International Journal of Engineering Technology Science and Research
IJETSR
www.ijetsr.com
ISSN 2394 – 3386
Volume 2 Issue 8
August 2015

Calculations of Photocurrent from Semiconductors

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Abstract: *Photocurrent calculations from semiconductors are done using initial state wavefunction deduced by Green function. To define the crystal potential Kronig Penny model is used and a spatially dependent vector potential is used in the calculation. Photocurrents are calculated from GaAs and PbS.*

Keywords : Photocurrent, Photoemission, Kronig Penny model, semiconductors

1. INTRODUCTION:

The photocurrent density formula given by Fermi Golden rule [1] directly involved the evaluation of the matrix element $\langle \psi_f | H' | \psi_i \rangle$ In this model the initial state wavefunction is deduced by solving Schrodinger equation using Green function [2]. Spatially dependent vector potential is incorporated in the calculation which is a modified form of the dielectric model used by Bagchi and Kar [3]. To define the crystal potential Kronig Penny model is used. For the surface state photoemission, the initial state wavefunction ψ_i is described by the normalized Gaussian state wavefunction. The model is applied to semiconductors GaAs and PbS.

2. FORMALISM:

The photocurrent density formula from golden rule[1] approximation can be written as

$$\frac{dj(E)}{d\Omega} = \frac{2\pi}{\hbar} \sum |< \psi_f | H' | \psi_i >|^2 \, \delta(E - E_f) \delta(E_f - E_i - \hbar\omega) f_o(E - \hbar\omega)[1 - f_o(E)] \qquad (1)$$

where $\psi_i (\psi_f)$ refer to the initial (final) state wavefunctions and the perturbation H' can be written as

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

where *m* is the mass of the electron, ***p*** the one-electron momentum operator and ***A*** the vector potential of the incident photon field.

The photon field vector formulae used in our calculations is obtained by using the dielectric model of Bagchi and Kar[2]. With simple modifications, we can write the photon field vector as

$$\tilde{A}_\omega(z) = \begin{cases} A_1 , & z \le -a \quad (Bulk) \\ \dfrac{A_1 a \, \varepsilon(\omega)}{[1 - \varepsilon(\omega)] z + a} , & -a \le z \le 0 \quad (Surface) \\ A_1 \varepsilon(\omega) , & z \ge 0 \quad (Vacuum) \end{cases} \qquad (3)$$

where $A_1 = - \dfrac{\sin 2\theta_i}{[\varepsilon(\omega) - \sin^2 \theta_i]^{1/2} + \varepsilon(\omega) \cos\theta_i}$ is a constant depending on the dielectric function $\varepsilon(\omega)$, photon energy $\hbar\omega$ and angle of incidence θ_i.

The initial state wavefunction deduced by using Green's function method is given by

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$$\psi_i(z)=\begin{cases}\dfrac{-4\pi pC\sin^2 k_i a}{k_i a\left(k_i\cos k_i a+k_i-\chi\sin k_i a\right)\left(1+e^{-ik_i a}\right)\left(1+\cos k_i a\right)}\left\{k_i\cos k_i z-\chi\sin k_i z\right\}e^{-\mu z} & z<0\\ \dfrac{-4\pi pC\sin^2 k_i a}{k_i a\left(k_i\cos k_i a+k_i-\chi\sin k_i a\right)\left(1+e^{-ik_i a}\right)\left(1+\cos k_i a\right)}k_i e^{-\chi z} & z>0\end{cases} \quad (4)$$

where $C=\left(\dfrac{m_e}{2\pi k_i}\right)^{1/2}$, $k=\pm\dfrac{\pi}{a}$, $k_i^2=\dfrac{2mE_i}{\hbar^2}$, $\chi^2=\dfrac{2m}{\hbar^2}(V_o-E_i)$, $\mu=k_i-\pi/d$.

In equation (4), for the surface state photoemission calculations, $\psi_i(z)$ is replaced by a properly normalized Gaussian form of the wavefunction located at $z = z_o$ plane and is given by

$$\Psi_i(z)=\left(2\beta/\pi a^2\right)^{1/4}\exp\left[-\beta(z-zo)^2/a^2\right] \quad (5)$$

where β describes the width of the Gaussian and is a dimensionless quantity, a is the surface width.

The final state wavefunction ψ_f is the scattering state due to the existence of a step potential at the surface plane $z = 0$. This potential is defined by $V(z)=-V_o\theta(z)$, where $\theta(z)$ is a unit function. Therefore ψ_f is given by

$$\psi_f(z)=\begin{cases}\left(\dfrac{m}{2\pi\hbar^2 k_f}\right)^{\frac{1}{2}}\dfrac{2k_f}{q_f+k_f}e^{ik_f z}e^{-\alpha|z|}, & z<0 \quad (bulk\ \&\ surface)\\ \left(\dfrac{m}{2\pi\hbar^2 k_f}\right)^{\frac{1}{2}}\left(e^{ik_f z}+\dfrac{k_f-q_f}{q_f+k_f}e^{-ik_f z}\right), & z>0 \quad (vacuum)\end{cases} \quad (6)$$

where $k_f^2=\dfrac{2mE_f}{\hbar^2}$ and $q^2=\dfrac{2m}{\hbar^2}(E_f-V_0)$ and $E_f=E_i+\hbar\omega$. The factor $e^{-\alpha|z|}$ is included on the bulk to take into account the inelastic scattering of the electrons. The photocurrent was calculated by evaluating the matrix element in equation (1) and by using the above wavefunctions in equations. (4), (5) and (6).

The matrix element when expanded is given by

$$I=\left\langle\psi_f\left|\tilde{A}_\omega(z)\frac{d}{dz}+\frac{1}{2}\frac{d}{dz}\tilde{A}_\omega(z)\right|\psi_i\right\rangle$$

$$=\int_{-\infty}^{-a}\psi_f^*\tilde{A}_\omega\psi_i dz+\int_{-a}^{0}\psi_f^*\tilde{A}_\omega\frac{d\psi_i}{dz}dz+\frac{1}{2}\int_{-a}^{0}\psi_f^*\frac{d\tilde{A}_\omega}{dz}\psi_i dz+\int_{0}^{\infty}\psi_f^*\tilde{A}_\omega\frac{d\psi_i}{dz}dz. \quad (7)$$

Some of the matrix element could not be solved analytically, hence FORTRAN programs were written to solve it. Using the above model, photocurrents were calculated for GaAs and PbS.

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3. RESULTS AND DISCUSSIONS:

We have applied the model developed to calculate photocurrent from semiconductors *GaAs*and *PbS*.

Photocurrent was calculated as a function of photon energy $\hbar\omega$ for the location of the initial state wavefunction ψ_i at different values of z_o and for the same values of the surface width given by $a = 5.29\,\text{Å}$.Width of the Gaussian form of wavefunction is taken to be 1. i.e. $\beta = 1$

In Figure 1, a graph of photocurrent against photon energy is plotted for semiconductor *GaAs* for values of z_o = 0, - 2.645 and – 5.29Å. We have taken the height of the step potential V_0 = 15 eV and the initial state energy E_i = 0.3 eV below the Fermi level. In this figure, we find that for z_o= - 2.645 Å, as the photon energy $\hbar\omega$ is increased, photocurrent increases till a maximum is obtained at $\hbar\omega$ =11 eV and then starts decreasing until a minimum occurs at $\hbar\omega$ =15 eV. This value of the plasmon energy is in good agreement with experimental data obtained by Manzke [4]. This result is also in good agreement with the theoretical result of Thapa and Kar [5]. Such kind of a graph is not observed for the other locations of the initial state wavefunction ψ_i, that is, at z_o = 0 and – 5.29 Å.

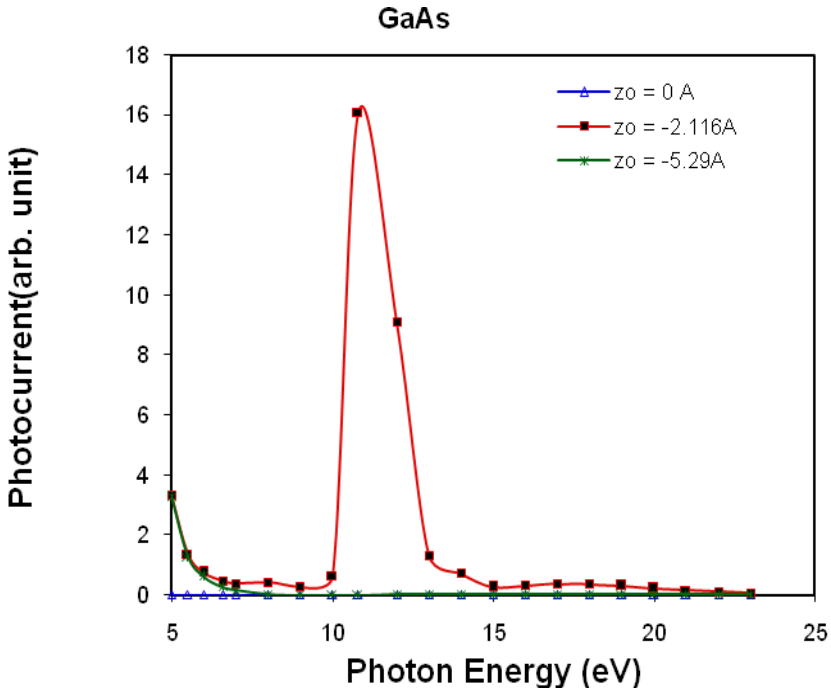

Figure 1: Plot of photocurrent variation against photon energy $\hbar\omega$ for GaAs at three different locations of the initial state

Figure 2 shows variation of photocurrent against photon energy ($\hbar\omega$) for three different locations of the initial state wavefunction namely z_o = 0, - 2.116 and – 5.29 Å for *PbS*. Here also the height of the step potential $V_0$is taken to be 15 eV and the initial state energy E_i = 0.3 eV below the Fermi level. We find that for the location of the initial state wavefunction at the surface region, that is at z_o = - 2.116 Å, with the increase in the photon energy, the photocurrent increases and a peak is observed at photon energy $\hbar\omega$ = 7 eV and

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further increase in photon energy shows a decrease in photocurrent and a minimum is observed at $\hbar\omega$ = 14.5 eV which is near the plasmon energy of PbS given by 14.4 eV. For the location of the initial state wavefunction at the vacuum region given by z_o = 0 Å, the photocurrent is found to decrease with the increase in the photon energy and does not show a maximum or a minimum in photocurrent. Such maximum and minimum values are also not observed for the location of the initial state wavefunction in the bulk region given by z_o = – 5.29 Å. In this case, the photocurrent decreases initially with the increase in photon energy and attains a constant value after around photon energy $\hbar\omega$ = 6 eV.

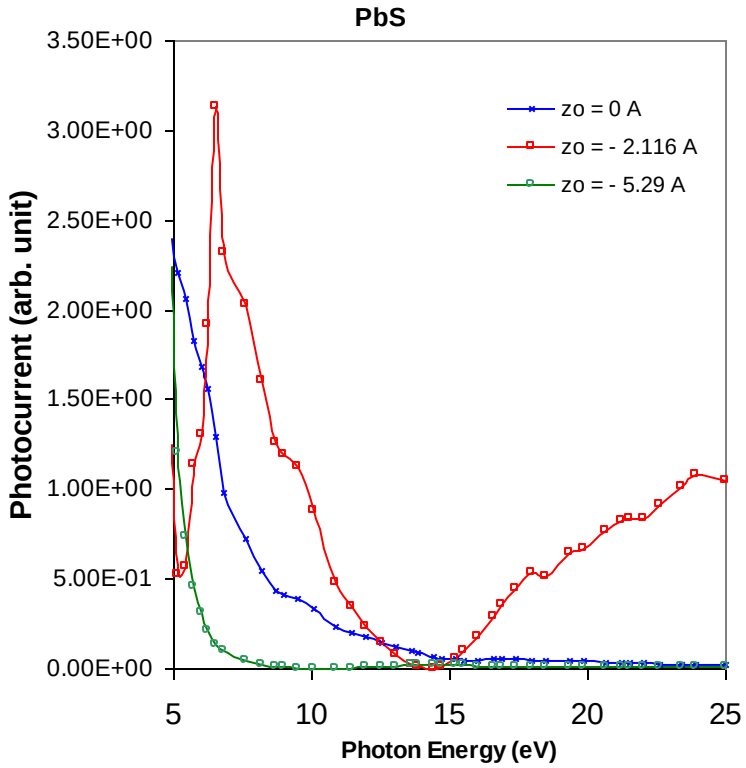

Figure 2: Plot of photocurrent variation against photon energy $\hbar\omega$ for *PbS* at three different locations of the initial state wavefunction ψ_i given by z_o = 0, - 2.116 and - 5.29 Å.

4. CONCLUSION:

Using the model presented and the results obtained photocurrent calculations show maximum below the plasmon energy and minimum at the plasmon energy for the surface region as expected. The model presented here produces results comparable with other experimental [4] and theoretical models [5],[6] and [7]. We can therefore conclude that the photocurrent calculations using initial state wavefunction deduced by solving one dimensional schrodinger equation using Green function and considering Kronig Penny model for the periodic potential works for semiconductors such as GaAs and PbS and may be applicable for other semiconductor as well.

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