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Photoemission study from Si and GaAs using a spatially varying vector potential

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Abstract

Photoemission calculations in the case of semiconductors like gallium arsenide (GaAs) and silicon (Si) using a spatially dependent vector potential is presented here. The logarthmic dielectric model of Gurung and Thapa is used for the calculation of vector potential. The vector potential thus developed is used for the calculation of photocurrent for which Kronig-Penney potential has been used to define the crystal potential from which the initial state wave-function for the surface state is derived.

Key words: Photoemission; photocurrent; vector potential; dielectric function.

Introduction

Photoemission from a metal, in which an electron is excited by an incident photon and escapes to the vacuum by overcoming the surface potential barrier is well established as a technique for studying the electronic states of solids. Many methods of photoemission calculation have been developed where wave function for the semi-infinite solids are constructed accurately.[1] However, in these calculations, the spatial variation of the photon field has been generally neglected. An accurate calculation of the electromagnetic field in the surface of a solid is a complex problem and first principle calculations are available only for jellium model.[2] On the other hand, empirical calculations of fields near the surface with 'local' dielectric function have been used to explain certain qualitative features of photoemission data. Bagchi and Kar have developed a dielectric model to deduce vector potential using a simple 'local' dielectric function and applied the same to study photoemission from tungsten.[3] This model had been used by Thapa *et al.* in explaining the surface photoemission from metals like aluminium,[4,5] palladium,[6] copper and molybdenum[7] and semiconductors like silicon[8,9] and gallium arsenide.[9]

In this report, photoemission calculations from semiconductors Si and GaAs using the dielectric model is presented as proposed by Gurung and Thapa.[10]

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FORMALISM

The Golden rule formula[11] for calculating photocurrent density can be written as

$$\frac{dj(E)}{d\Omega} = \frac{2\pi}{\hbar}\sum_{f,i}\left|\langle\psi_f|H'|\psi_i\rangle\right|^2\delta\left(E_f - E_i - \hbar\omega\right) \times f_o(E-\hbar\omega)\left[1-f_o(E)\right] \quad (1)$$

where ψ_i and ψ_f are the initial and final state wave-functions and

$$H' = \left(\frac{e}{2mc}\right)(\boldsymbol{A}\cdot\boldsymbol{p} + \boldsymbol{p}.\boldsymbol{A})$$

is the perturbing Hamiltonian, $\boldsymbol{A}$ being the vector potential of the photon field and $\boldsymbol{p}$ the one electron momentum operator. To evaluate the matrix element, we have to evaluate $\boldsymbol{A}$ and construct ψ_i and ψ_f.

DIELECTRIC MODEL AND VECTOR POTENTIAL

We consider the solid to occupy all space to the left of $z = 0$ plane with surface parallel to the x-y plane and assume the surface region to extend from $z = 0$ to $z = -d$ such that the surface thickness is d.

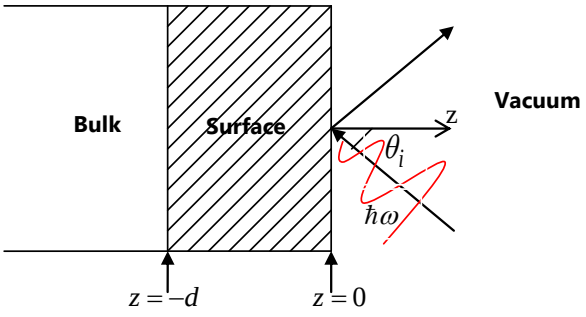

Figure 1. Diagram for model dielectric function.

The model dielectric function[10] for the bulk ($z \le -d$), surface ($-d \le z \le 0$) and vacuum ($z \ge 0$) is given by,

$$\varepsilon(\omega,z) = \begin{cases} \varepsilon_b(\omega) & ;\ z \le -d \\ 1 + \dfrac{(\varepsilon_b - 1)}{\log_e 2}\log_e\left(1 - \frac{z}{d}\right) & ;\ -d \le z \le 0 \\ 1 & ;\ z \ge 0 \end{cases} \quad (2)$$

where $\varepsilon_b(\omega) \cong \varepsilon_1(\omega) + i\varepsilon_2(\omega)$ is the bulk dielectric function. For a p-polarized light, the magnetic field $B(z) = B(\boldsymbol{K},\omega,z)$, where $\boldsymbol{K} = \frac{\omega}{c}Sin\theta_i$ is in the y-direction and it obeys the following equation[12]

$$\frac{\partial}{\partial z}\left(\frac{1}{\varepsilon}\frac{\partial B}{\partial z}\right) + \left(\frac{\omega^2}{c^2} - \frac{K^2}{\varepsilon}\right)B = 0 \quad (3)$$

To solve the above equation, we follow the prescription of Landau and Lifsitz[12] and use $\boldsymbol{B} = u(z)\sqrt{\boldsymbol{\varepsilon}(z)}$, so that Eq. (3) becomes,

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

Using Eq. (2) and the boundary conditions that B and $\frac{\partial B}{\partial z}$ are continuous at $z = 0$ and $z = -d$, we obtain the magnetic field components for the three regions as

$$B(z) = \begin{cases} \left(e^{-ik\cos\theta_i\cdot z} + ye^{ik\cos\theta_i\cdot z}\right) & ;\ (vacuum) \\ p\left[\left(1 + \dfrac{\xi^3}{6}\right) + x\left(\xi + \dfrac{\xi^2}{12}\right)\right](\varepsilon)^{\frac{1}{2}} & ;\ (surface) \\ pq\sqrt{\varepsilon_b}e^{-ik\sqrt{\varepsilon_b - \sin^2\theta_i}\cdot z} & ;\ (bulk) \end{cases} \quad (5)$$

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

$$E^x(\boldsymbol{K},\omega,z) = \frac{c}{i\omega\varepsilon}\frac{dB}{dz} \text{ and } E^z(\boldsymbol{K},\omega,z) = -\frac{Sin\theta_i}{\varepsilon}B$$

Thus, the vector potential in three regions are

$$\tilde{A}_\omega(z)=\frac{A_\omega^z(z)}{A_o}=\frac{E^z(\boldsymbol{K}\to 0,\omega,z)}{E_o}$$

$$=\begin{cases}-\sin\theta_i\left[e^{-ik\cos\theta_i z}+ye^{ik\cos\theta_i z}\right], & (vacuum)\\ \dfrac{-\sin\theta_i}{\sqrt{\varepsilon}}p\left[1+\dfrac{\xi^3}{6}+x\left(\xi+\dfrac{\xi^4}{12}\right)\right], & (surface)\\ \dfrac{-\sin\theta_i}{\sqrt{\varepsilon_b}}pqe^{-ik\sqrt{\varepsilon_b-\sin^2\theta_i}\cdot z}, & (bulk)\end{cases} \quad (6)$$

Various parameters in Eq. (6) are defined as

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

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

$$y=\frac{ik\cos\theta_i\left(\sigma+x\phi\right)-\left[\dfrac{a^{\frac{1}{3}}}{2}\eta^2+\rho\sigma\right]+x\mu}{\dfrac{a^{\frac{1}{3}}}{2}\eta^2+\rho\sigma+x\mu+ik\cos\theta_i\left(\sigma+x\phi\right)} \quad (7)$$

where ϕ,μ,λ,β, etc. in Eq. (7) are given by,

$$\sigma=1+\frac{\eta^3}{6},\ \phi=\eta+\frac{\eta^4}{12},\ \mu=a^{\frac{1}{3}}\left(1+\frac{\eta^3}{3}\right)+\rho\phi$$

$$\lambda=ik\sqrt{\varepsilon_b-\sin^2\theta_i},\ \beta=\frac{\varepsilon_b-1}{4d\sqrt{\varepsilon_b}\log_e 2},$$

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

Matrix Element

Matrix element in Eq. (1) for transition from initial to final state can be written in expanded form as

$$\left\langle\psi_f\left|H'\right|\psi_i\right\rangle$$
$$=\int_{vac}\psi_f^*H'\psi_i d^3r+\int_{surf}\psi_f^*H'\psi_i d^3r+\int_{bulk}\psi_f^*H'\psi_i d^3r \quad (8)$$

where in each region, the wave functions and the vector potentials corresponding to that region have to be used. The final state wave function (ψ_f) is taken to be free electron type[13], given by the following expression

$$\psi_f(z)=\begin{cases}\left(\dfrac{m}{2\pi\hbar^2\mu}\right)^{\frac{1}{2}}\dfrac{2\mu}{\mu+k_f}e^{-\alpha|z|}e^{ik_f z}\ ;\ (z\le 0)\\ \left(\dfrac{m}{2\pi\hbar^2\mu}\right)^{\frac{1}{2}}\left[e^{i\mu z}+\dfrac{\mu-k_f}{\mu+k_f}e^{-i\mu z}\right];(z\ge 0)\end{cases} \quad (9)$$

where, $k_i^2=\frac{2m}{\hbar^2}E_i$, $k_f^2=\frac{2m}{\hbar^2}E_f$, $E_f=E_i+\hbar\omega$ and $\mu^2=\frac{2m}{\hbar^2}\left(E_f-Vo\right)$. Here, the factor $e^{-\alpha|z|}$ is introduced for the region $z\le 0$ to take into account the inelastic scattering of the electron.[14]

Deduction of Initial State Wave Functions

To deduce the initial state wave function (ψ_i) in Kronig Penney potential,[15] one generally solves the one dimensional Schrodinger's equation which can be written as

$$\frac{d^2\psi(z)}{dz^2}+k_i^2\psi(z)=-2V(z)\psi(z) \quad (10)$$

where $k_i^2=\frac{2mE}{\hbar^2}$

and $V(z)$ is the δ-function potential of the Kronig-Penney model. Let $\phi(z)$ denote the Bloch wave function deep in the metal and $\phi^*(z)$ the time reversal version of $\phi(z)$. The eigenfunction in the semi-infinite solid ($z<0$) has been chosen to have the form

$$\psi_i(z) = \phi(z) - P\phi^*(z) \quad (11)$$

where P is the reflection coefficient obtained by matching the wave functions and its derivative at $z = 0$. One can then show that the initial state wave function for $z < 0$ may be written as

$$\psi_i(z) = (1 - iPe^{-i\delta}\sin\delta)e^{ik_i(z)} - (P - ie^{i\delta}\sin\delta)e^{-ik_i(z)} \quad (12)$$

where $\cot\delta = -\frac{\hbar^2 k_i}{mg}$ with g being the strength of the potential. The initial state wavefunction outside the metal ($z < 0$) is

$$\psi_i(z) = Te^{-\chi z} \quad (13)$$

where, T is the transmission coefficient across the boundary plane and $\chi^2 = 2(V_0 - E)$ with V_0 being the step potential at the surface. By matching the wave function and its derivative at $z < 0$, we get

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

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

Thus, the initial state wavefunction can be written as

$$\psi_i(z) = \begin{cases} \left(1 - iPe^{-i\delta}\sin\delta\right)e^{ik_i z}\left(P - ie^{i\delta}\sin\delta\right)e^{-ik_i z} & (z \le 0) \\ Te^{-\chi z} & (z \ge 0) \end{cases} \quad (14)$$

Using the expressions of ψ_f and ψ_i (Eqs. 9 and 14) and the vector potential as given by Eq. (6), the matrix element in Eq. (8) can be evaluated for each region to calculate photocurrent.

Results and Discussion

Figure 2 depicts the plot of photocurrent in the case of Si as a function of photon energy. As can be seen from the figure, the photocurrent plot shows a maximum at around 16eV followed by a minimum at around 17eV, the plasmon energy of Si. A second maximum in the photocurrent is obtained at about 18.5 eV, beyond which the photocurrent decreases with increase in photon energy.

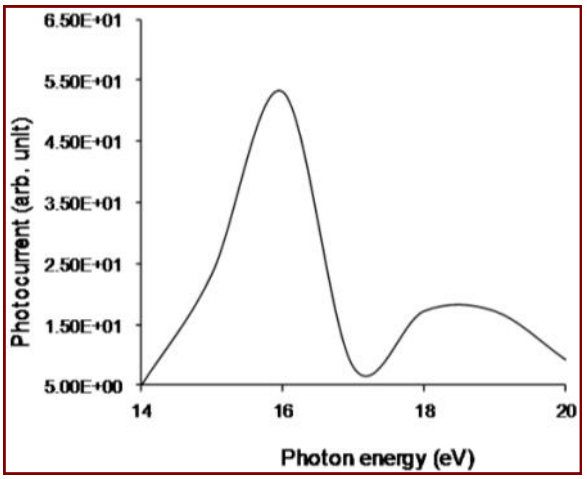

Figure 2. Plot of Photocurrent as a function of Photon energy for Si.

Figure 3 shows the photocurrent plot of GaAs as a function of photon energy. In this case also, we see similar trend with a peak around 13 eV followed by a minimum around 15 eV, the plasmon energy of GaAs along with a peak of lower height around 15.5 eV. The gen-

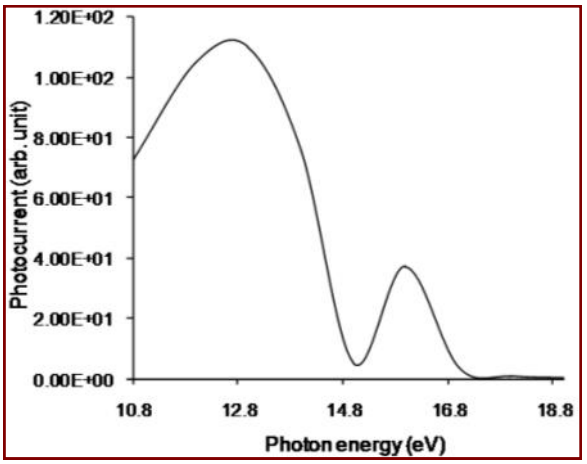

Figure 3. Plot of Photocurrent as a function of Photon energy for GaAs.

eral nature of the photocurrent plot agrees well with those of other metals like Al and Be,[10] W[16] and also semiconductors Si[8] and GaAs.[9] The present calculation shows better agreement as far as the location of minimum in the photocurrent plot at the Plasmon energy is concerned than earlier calculations.[8,9]

CONCLUSION

The location of minimum at the plasmon energy along with peaks before and after it in the case of both Si and GaAs show that the dielectric model being employed in the calculation of vector potential can be used in the study of photoemission from semiconductors also. I wish to test the model for other semiconductors also which will be reported later.

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