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Calculation of photofield emission from band states using Kronig-Penney model and spatially varying photon field

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Abstract : A model photofield emission calculation is discussed which takes into consideration the band states and spatially dependent vector potential of the incident radiation. The initial state wavefunction is the one derived by using the Kronig-Penney potential model for the bulk and the surface region of metal.

Keywords Photofield emission, vector potential, Kronig-Penney model

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1. Introduction

Photofield emision (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 workfunction (ϕ) of the metal surface under investigation. The incident radiation photoexcites the electrons to final state which lies between the Fermi level and the vacuum level, hence these electrons are confined within the metal surface. A strong electric field (~ 10^9 Vm^{-1}) is applied to the surface of the metal which then 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 photofield emission current. Unlike in photoemission where only the states below the Fermi level are probed, in PFE, electron states below and above the Fermi level can be studied. As incident radiation in PFE can be used to probe the electron states between the Fermi level and the vacuum level, the initial state of the electron can play an important role in determining the shape of the final state energy distribution. This allows one therefore, to see the effect of initial state energy bands on PFE.

There had been a number of theoretical studies on PFE [1-7] which have included the effect of surface photoexcitation mechanism. For example, Caroli *et al* [8] emphasized the non-equilibrium aspects of PFE and presented the phenomena in terms of second-order perturbation theory. Taranko [9], Bagchi [10], Schwartz and Cole [11] calculated photofield energy distribution assuming different surface potential barriers. A general characteristic of these theories is the triangular-shaped energy distribution. Lee [1], Gao and Reifenberger [3], and Schwartz and Schaich [4] have considered also the effect of image potential barrier on the work function of metal in their calculations of PFE. The transmission probability function was appropriately calculated by them. In most of the theoretical considerations of PFE, it has been seen that a free electron model potential was used to define the bulk and surface potential. However in these cases, the initial state wavefunction was not appropriately defined. Further, photoexcitation in PFE is a surface photoeffect process, which involves the spatial variation of the vector potential of the incident radiation due to the presence of the term $\nabla \cdot A$ in the matrix element for photoexcitation. This demands for an accurate description of vector potential of the incident radiation.

In this paper, we present a simple model for PFE calculations in which band states are defined by Kronig-Penney potential. The electron states which defines the initial and final state

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wavefunctions are derived by matching the wavefunction and its derivative at $z = 0$ plane.

2. Theoretical formalism

A p-polarized radiation of photon energy $\hbar\omega$ is incident on the metal surface at an angle θ_i with respect to the surface normal. Surface normal is defined by z-axis which is perpendicular to xy-plane. This incident radiation usually a laser beam, causes the transition of electrons from the initial state $|i\rangle$ to final state $|f\rangle$ and the matrix element for this transition can be written as

$$M_{fi} = \langle f|A.p + p.A|i\rangle$$

$$= \frac{2i}{\hbar\omega}\left\{\hbar\langle f|A\nabla\cdot V|i\rangle + \frac{i\hbar}{2m}\langle f|A^2\nabla\cdot p|i\rangle - \frac{\hbar}{m}\langle f|\nabla(A.p)\cdot p|i\rangle\right.$$

$$\left. - \frac{\hbar^2 w}{2}\langle f|\nabla\cdot A|i\rangle\right\}, \qquad (1)$$

where A is the vector potential of the incident radiation and p the momentum operator. The important ingredients of eq. (1) are : (i) initial (final) state wavefunction $\psi_i(\psi_f)$ and (ii) vector potential A of the incident radiation. The initial state wavefunctions ψ_i will be the one used by Thapa [12] for photoemission calculations. This is discussed briefly in the next section.

In photofield emission, the dominant contribution to the photocurrent comes from the surface photoeffect. As evidenced by several authors, for example, Levinson *et al* [13], Feibelman [14], Kliewer [15], main contribution to the surface photoeffect is due to spatial variation of photon field vector A. A systematic calculation of this effect on surface photoeffect had also been done by Thapa [12]. It is therefore, necessary that one needs a detail theory of dielectric model for the appropriate formulations of A. In this formalism here, we will use the modified form of the inhomogeneous dielectric model of Bagchi and Kar [16] which takes into account the dependence of A not only on frequency ω but also on the z-coordinate. The vector potential for the bulk $(z < -a)$, surface $(-a \le z \le 0)$ and vacuum $(z > 0)$ regions is given by

$$\bar{A}_\omega(z) = \begin{cases} -A_0 & z < -a, \\ -A_0\dfrac{a\varepsilon(\omega)}{[1-\varepsilon(\omega)]z + a}, & -a \le z \le 0, \\ -A_0.\varepsilon(\omega), & z > 0, \end{cases} \qquad (2)$$

where $A_0 = \dfrac{\sin 2\theta_i}{\left[\varepsilon(\omega) - \sin^2\theta_i\right]^{\frac{1}{2}} + \varepsilon(\omega)\cos\theta_i}$

The matrix element of eq. (1) can be written now in one dimension as

$$M_{fi} = \int_{-\infty}^{-a}\psi_f^* A_z\frac{dV}{dz}\psi_i dz + \int_{-a}^{0}\psi_f^* A_z\frac{dV}{dz}\psi_i dz + \int_{0}^{\infty}\psi_f^* A_z\frac{dV}{dz}\psi_i dz$$

$$+ \int_{-a}^{0}\psi_f^*\frac{d^2A_z}{dz^2}\left(-i\hbar\frac{d}{dz}\right)\psi_i dz + \int_{-a}^{0}\psi_f^*\frac{dA_z}{dz}\left(-\hbar^2\frac{d^2}{dz^2}\right)\psi_i dz$$

$$+ \int_{-a}^{0}\psi_f^*\frac{dA_z}{dz}\psi_i dz. \qquad (3)$$

The photoexcited electrons are now in the final state with energy $E_f = E_i + \hbar\omega$ due to absorption of photon energy $\hbar\omega$, but lies below the vacuum level (as $E_f < \phi$ the work function of metal). A strong static field when applied to the surface of the metal will now cause the photoexcited electrons to be transmitted across the surface potential barrier to vacuum region. The high static field causes the reduction of the work function of the metal causing thereby the Schottky effect which brings the image potential effect. This will reduce the height of the step potential and the work function at the surface as shown in Figure 1. The

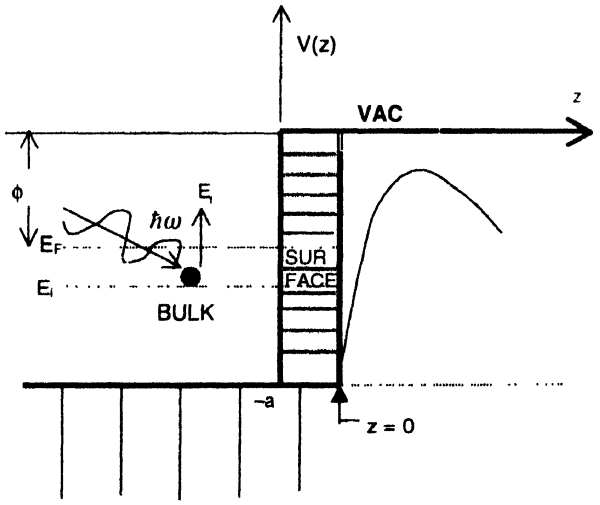

Figure 1. Model potential used in photofield emission calculations for describing the band states with a surface of width a included. The effect of the applied field on the potential is also shown.

photofield emission current density formula as given by Gao and Reifenberger [3] is

$$\frac{dj}{dE} = -\frac{e}{2\hbar^4\omega^3}\frac{n}{\Omega}(\hat{\varepsilon}.\hat{z})^2 f(E-\hbar\omega)\int_0^{D(W)|M} dW \frac{}{[W(W-\hbar\omega)]^{\frac{1}{2}}}, \qquad (4)$$

In eq. (4), $f(E-\hbar\omega)$ is the Fermi-Dirac distribution function, $D(W)$ is the quantum mechanical transmission probability and the energy of the photoexcited electrons is $E = W + \dfrac{\hbar^2 k_\parallel^2}{2m}$. These electrons will travel across the surface potential barrier which is deformed by the applied electrostatic field and the image potential barrier. Here, W is the normal component of

energy E. $D(W)$ in this model is as given by Soven *et al* [17] and is

$$D(W) = \left[W(V_0 - W)\right]^{1/2} \exp\left[-\frac{4}{3}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \frac{(-W)^{3/2}}{eF}\right] \quad (5)$$

and $$V(z) = V_0 - eFz - \frac{e}{4z}. \quad (6)$$

Potential given by eq. (6) is image rounded barrier which is shown in Figure 1. Photofield emission current (PFEC) given by eq (4) can be calculated by writing FORTRAN programs, as the integrals involved in matrix element M_{fi} cannot be evaluated analytically.

3. Description of the initial and final state wavefunctions

To study surfaces, we have to solve the Schroedinger's equation both in the metallic and vacuum region outside the metal. One general approach is to calculate the wavefunctions in the two regions and make sure that it matches properly as regards to ψ and $\frac{d\psi}{dz}$ on the boundary plane $z = 0$. Let $\phi(z/E)$ denote the Bloch wavefunction deep in the metal and $\phi^*(z/E)$ is the time reversed version of ϕ. The eigenfunction in the semi infinite metallic region has been chosen to have the form as:

$$\psi_i(z/E) = \phi(z/E) - P\phi^*(z/E),$$

where P is to be determined by matching slope and value at $z = 0$. To find $\phi(z/E)$, let us consider an electron with energy $E_i = \frac{\hbar^2 k_i^2}{2m}$ to be incident on the single barrier potential $v(z)$ of width a_0. We consider the potential (Figure 1) to be one-dimensional Kronig-Penney type described by

$$v(z) = \sum_n g\delta\left[z - (2n+1)\frac{a_0}{2}\right]. \quad (7)$$

Since $v(z) = 0$ for $|z| \geq \frac{a_0}{2}$, the wavefunction $\phi(z)$ in these regions:

$$\phi(z) = \begin{cases} e^{ik_i z} + re^{-ik_i z}, & z \leq -\frac{a_0}{2}, \\ te^{ik_i z} & z \geq \frac{a_0}{2}. \end{cases}$$

where r and t are the reflection and transmission coefficients through this potential. Their values for the Kronig-Penney model is $r = i\sin\delta\exp(i\delta)$, $t = \cos\delta\exp(i\delta)$ where δ is the phase shift introduced in the transmitted wave given by $\cot\delta = -\frac{\hbar^2 k_i}{mg}$. Here, g is the strength of the potential. The initial state wavefunction can then be written as

$$\psi_i(z/E) = \begin{cases} \left(1 - iPe^{i\delta}\sin\delta\right)e^{ik_i z} & z < 0, \\ -\left(P - ie^{i\delta}\sin\delta\right)e^{-ik_i z}, & \\ Te^{\chi z}, & z > 0, \end{cases} \quad (8)$$

where P and T are reflection and the transmission coefficients across the boundary plane and

$$\chi = \left[\frac{2m}{\hbar^2}(V_0 - E_i)\right]^{\frac{1}{2}}$$

V_0 is the step potential at the surface (measured from the bottom of the well) which an electron encounters while transmitting through the boundary. Imposing the boundary conditions on eq. (8) gives

$$P = \frac{(\chi - ik_i) - (k_i - \chi)e^{i\delta}\sin\delta}{(\chi - ik_i) + (k_i - \chi)e^{-i\delta}\sin\delta} \quad (9)$$

and

$$T = \frac{2k_i \sin 2\delta}{(\chi - ik_i) + (k_i - \chi)\sin\delta\, e^{i\delta}}. \quad (10)$$

The values of P and T enables one to write appropriately the initial state electron wavefunction in the vicinity of the surface both in the metallic and the vacuum region. The final state wavefunction is given by

$$\psi_f(z) = \begin{cases} \left(\frac{2\pi\hbar^2 q_f}{m}\right)^{\frac{1}{2}} \frac{2q_f}{q_f + k_f} e^{ik_f z} e^{-\alpha|z|}, & z < 0, \\ \left(\frac{m}{2\pi\hbar^2 q_f}\right)^{\frac{1}{2}} \left(e^{iq_f z} + \frac{q_f - k_f}{q_f + k_f} e^{-iq_f z}\right), & z > 0, \end{cases} \quad (11)$$

Here, $k_f^2 = \frac{2m}{\hbar^2}E_f - k_\parallel^2$ and $q_f^2 = \frac{2m}{\hbar^2}(E_f - V_0) - k_\parallel^2$.

4. Conclusion

A simple model for PFE calculation has been presented in the context of a periodic type Kronig-Penney potential model which considers the band state of electron. A free electron model as used by Gao and Reifenberger [3] in the case of W is not a fitting type of potential as W is a strongly bonded metal. Further Gao and Reifenberger [3] had also not taken into consideration the effect of the dielectric response function for the bulk, surface and vacuum regions of metal which causes the change in the vector potential of incident radiation. We have presented here a model which will take into account the bulk and the surface

state bands of different symmetries and also the effect of variation of vector potential. The success of this model applied to photoemission calculations has encouraged us to expect that the model proposed here would be able to reproduce at least the qualitative features.

However, the main drawback of the model is the initial state wavefunction used for the surface region. The same initial state wavefunction describing the band states, had been used also for the surface states especially in the expansion of matrix element given by eq. (3). Further, we have not considered any specific kind of potential to describe the surface potential.

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