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A MODEL CALCULATION OF PHOTOFIELD EMISSION BY USING VECTOR POTENTIAL AND GROUP THEORY

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ABSTRACT

A model calculation of photofield emission is discussed in which initial state wave function has been deduced by using projection operator method of group theory. A spatial dependent vector potential is used to evaluate the matrix element for calculating the photofield emission current density.

Key words : Photofield emission, Projection operator, Vector potential.

1 INTRODUCTION

Photofield emission (*PFE*) is a technique in which a metal is irradiated by an incident laser radiation of photon energy $\hbar\omega$. Photo energy is usually less than the workfunction (ϕ) of the metal under investigation. The incident radiation photoexcites the electrons 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 electron to tunnel through the surface potential barrier into the vacuum region constitutes the photofield emission current (PFEC). In photofield emission, in addition, in addition to transmission probability *D(W)*, the transition matrix element $\langle\psi_f|A.p + p.A|\psi_i\rangle$ 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 methods of deducing the initial state wavwfunction ψ_i and the exactness of the model developed or used can correctly interpret the results in photofield emission calculation. For example, the LEED (low energy electron diffraction) states deduced by Pendry [1], [2] for band structures and photoemission calculation are accurate, but the method is too complex and involves heavy computations. One also uses the Green function method for obtaining the appropriate wavefunctions as has done by Bagchi [3] and Modinos [4] . Multiple scattering technique and density functional theory [5], [6], [7] are also being used in the interpretation of results of photofield emission.

The incident radiation in PFE can be used to probe the electron states between the Fermi level and the vacuum level. Therefore, 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.

In this report, we are presenting a model calculation of photfield emission current by using the initial state wavefunction ψ_i

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which is deduced by projection operator method of group theory. As an example, basis function were derived for $W(100)$ surface state. An appropriate dielectric model and vector potential A also will be used for the surface region.

2 Theoretical Formalism

We have considered a *p*-polarised radiation of photon energy $\hbar\omega$ 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 is usually a laser beam, causes the transition of electrons from the initial state $|i\rangle$ to final $|f\rangle$. We consider initial states to be electron states lying below the Fermi level, and final states are states in the vacuum (detector). Therefore, the photofield emission current density measured can be written [8] as,

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

where $\frac{n}{\Omega}(\hat{\varepsilon}.\hat{z})^2 = \left|\frac{A_\omega(z)}{A_0}\right|^2 = \left|\tilde{A}_\omega(z)\right|^2$ and $A_\omega^z(z)$ is the *z*-component of vector potential along *z*-axis, A_0 is the amplitude of vector potential associated with the incident radiation. Also $f\left(E-\hbar\omega\right)$ is the Fermi-Dirac distribution function. The matrix element M_{fi} when expanded in one dimension along *z*-axis is given by,

$$M_{fi} = \int_{-d}^{0}\psi_f^* A_z\frac{dV}{dz}\psi_i dz + \int_{-d}^{0}\psi_f^*\frac{d^2A_z}{dz^2}\left(-i\hbar\frac{d}{dz}\right)\psi_i dz + \int_{-d}^{0}\psi_f^*\frac{dA_z}{dz}\left(-\hbar^2\frac{d^2}{dz^2}\right)\psi_i dz + \int_{-d}^{0}\psi_f^*\frac{dA_z}{dz}\psi_i dz. \tag{2}$$

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

$$E = W + \frac{\hbar^2.k_{\parallel}^2}{2m} \tag{3}$$

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 Eq. (1) is obtained by solving [9] Airy's differential equation and is given by

$$D(W) = \frac{W^{\frac{1}{4}}\sqrt{\pi}}{(\hbar eF)^{\frac{1}{6}}}\left(\frac{2ik_i}{ik_i+\chi}\right)(2m)^{\frac{1}{12}}\exp\left[-i\left(\frac{2}{3}\frac{W^{\frac{3}{2}}\sqrt{2m}}{\hbar eF}+\frac{\pi}{4}\right)\right] \tag{4}$$

3. Dielectric Model and Vector Potential

In photofield emission, the dominant contribution to the photocurrent comes from the surface photeffect. As evidenced by several authors, for example, Levinson [10] *et.al.*, Fiebelman [11], Kliewer [12], the 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 been also done by Thapa [13] *et.al.* It is, therefore, necessary that a detailed theory of dielectric model is developed at first for the appropriate formalism of ***A***. In this formalism here, we will employ the dielectric model of Bagchi and Kar [14], which takes into account the dependence of ***A*** not only on frequency ω but also on *z*-coordinate. Therefore, the vector potential for the surface region $\left(-d \le z \le 0\right)$ in one dimension is given by,

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$$A_z(\omega, z) = -\frac{A_o d\varepsilon(\omega)}{\left[1-\varepsilon(\omega)\right]z + d} \quad (5)$$

where

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

In the above equation, θ_i is the angle of incident photon radiation with respect to the surface normal.

4. Description of Initial and Final state wave functions

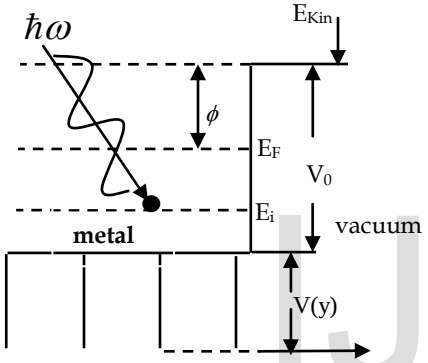

Fig : Schematic representation of Kronig-Penney δ -potential model for calculating the initial state wave function by using projection operator method of Group Theory.

To calculate the initial state wavefunction ψ_i, we have assumed the crystal potential of the solid which is defined by $\hat{\partial}$ - potential and represented by the Kronig-Penny potential. The potential is periodic with the periodicity of the lattice as shown in Fig. In one dimension, one can write ψ_i as

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

where $\psi^*(z)$ is the complex conjugate of $\psi(z)$, R is the reflection coefficient, T is the transmission coefficient across the boundary plane and $\chi_0^2 = \frac{2m}{\hbar^2}(-V_0 - E_i)$ with V_0 as the potential at the surface which an electron encounters while transmitting through the boundary surface. Matching the wavefunction and its derivatives at z = 0 gives the value of coefficients R and T as

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

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

where $$\sigma = \frac{p}{k_i a}\psi(0)\frac{\sin k_i a}{\cos ka - \cos k_i a} \quad (9)$$

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

Also p is the strength of the $\hat{\partial}$ - potential barrier and it is assumed to be positive and μ is used as converging factor.

For W (100) surface state occurs [15] in the energy band gap $\left(\Delta_2 - \Delta_2'\right)$. The linear combination of atomic orbital (LCAO) representation for Δ_2' is $\frac{1}{3}\left(3z^2 - r^2\right)$, 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}. We have obtained the basis function for the C_{4v} point group corresponding to W (100) surface state by using projection operator formula [16]

$$\mathcal{P}^p_{mn} = \frac{l_p}{g}\sum_T \Gamma^p(T)^*_{mn} P(T) \quad (11)$$

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

Now introducing the atomic orbital $\Phi(z)$, which includes the

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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

$$\psi_i(z)=\begin{cases}\sigma\left[\Phi(z)e^{ik\,z}+R\Phi^{*}(z)e^{-ik\,z}\right], & bulk\ \&\ surface\ z\le 0\\ T\,e^{-\chi\,z}, & vacuum\ z\ge 0\end{cases} \qquad (12)$$

The initial state wavefunction given by Eq. (12) has been used in conjunction with final state wavefunction ψ_f given by Eq. (5) and vector potential $A_\omega(z)$ of Eq. (3), to calculate photofield emission current by using the formula given in Eq. (1). For calculation of *PFEC* with inclusion of ψ_i defined in Eq. (12) are evaluated by writing FORTRAN programme.

The description of the final state wavefunction $|\psi_f\rangle$ used is already given elsewhere [17].

4. Conclusion

Gao and Reifenberger [8] have given a detailed study of photofield emission from *W* but the theoretical interpretation was based on free electron concept. Keeping in mind that *W* is a strongly bonded metal and application of free electron model may not be appropriate, we have presented here a model for photofield emission calculation. This model has also been used by Thapa *et al* [18] in photoemission calculations and the results on metal and semiconductors showed qualitative agreement with the experimental results. However the point of difference with the model presented here is the dielectric model for the calculation of vector potential. With this vector potential, we intend to calculate photofield emission current in the strongly bonded metals like *W*, *Mo* etc. and compare the results with the other methods of calculations and the eperimental values as given by Gao *et al* [8].

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