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PHOTOFIELD EMISSION CALCULATIONS BY USING PROJECTION OPERATOR METHOD

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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.

Keywords: Photofield emission; vector potential; projection operator.

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1. Introduction

Photofield emission (PFE) is a technique 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 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 electrons to tunnel through the surface potential barrier into the vacuum region which then constitutes the photofield emission current (PFEC). In photofield emission, in addition to transmission probability $D(W)$, the transition matrix element $\langle\psi_f|A\cdot p + P\cdot A|\psi_i\rangle$ 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 wavefunction ψ_i and the exactness of the model developed or used can hence 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 calculations 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 been 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 emissions.

In this report, we are presenting a model calculation of photofield emission current by using the initial state wave function ψ_i which is deduced by projection operator method of group theory. As an example, basis functions were derived for W (100) surface states. The vector potential A will be the one deduced by Thapa *et al.*[8]

2. Theoretical Formalism

A p-polarized radiation of photon energy $\hbar\omega$ 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, 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 written[9] as

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

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 the 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 the z-axis is given by

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

$$+\int_{-d}^{0}\psi_f^*\frac{dA_\omega^z(z)}{dz}\left(-\hbar^2\frac{d^2}{dz^2}\right)\psi_i dz + \int_{-d}^{0}\psi_f^*\frac{dA_\omega^z(z)}{dz}\psi_i dz\,. \tag{2}$$

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

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

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

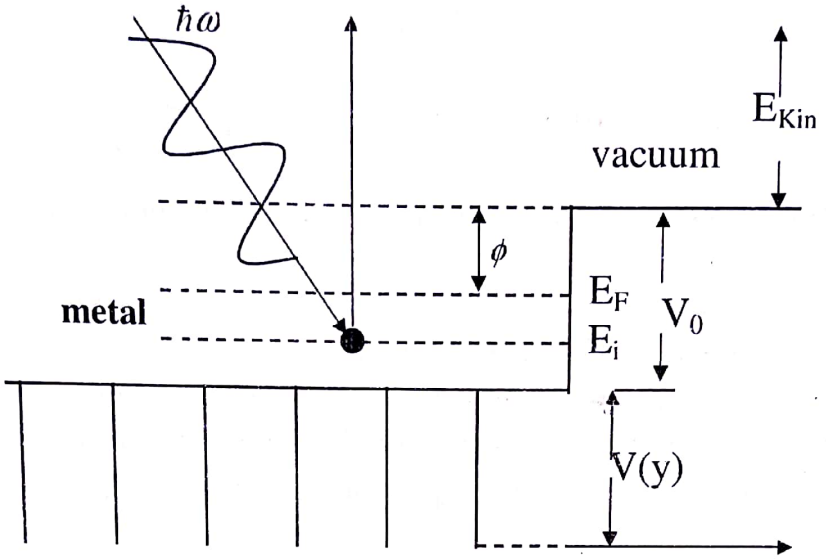

Fig. 1. Schematic representation of Kronig Penney δ-potential model for calculating the initial state wave function.

of energy E. $D(W)$ used in Eq. (1) is obtained by solving[10] the 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. Description of Initial and Final State Wavefunctions

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 Fig. 1. In one dimension, one can write ψ_i as

$$\psi_i(z) = \begin{cases} \psi(z) + R\psi^*(z) & z \leq 0 \text{ (bulk and surface)} \\ Te^{-\chi z} & z \geq 0 \text{ (vacuum)} \end{cases} \tag{5}$$

where $\psi^*(z)$ is the complex conjugate of $\psi(z)$, R is the reflection coefficient, 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

$$R = \frac{-\chi + \mu - ik}{\chi - \mu - ik} \tag{6}$$

and

$$T = \sigma\left(\frac{-2ik}{-\chi - \mu - ik}\right) \tag{7}$$

where

$$\sigma = \frac{p}{k_i a}\psi(0)\frac{\sin k_i a}{\cos ka - \cos k_i a} \tag{8}$$

and

$$\psi(0) = -2iC\frac{\sin k_i a}{1 + \cos k_i a - i \sin k_i a}\,. \tag{9}$$

In the above equations, p is the strength of the δ-potential barrier and is assumed to be positive, and μ is used as the converging factor.

For $W(100)$, surface state occurs[11] in the energy band gap $(\Delta_2 - \Delta_2')$. The linear combination of atomic orbital (LCAO) representation for Δ_2' is $\frac{1}{3}(3z^2 - r^2)$, 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 formula[12]

$$P^p_{mn} = \frac{l_p}{g}\sum_T \Gamma^p(T)^*_{mn} P(T)\,. \tag{10}$$

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. (10), the final form of the initial state wavefunction can be represented by

$$\psi_i(z) = \begin{cases} \sigma[\Phi(z)e^{ikz} + R\Phi^*(z)e^{-ikz}] & z \le 0\,, \\ Te^{-\chi z} & z \ge 0\,. \end{cases} \tag{11}$$

The description of the final state wavefunction ψ_f is already given elsewhere.[13]

4. Dielectric Model and Calculations of Vector Potential

We consider the metal to occupy all space to the left of $z = 0$ plane. The model dielectric function (Fig. 2) for the bulk ($z \le -d$), surface ($-d \le z \le 0$) and vacuum

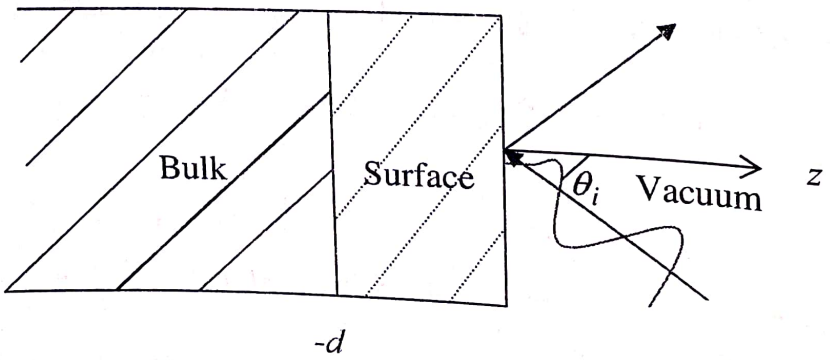

Fig. 2. Schematic diagram of model for dielectric

$(z \geq 0)$ is given by

$$\varepsilon(\omega, z) = \begin{cases} \varepsilon_b(\omega) & z \leq -d \\ 1 + \dfrac{(\varepsilon_b - 1)}{\log_e 2} \log_e \left(1 - \dfrac{z}{d}\right) & -d \leq z \leq 0 \\ 1 & z \geq 0 \end{cases} \tag{12}$$

where $\varepsilon_b(\omega) \cong \varepsilon_1(\omega) + i\varepsilon_2(\omega)$ is the bulk dielectric function. For p-polarized light, $B(z) = B(\mathbf{K}, \omega, z)$ (where $\mathbf{K} = \frac{\omega}{c} \sin\theta_i$ is small) and it obeys the equation

$$\frac{\partial}{\partial z}\left(\frac{1}{\varepsilon}\frac{\partial B}{\partial z}\right) + \left(\frac{\omega^2}{c^2} - \frac{K^2}{\varepsilon}\right) B = 0 . \tag{13}$$

To solve the above equation, we follow the prescription of Landau and Lifshitz where $B = u(z)\sqrt{\varepsilon(z)}$, so that

$$\frac{d^2u}{dz^2} + k^2(\varepsilon - \sin^2\theta_i)u + \left(\frac{1}{2\varepsilon}\frac{d^2\varepsilon}{dz^2} - \frac{3}{4}\frac{1}{\varepsilon^2}\left(\frac{d\varepsilon}{dz}\right)^2\right) u = 0 . \tag{14}$$

In the surface region,

$$\frac{d\varepsilon}{dz} = \frac{\varepsilon_b - 1}{(z-d)} \frac{1}{\left[\log_e 2 + (\varepsilon_b - 1)\log_e\left(1 - \dfrac{z}{d}\right)\right]}$$

and

$$\frac{d^2\varepsilon}{dz^2} = \frac{-(\varepsilon_b - 1)}{\log_e 2} \frac{1}{(z-d)^2} .$$

As

$$\left[\frac{1}{2\varepsilon}\frac{d^2\varepsilon}{dz^2} - \frac{3}{4}\left(\frac{1}{\varepsilon}\frac{d\varepsilon}{dz}\right)^2\right] \ll k^2(\varepsilon - \sin^2\theta_i) ,$$

hence Eq. (3) for the surface region becomes,

$$\frac{d^2u}{dz^2} + (az + b)u = 0 \tag{15}$$

where $a = \frac{k^2}{d\log_e 2}(1 - \varepsilon_b)$ and $b = \frac{k^2}{2}$. Thus the solution of Eq. (15) is $u(z) = A_i(\xi) + B_i(\xi)$ where $\xi = \frac{-(az+b)}{a^{\frac{2}{3}}}$ and $A_i(\xi)$ and $B_i(\xi)$ are Airy functions[8] given by

$$A_i(\xi) = \left[3^{\frac{2}{3}}\Gamma\left(\frac{2}{3}\right)\right]^{-1}(1 + \sqrt{3})\left(1 + \frac{1}{3!}\xi^3 + \cdots\right)$$

$$B_i(\xi) = \left[3^{\frac{1}{3}}\Gamma\left(\frac{1}{3}\right)\right]^{-1}(\sqrt{3} - 1)\left(\xi + \frac{2}{4!}\xi^4 + \cdots\right) .$$

Absorbing the numerical coefficients and neglecting higher terms, we write the solution in the surface region as

$$u(z) = A_2\left(1 + \frac{1}{3!}\xi^3\right) + B_2\left(\xi + \frac{2}{4!}\xi^4\right) . \tag{16}$$

As $B(z) = u(z)\sqrt{\varepsilon(z)}$, and using the boundary conditions that B and $\frac{\partial B}{\partial z}$ are continuous at $z = 0$ and $z = -d$, we obtain

$$B(z) = \begin{cases} \left(e^{-ik\cos\theta_i \cdot z} + ye^{ik\cos\theta_i \cdot z}\right) & \text{(vacuum)} \\ p\left[\left(1 + \frac{\xi^3}{6}\right) + x\left(\xi + \frac{\xi^2}{12}\right)\right](\varepsilon)^{\frac{1}{2}} & \text{(surface)} \\ pq\sqrt{\varepsilon_b}e^{-ik\sqrt{\varepsilon_b - \sin^2\theta_i}\cdot z} & \text{(bulk)}. \end{cases} \tag{17}$$

The electric field components can be obtained from the magnetic field by using the relation

$$E^x(\mathbf{K}, \omega, z) = \frac{c}{i\omega\varepsilon}\frac{dB}{dz}$$

$$E^z(\mathbf{K}, \omega, z) = -\frac{\sin\theta_i}{\varepsilon}B\,.$$

Thus, we can write in the long wavelength limit ($\frac{\omega d}{c} \to 0$) the vector potential for the surface region $-d \le z \le 0$ as

$$\tilde{A}_\omega(z) = \frac{A^z_\omega(z)}{A_0} = \frac{E^z(\vec{K} \to 0, \omega, z)}{E_0} = \left\{\frac{-\sin\theta_i}{\sqrt{\varepsilon}}p\left[1 + \frac{\xi^3}{6} + x\left(\xi + \frac{\xi^4}{12}\right)\right]\right\}, \tag{18}$$

where

$$p = \frac{y+1}{1 + \frac{\eta^3}{6} + x\left(\eta + \frac{\eta^4}{12}\right)}, \qquad q = \frac{1 + \frac{\gamma^3}{6} + x\left(\gamma + \frac{\gamma^4}{12}\right)}{\sqrt{\varepsilon_b}e^{\lambda d}},$$

$$x = \frac{a^{\frac{1}{3}}\sqrt{\varepsilon_b}\gamma^2 + \left(\beta - \sqrt{\varepsilon_b}\lambda\right)\left(1 + \frac{\gamma^3}{6}\right)}{\left(\sqrt{\varepsilon_b}\lambda - \beta\right)\left(\gamma + \frac{\gamma^4}{12}\right) - \sqrt{\varepsilon_b}a^{\frac{1}{3}}\left(1 + \frac{\gamma^3}{3}\right)},$$

$$y = \frac{ik\cos\theta_i\left(1 + \frac{\eta^3}{6} + x\left(\eta + \frac{\eta^4}{12}\right)\right) - \left(\frac{a^{\frac{1}{3}}}{2}\eta^2 + \rho\left(1 + \frac{\eta^3}{6}\right)\right) + x\left(a^{\frac{1}{3}} + a^{\frac{1}{3}}\frac{\eta^3}{3} + \rho\left(\eta + \frac{\eta^4}{12}\right)\right)}{\frac{a^{\frac{1}{3}}}{2}\eta^2 + \rho\left(1 + \frac{\eta^3}{6}\right) + x\left(a^{\frac{1}{3}} + a^{\frac{1}{3}}\frac{\eta^3}{3} + \rho\left(\eta + \frac{\eta^4}{12}\right)\right) + ik\cos\theta_i\left(1 + \frac{\eta^3}{6} + x\left(\eta + \frac{\eta^4}{12}\right)\right)} \tag{19}$$

$$\lambda = ik\sqrt{\varepsilon_b - \sin^2\theta_i}. \qquad \beta = \frac{\varepsilon_b - 1}{4d\sqrt{\varepsilon_b}\log_e 2}, \qquad \gamma = \frac{ad - b}{a^{\frac{2}{3}}},$$

$$\eta = \frac{-b}{a^{\frac{2}{3}}}, \qquad \text{and} \qquad \rho = \frac{\varepsilon_b - 1}{2d\log_e 2}.$$

5. Conclusion

Gao and Reifenberger[9] have given a detailed study of photofield emission from W but the theoretical interpretation was based on the 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 had also been used by Thapa *et al.*[8] 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.*[9]

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References

1. J. B. Pendry, *Low Energy Electron Diffraction* (Academic Press, London, 1974).
2. J. B. Pendry, *Surf. Sci.* **57** (1976) 679.
3. A. Bagchi, *Phys. Rev. B* **10** (1974) 542.
4. A. Modinos, *J. Phys. C: Solid State Phys.* **9** (1976) 3867.
5. A. Ernst, J. Henk and R. K. Thapa, *J. Phys. Condens. Mat.* **17** (2005) 5269.
6. P. J. Durham, *J. Phys. F* **11** (1981) 2475.
7. M. J. Haggmann, *Int. J. Quantum Chemistry* **65** (1997) 857.
8. R. K. Thapa, S. R. Gurung, G. Das and R. Bhattacharjee, *Indian J. Phys.* **80** (2006) 361.
9. Y. Gao and R. Reifenberger, *Phys. Rev.* **35** (1987); *ibid.* **35** (1987) 8301.
10. G. Das, A theoretical study of photofield emission from metals incorporating the spatially dependent photon fields, Ph.D. Thesis, Assam University (2005).
11. E. Bertel, *Phys. Rev. B* **50** (1994) 4925.
12. J. F. Cornwell, *Group Theory and Electronic Energy Band in Solids* (North Holland, 1969), p. 54.
13. R. K. Thapa and G. Das, *Int. J. Mod. Phys.* **19** (2005) 3141.