

A model calculation of photofield emission by using a simple vector potential

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ABSTRACT

A simple model of photofield emission calculation is discussed. A spatially dependent vector potential is used to evaluate the matrix element for calculating the photofield emission current density. We have presented a model in which Projection Operator method of group theory has been applied to deduce initial state wave function Ψ_i for a particular surface state pertaining to a particular point group. The model will also take into account the bulk and the surface state bands of different symmetry and also considers the effect of variation of vector potential. We have considered the point Δ_2' for which the point group is C_{4v} which corresponds to the surface states. By introducing the atomic orbital $\Phi(z)$, the final form of initial state wavefunction is calculated.

Key words: Photofield emission; Projection Operator; vector potential; wavefunction.

INTRODUCTION

Photofield emission (PFE) is a novel investigative method in which a metal is irradiated by a laser radiation of photon energy $\hbar\omega$. Photon energy is usually less than the workfunction (ϕ) of the metal under investigation. The incident radiation photo excites the electrons to a final state which lies below the vacuum level; hence these electrons are confined within the metal surface. A strong static electric field of the order of 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 which then constitutes the

photofield emission current (PFEC).

In PFE, in addition to transmission probability $D(W)$, the transition matrix element $\langle \psi_f | \mathbf{A} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{A} | \psi_i \rangle$ also plays an important role. In this matrix element, we find that the important ingredients are the vector potential A , initial state wave function Ψ_i and final state wave function Ψ_f . There are several methods¹⁻⁷ of deducing the initial state wavefunction Ψ_i and the exactness of the model developed or used can hence correctly interpret the results in PFE calculations.

In this report, we are presenting a model for the calculation of PFEC in which Ψ_i is deduced by projection operator method of group theory.

METHODS

A p -polarised radiation of photon energy $\hbar\omega$

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is considered to be incident on the metal surface. The surface normal is defined by the z -axis which is perpendicular to the xy -plane. The incident radiation of a laser beam causes the transition of electrons from the initial state Ψ_i to final state Ψ_f . We consider the electron states to be lying below the Fermi level, and final states are states in the vacuum (detector). Therefore, the photofield emission current density formula can be written⁸ as,

$$\frac{dj}{dE} = -\frac{e^3}{2\hbar^4\omega^3} \frac{n}{\Omega} (\hat{\varepsilon} \cdot \hat{z})^2 f(E - \hbar\omega) \int_{-V_0 + \hbar\omega}^E dW \frac{D(W) |M_{fi}|^2}{[W(W - \hbar\omega)]^{\frac{1}{2}}} \quad (1)$$

where,

$$\frac{n}{\Omega} (\hat{\varepsilon} \cdot \hat{z})^2 = \left| \frac{A_\omega^z(z)}{A_0} \right|^2 = |\tilde{A}_\omega(z)|^2$$

and $A_\omega^z(z)$ is the z -component of vector potential along z -axis with frequency ω , A_0 is the amplitude of vector potential associated with the incident radiation, $f(E - \hbar\omega)$ is the Fermi-Dirac distribution function. The matrix element M_{fi} when expanded in one dimension along z -axis is given by,

$$M_{fi} = \int_{-d}^0 \psi_f^* A_\omega^z(z) \frac{dV}{dz} \psi_i dz + \int_{-d}^0 \psi_f^* \frac{d^2 A_\omega^z(z)}{dz^2} \left(-i\hbar \frac{d}{dz} \right) \psi_i dz + \int_{-d}^0 \psi_f^* \frac{dA_\omega^z(z)}{dz} \left(-\hbar^2 \frac{d^2}{dz^2} \right) \psi_i dz + \int_{-d}^0 \psi_f^* \frac{dA_\omega^z(z)}{dz} \psi_i dz. \quad (2)$$

To compute the vector potential $A_\omega^z(z)$, we will employ the dielectric model as discussed by Thapa *et al.*⁹ which takes into account the dependence of vector potential not only on frequency ω , but also on the z -axis. Therefore, the vector potential for the surface region ($-d \leq z \leq 0$) in one dimension is given by,⁹

$$\tilde{A}_\omega(z) = \frac{A_\omega^z(z)}{A_0} = \frac{-s \sin \theta_i}{\sqrt{\varepsilon}} p \left[1 + \frac{\xi^3}{6} + \alpha \left(\xi + \frac{\xi^4}{12} \right) \right], \quad (3)$$

where p and α are constants and $\xi = f(z)$. In the above equation, θ_i is the angle of incident photon radiation with respect to the surface normal.

RESULTS AND DISCUSSIONS

The transmission probability $D(W)$ in Eq. 1, which describes the quantum mechanical transmission probability that the photoexcited electrons with energy

$$E = W + \frac{\hbar^2 k_{\parallel}^2}{2m}$$

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 . $D(W)$ used in Eq. (1) is obtained by solving the Airy's differential equation⁹ and is given by,

$$D(W) = \frac{W^{\frac{1}{4}} \sqrt{\pi}}{(\hbar e F)^{\frac{1}{6}}} \left(\frac{2ik_i}{ik_i + \chi} \right) (2m)^{\frac{1}{2}} \exp \left[-i \left(\frac{2}{3} \frac{W^{\frac{3}{2}} \sqrt{2m}}{\hbar e F} + \frac{\pi}{4} \right) \right] \quad (4)$$

The final state wavefunction Ψ_f used is the scattering state of the step potential which is encountered by the electron at the surface. Step potential is defined by $V_z = -V_0 \theta(z)$, where $\theta(z)$ is unit function such that $\theta(z) = 1(0)$ for $z > 0$ ($z < 0$). Ψ_f is, therefore, given by,

$$\Psi_f(z) = \begin{cases} \left(\frac{m}{2\pi \hbar^2 q_f} \right)^{\frac{1}{2}} \frac{2q_f}{q_f + k_f} e^{-\alpha|z|} e^{ik_f z} \cdot e^{ik_f \cdot \eta}, & z < 0 \text{ (below surface)} \\ \left(\frac{m}{2\pi \hbar^2 q_f} \right)^{\frac{1}{2}} \left[e^{iq_f z} + \frac{q_f - k_f}{q_f + k_f} e^{-iq_f z} \right] e^{ik_f \cdot \eta}, & z > 0 \text{ (vacuum)} \end{cases} \quad (5)$$

where,

$$k_f^2 = \frac{2mE_f}{\hbar^2} - k_{\parallel}^2; \quad q_f^2 = \frac{2m}{\hbar^2} (E_f + V_0) - k_{\parallel}^2,$$

and

$$E_f = E_i + \hbar\omega$$

In Eq. (5), the factor $e^{-\alpha|z|}$ is included on the surface and bulk side to take into accounts the inelastic scattering of the electrons.

To calculate the initial state wavefunction Ψ_i , we have assumed the crystal potential to be defined by δ -potential and represented by the Kronig-Penney potential. The potential is periodic with the periodicity of the lattice as shown in Figure 1. In one dimension, one can write Ψ_i as,

$$\psi_i(z) = \begin{cases} \psi(z) + R\psi^*(z) & z \leq 0 \text{ (bulk \& surface)} \\ T e^{-\chi z} & z \geq 0 \text{ (vacuum)} \end{cases} \quad (6)$$

where $\Psi^*(z)$ is the complex conjugate of $\Psi(z)$, R is the reflection coefficient and T is the transmission coefficient across the boundary plane. Matching the wavefunction and its derivatives at $z = 0$ gives the value of coefficients R and T as,

$$R = \frac{-\chi + \mu - ik}{\chi - \mu - ik} \quad (7)$$

$$\text{and } T = \sigma \left(\frac{-2ik}{-\chi - \mu - ik} \right) \quad (8)$$

$$\text{where } \sigma = \frac{p}{k_1 a} \psi(0) \frac{\sin k_1 a}{\cos k_1 a - \cos k_2 a} \quad (9)$$

$$\text{and } \psi(0) = -2iC \frac{\sin k_1 a}{1 + \cos k_1 a - i \sin k_1 a} \quad (10)$$

Here p is the strength of the δ -potential barrier and it is assumed to be positive and μ is used as converging factor.

For W (100), surface state occurs¹⁰ in the energy band gap ($\Delta_2 - \Delta_2'$). The linear combination of atomic orbital (LCAO) representation for Δ_2' is

$$\frac{1}{3}(3z^2 - r^2), \text{ where } r^2 = x^2 + y^2 + z^2.$$

We have, therefore, considered the point Δ_2' for which the point group is C_{4v} . The basis function for the C_{4v} point group corresponding to W (100) surface state by using projection operator formula¹¹ is given by,

$$P_{mm}^p = \frac{l_p}{g} \sum_T \Gamma^p(T)_m^* P(T) \quad (11)$$

Here l_p is the dimension of the unitary irreducible representation of the group G , g is order of G and \sum_T is the summation over all the transformation T of G .

Now introducing the atomic orbital $\Phi(z)$, which includes the basis function derived by projection operator method of group theory obtained from Eq. (11), the final form of initial state wavefunction can be represented by,

$$\psi_i(z) = \begin{cases} \sigma [\Phi(z)e^{ikz} + R\Phi^*(z)e^{-ikz}], & z \leq 0 \\ T e^{-\chi z}, & z \geq 0 \end{cases} \quad (12)$$

The initial state wavefunction given by Eq. (12) can be used in conjunction with final state wavefunction Ψ_f given by Eq. (5) and vector potential $A_\omega(z)$ of Eq. (3), to calculate photo-field emission current given by Eq. (1).

CONCLUSIONS

A model photofield emission calculation has been presented in the context of a periodic type Kronig-Penney potential model which considers the band state of the electron. *PFE calculation* by using a free electron model as used by Gao and Reifenberger¹², and also by Thapa *et al.*¹³ in the case of W is not a fitting type of potential as W is a strongly bonded metal. Further, they have considered the free electron approximation in which the bulk crystal potential is empty. Also

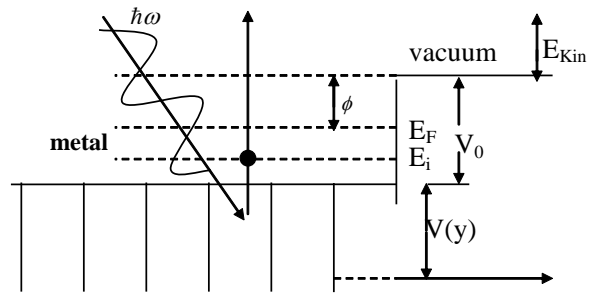


Figure 1. Schematic representation of Kronig-Penney δ -potential model for calculating the initial state wave function.

the initial state wave function describing the band states had been used also for the surface states especially in the expansion of matrix element given by Eq. (3) in the case of $W(100)$. Here we have presented a model in which Projection Operator method of group theory has been applied to deduce initial state wave function Ψ_i for a particular surface state pertaining to a particular point group. The model which we have presented here will also take into account the bulk and the surface state bands of different symmetry and also considers the effect of variation of vector potential.

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