Calculation of photofield emission current by using the projection operator method of group theory

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

1. Introduction

Photofield emission (PFE) is a technique in which a metal is irradiated by an incident laser radiation of photon energy. Photon energy is usually less than the work function of the metal under investigation. The incident radiation photoexcites 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 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 $\psi_i$ and final state wave function $\psi_f$. There are several methods of deducing the initial state wavefunction $\psi_i$ and the exactness of the model developed or used can correctly interpret the results in photofield emission calculations. 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.

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 [5-7] 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 calculation of photofield emission current by using the initial state wavefunction $\psi_i$ which is deduced by projection operator method of group theory. As an example, basis function was 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

2.1. Matrix element and transmission probability

We have considered a $p$-polarised radiation of photon energy $\omega$ 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 to final. 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

$$
\frac{dI_i}{dE} = -\frac{e^3}{2\hbar^2\omega} \frac{n}{\Omega} \langle \hat{\varepsilon} \cdot \hat{z} \rangle^2 f(E - \hbar\omega) \int_{-\omega, \omega} dW \frac{D(W) |M_f|^2}{[W(W - \hbar\omega)]^2}.
$$

(1)

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

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

$$
\int_{-d}^{0} \psi_f^* \frac{dA_s}{dz} \left( -\eta^2 \frac{d^2}{dz^2} \right) \psi_i dz + \int_{-d}^{0} \psi_f^* \frac{dA_s}{dz} \psi_i dz.
$$

(2)

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

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

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 $E$. $D(W)$ in Eq. (1) is obtained by solving [9]Airy’s differential equation and is given by

$$
D(W) = \left( \frac{W^2 - \sqrt{\pi} \left( \frac{2\eta \kappa_i}{\sqrt{\eta F}} \right)^2 \left( \sqrt{2m} \right)^{\frac{1}{3}} \exp \left[ -i \left( \frac{2 W^{\frac{2}{3}} \sqrt{2m}}{\eta F} + \frac{\pi}{4} \right) \right] \right)
$$

(4)

2.2. Dielectric Model and Vector Potential

In photofield emission, the dominant contribution to the photocurrent comes from the surface photo effect. As evidenced by several authors, for example, Levinson et al., [10] 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 $\omega$ but also on $z$-coordinate. Therefore, the vector potential for the surface region $(-d \leq z \leq 0)$ in one dimension is given by,

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

(5)

where

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

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

3. Description of Initial and Final state wave Functions

![Figure 1](image-url)  

**Figure 1**: Schematic representation of Kronig-Penney $\delta$-potential model for calculating the initial state wave function by using projection operator method of Group Theory.

To calculate the initial state wavefunction $\psi_i$, we have assumed the crystal potential of the solid which is defined by $\delta$ - 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 $\psi_i$ as

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

(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 $Z_0^2 = \frac{2m}{\hbar^2} (-V_0 - E_i)$ 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
$R = -\frac{\chi + \mu - ik}{\chi - \mu - ik}$ \hspace{1cm} (7)

and \( T = \sigma \left( \frac{-2ik}{-\chi - \mu - ik} \right) \) \hspace{1cm} (8)

where \( \sigma = \frac{P}{k_a} \psi(0) \frac{\sin k_a}{\cos k_a - \cos k_a} \) \hspace{1cm} (9)

and \( \psi(0) = -2iC \frac{\sin k_a}{1 + \cos k_a - i \sin k_a} \) \hspace{1cm} (10)

Also, \( p \) is the strength of the $\partial$- potential barrier and it is assumed to be positive and \( \mu \) is used as converging factor.

For \( W(100) \) surface state occurs [15] in the energy band gap \( \Delta_2 - \Delta_2' \). The linear combination of atomic orbital (LCAO) representation for \( \Delta_2' \) is \( \frac{1}{3} (3z^2 - r^2) \), where \( r^2 = x^2 + y^2 + z^2 \). We have, therefore, considered the point \( \Delta_2' \) 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]

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

Here \( l_p \) is the dimension of the unitary irreducible representation of the group \( G \), \( g \) is the 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

\[
\psi_i(z) = \begin{cases} \sigma \Phi(z)e^{ikz} + R \Phi^*(z)e^{-ikz}, & \text{bulk \& surface} z \leq 0 \\ T e^{-\chi z}, & \text{vacuum} z \geq 0 \end{cases}
\] \hspace{1cm} (12)

The initial state wavefunction given by Eq. (12) has been used in conjunction with final state wavefunction \( \psi_f \) given by Eq. (5) and vector potential \( A_y(z) \) of Eq. (3), to calculate photofield emission current by using the formula given in Eq. (1).

For calculation of \( PFEC \) with the inclusion of \( \psi_f \) defined in Eq. (12) are evaluated by writing FORTRAN programme.

The description of the final state wavefunction \( \psi_f \) used is already given elsewhere [17] as
Where,

$$k_j^2 = \frac{2mE_j}{\eta^2} - \frac{\rho^2}{\eta^2}; \quad q_j^2 = \frac{2m}{\eta^2}(E_j + V_j) - \frac{\rho^2}{\eta^2} \quad \text{and} \quad E_j = E_i + \eta\omega$$
Figure 4. Variation of matrix element $M_{fi}$ against photon energy ($\eta\Omega$).

Figure 5. Plot of variation of vector potential $|A_z|^2$ against photon energy ($\eta\Omega$).
4. Results and Discussions

We discuss here the photofield emission current \((PFEC)\) in the case of metal \(W\) as a function of initial state energy \((E_i)\), photon energy \((\hbar \omega)\) and the applied high static electric field \((F)\). We have also plotted the variation of \(A_i^2\) against photon energy \((\hbar \omega)\).

In Fig. 2, we show the plot of variation of photofield emission current \((PFEC)\) as a function of applied field for \(E_i = 2.1488 \text{ eV}, \ \theta_i = 45^0\) for three values of photon energies \(1.96 \text{ eV}, 2.70 \text{ eV}\) and \(3.54 \text{ eV}\). Here also, we find that the magnitude of \(PFEC\) is higher for low photon energies and decreases as photon energies increase. However, the variation in \(PFEC\) as applied field increases shows similar trends for all the three cases of photon energies. The decrease in \(PFEC\) is found to be exponential with the further decrease in the applied field.

We have also shown in Fig. 3, the variation of \(PFEC\) as a function of initial state energy of the electron with respect to Fermi level \((E_F)\) as a reference level. In this case, also, \(PFEC\) is plotted for the same three photon energies \(\eta \omega = 1.96 \text{ eV}, 2.70 \text{ eV}\), and \(3.54 \text{ eV}\), but for values of applied field \(F = 3.08 \times 10^{11} \text{ V/m}\) and \(\theta_i = 45^0\). In this case also, for low photon energies \(\eta \omega = 1.96 \text{ eV}\), the variation of \(PFEC\) is interesting. It showed a maximum in \(PFEC\) at \(E_i = 0.75 \text{ eV} \) below \(E_F\), and decreases with the value of \(E_i\) located further away from \(E_F\). For other values of photon energies, we find that the values of \(PFEC\) are very low in magnitude remaining constant without exhibiting any peaks.

Fig. 4 shows the plots of variation of matrix element \(M_{fi}\) against photon energy \((\eta \omega)\) for the value of applied field \(F = 3.08 \times 10^{11} \text{ V/m}, E_i = 2.1488 \text{ eV}\) below \(E_F\) and \(\theta_i = 45^0\). It is interesting to note here that as the values of photon energy of the incident radiation increases for low value, \(M_{fi}\) increases and showed a maximum at \(\eta \omega = 0.50 \text{ eV}\). Beyond \(\eta \omega = 0.50 \text{ eV}\), \(M_{fi}\) decreases and with
the further increase in \( \eta \phi \), it constantly showed a minima value. We have plotted \( M_{fi} \) only within very low photon energy values for \( \eta \phi \geq 0 \) to 3 eV.

The occurrence of origin of the peak in \( M_{fi} \) as shown in Fig. 4 can be understood from the plot of \( |A_z|^2 \) against \( \eta \phi \) as shown in Fig. 5. We find that \( |A_z|^2 \) slowly increases as \( \eta \phi \) is increased and showed a maximum at \( \eta \phi = 1.0 \) eV. With the further increase in \( \eta \phi \) beyond 1 eV, the value of \( |A_z|^2 \) decreased and a dip was shown at \( \eta \phi \sim 1.25 \) eV. The second hump of small height in \( |A_z|^2 \) was observed at \( \eta \phi \sim 1.5 \) eV. We can attribute the occurrence of maxima in \( M_{fi} \) at \( \eta \phi = 0.5 \) eV due to the occurrence of maxima in \( |A_z|^2 \) at \( \eta \phi = 0.5 \) eV, although the shift in \( \eta \phi \) is about 0.5 eV in the occurrence of maxima in \( M_{fi} \) and \( |A_z|^2 \).

In Fig. 6, the plot of \( PFEC \) as a function of photon energy is shown for values of applied field \( F = 3.08 \times 10^{11} \) V/m, \( E_i = 2.1488 \) eV and \( \theta_i = 45^0 \). We find that \( PFEC \) showed an exponential decrease with the decrease in applied field (Fig 2). It had shown high order magnitude in \( PFEC \) for low photon energies which is due to the occurrence of photon frequency in the formula of \( PFEC \) (Eq.1) where it varied inversely with frequency. The exponential decrease in \( PFEC \) is due to the presence of exponential term which is a predominant factor in photofield emission. This fact had been already seen also in the case of field emission [15]. However, in field emission due to dominant characteristics of the exponential term, usually a term called \( R \) factor is plotted which in fact nullifies the effect of an exponential factor to field emission current calculated.

We have also seen the effect of the variation of \( |A_z|^2 \) as a function of photon energies which in fact contribute to the values of the matrix element \( M_{fi} \). Thus, we find that matrix element \( M_{fi} \) is not a constant factor when checked with the variation of \( \eta \phi \). The change in \( M_{fi} \) in fact contributes to the photofield emission current. This is contradicting the report of Lee and Schaich[19] where it was observed that \( M_{fi} \) when plotted against \( \eta \phi \) remained constant. From our computations, we find therefore that calculation of the matrix element \( M_{fi} \) is equally important in photofield emission and its evaluation must be considered in details.

Just like in the case of free electron model, we find that the plot of photofield emission current as a function of initial state energy showed similar features. The peak height in \( PFEC \) is too low for higher photon energies. This implied that only at low photon energy, photofield effect is prominent.

5. Results and Discussions

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 experimental values as given by Gao et al[8].
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