathbf{A} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{A} | i \rangle \quad (1)$$

where  $\mathbf{p}$  is the one electron momentum vector and  $\mathbf{A}$  is the vector potential of the incident radiation. A gauge is chosen in which scalar potential  $\phi(r,t) = 0$ . We considered the photofield emission to take place along  $z$ -axis which is normal to the surface.

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For the evaluation of photofield emission current (PFEC), we need to know the initial state wavefunction  $\psi_i$  and final state wavefunction  $\psi_f$ . This was calculated by using free electron model as done by Thapa *et al.*<sup>1</sup> In this paper, PFEC is calculated in the case of tungsten and is compared with previously published results.<sup>2</sup>

### THEORY

The transfer Hamiltonian method takes into account the detailed electronic states of the electrons in solid. The Hamiltonian of an electron in one dimension is:

$$H = T + V_m \theta(-z) + V(z) - eFz \theta(z)$$

Here,  $T$  is one electron kinetic energy operator,  $V_m$  the periodic metal potential,  $V(z)$  the outside potential in the absence of field and  $F$  is the high static electric field. In transfer Hamiltonian formalism, the two left and right Hamiltonians are defined as

$$H_L = T + V_m \theta(-z) + V(z) \theta(z)$$

and  $H_R = T + V(z) \theta(z) - eFz \theta(z)$

The eigen functions of left and right Hamiltonian  $H_L$  and  $H_R$  are denoted by  $\psi$  and  $\chi$ , respectively. The transition matrix element from initial to final states can now be represented by

$$M_{fi} = \langle n | -eFz \theta(z) + H' | E_L \rangle$$

where the perturbation due to incident radiation (in one dimensional) is

$$H' = A_\omega(z) \frac{d}{dz} + \frac{1}{2} \frac{dA_\omega(z)}{dz}$$

Considering the effect of image potential on the transmitted electrons, the formula for current density is given by

$$j'(E) = \int_{-\infty}^{\infty} \frac{2\pi e}{\hbar} \left| \langle n | V_0 - eFz \theta(z) - \frac{e^2}{4z} + H' | E_L \rangle \right|^2 \times \delta(E_n - E_L) \delta(E - E_L) f(E_L) \quad (2)$$

Here,  $\chi_f$  is the final state and  $\psi_{E_L}$  is the initial state wavefunction of an electron. As photofield emission is a surface phenomenon, we consider only the surface region, therefore,

$$j'(E) \cong \int_0^d \frac{2\pi e}{\hbar} \left[ \psi_f^* \left( V_0 - eFz - \frac{e^2}{4z} + A(z) \frac{d}{dz} + \frac{1}{2} \frac{dA(z)}{dz} \right) \psi_i \right]^2 dz \quad (3)$$

On expansion, Eq. (3) becomes

$$j'(E) = \frac{2\pi e}{\hbar} \left[ \int_0^d \psi_f^* \left( V_0 - eFz - \frac{e^2}{4z} \right) \psi_i dz + \int_0^d \psi_f^* \left( A_\omega(z) \frac{d}{dz} \right) \psi_i dz + \frac{1}{2} \int_0^d \psi_f^* \frac{dA_\omega(z)}{dz} \psi_i dz \right]^2 \quad (4)$$

Photofield current  $j(E)$  can be calculated by evaluating the above integrals by writing FORTRAN programme.

### RESULTS AND DISCUSSIONS

We discuss here the results of PFEC in the case of metal tungsten, for which the following data are used to carry out the calculation:

Surface Width ( $d$ )	= 5.892 Å
Initial state energy ( $E_i$ )	= 2.148 eV
Potential barrier height ( $V_0$ )	= 15 eV
Work function ( $\phi$ )	= 4.928 eV
Fermi energy ( $E_F$ )	= 10.06 eV
Scattering factor ( $\alpha$ )	= 0.35

In Figure 1, the plot of the variation of

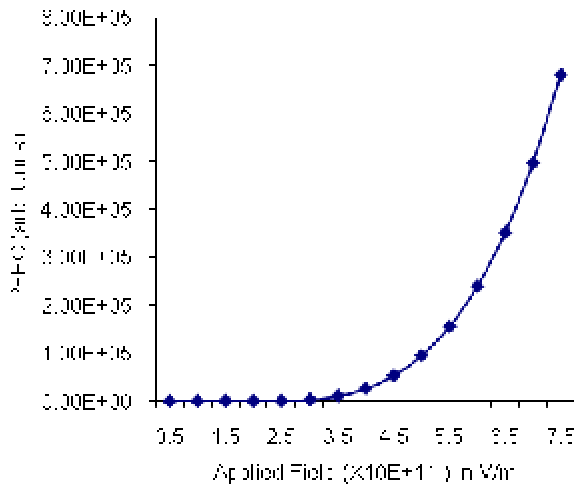


Figure 1. Plot of photofield emission current (PFEC) against applied field  $F$  (in the units of  $10^{11}$  / applied field (V/m)) for values of photon energy  $\hbar\omega = 1.96$  eV. Initial state energy  $E_i = 1$  eV below Fermi level ( $E_F = 0.0$ )

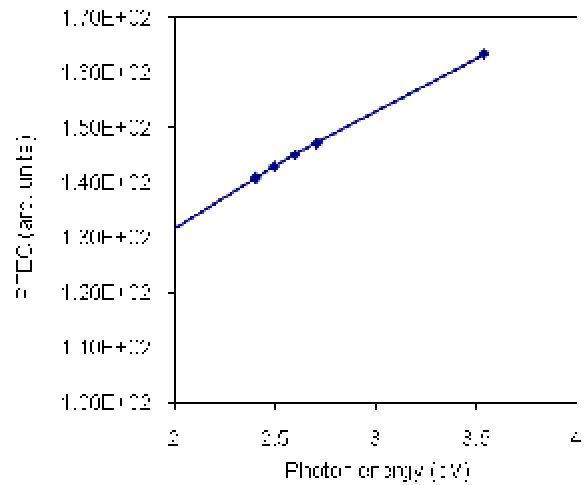


Figure 2. Plot of photofield emission current (PFEC) against photon energy and the applied field  $F = 3.08 \times 10^{11}$  V/m.

PFEC as a function of applied field for 1.96 eV photon energy is shown. It is seen from the plot that as the values of applied field increases, PFEC decreases exponentially. This observation had been also measured experimentally by Radon *et al.*<sup>3</sup> However, they have simply observed only decrease in PFEC, but exponential decrease was not seen.

In Figure 2, the plot of PFEC as a function of incident photon energy is shown. It is observed that PFEC is more or less remains constant for all values of photon energies. This is due to the reasons that matrix element does not change for all values of photon energies. Similar features have also been observed by Schwartz and Schaich<sup>4</sup> in the case of matrix element for transition.

## CONCLUSION

From the result of PFEC as a function of applied field and photon energy, it is seen that

the model developed could explain the variation of PFEC as obtained by Thapa and Das.<sup>5</sup> It also confirmed that PFEC varies exponentially and there is no oscillations in PFEC as observed earlier.<sup>4</sup> However, there are certain drawbacks in the model used. For example, the vector potential had been deduced without inclusion of the effect of high static field that is used in photofield emission.<sup>5</sup> Further perturbation effect should be included appropriately with initial conditions. However, the model developed is explaining to some extent the features associated in photofield emission that were observed previously by Gao and Reifenberger.<sup>2</sup>

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