Calculations of Photocurrent from BP and its band structures

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Abstract. We present here the results of photocurrent from boron pnictides namely BP. The photocurrent in this system had been calculated by using three types of potential namely free-electron, Kronig-Penney and Muffin-Tin potentials. Schrödinger’s equation has been solved by using these potentials to obtain the necessary initial and final state wave-functions for the electrons. These wave-functions are used for evaluating the matrix element $\langle \Psi_f | p \cdot A + A \cdot p | \Psi_i \rangle$ which is involved in the formula of photocurrent.

1. Introduction
Boron compounds have attracted research interest over the past few years as wide band gap semiconductors. For example, boron pnictides (BAs, BN and BP) are binary compounds belonging to III-V semiconductors, which crystallizes in zinc blende structure [1]. They are extensively under study and are highly attracted due to their high technological applications such as high-temperature, electronic and optical devices like linear and non-linear optics, solar cells, light-emitting diodes, etc. Photoemission studies from the surface of solids are mainly concerned with the excitation of electrons. These photoelectrons lying at the surface or at the bulk region needs sufficient energy to transport themselves across the barrier. However, the incident energy is too weak to provide the necessary momentum to excite the photoelectrons at the surface. Therefore, the spatial variations of vector potential at the surface are considered to be the main factor for the excitation of photoelectrons at the surface. For evaluation of the vector potential involved in the matrix element for transition from initial to final state, we require real and imaginary dielectric constants. These have been calculated by using the density functional theory based on full-potential approximation which is implemented in Wien2k code [2].

2. Methodology
The current density for photoemission is calculated by using the golden-rule approximations [3] as

$$\frac{dj}{d\Omega} = \frac{2\pi}{\hbar} \sum_f |\langle \Psi_f | H' | \Psi_i \rangle|^2 \delta(E - E_f) \delta(E_f - E_i - \hbar \omega) f_0(E - \hbar \omega)[1 - f_0(E)]$$

(1)

where $\Psi_i$ and $\Psi_f$ are the initial and final states wave-function and $H' = (e/2mc)(A \cdot p + p \cdot A)$. $A$ being the vector potential and $p$ the one-electron momentum operator. In order to evaluate the matrix element in Eq. (1), we need to construct $\Psi_i$ and $\Psi_f$ and determine vector potential $A$. Although the one-electron states are treated quite accurately in many photoemission calculations [4], the variation of the photon field $A$ in the surface region is usually neglected. We have used a simple model for calculations of $A$ as done by Bagchi and Kar [5].

We have used three types of potentials for calculating the wave function to evaluate the matrix element for calculating photocurrent. We will describe each one of these briefly here. First, the muffin-tin potential [6] had been used by which the initial state wavefunction derived is given by
\[ \Psi_i(r) = \begin{cases} \sum A(R)Y_l(\theta, \phi) & \text{spherical region} \\ \sum gL(\theta, \phi) + v_g e^{ik_g^+ R} & \text{interstitial region} \end{cases} \]

where \( k_g^+ = [(k + g)_\| \pm \sqrt{2(E_i - V_0) - |k - g|_\|} \) and \( R = r - C_j \) with the \( g \)'s denoting two-dimensional reciprocal lattice vectors and the \( C_j \)s is the origin at the \( j \)th layer.

The initial state wavefunction used for the free-electron model [7] is given by

\[ \Psi_i(r) = \begin{cases} e^{ik_iz} + \frac{ik_iz}{ik_iz} e^{ik_iz} & z \leq 0 \\ \frac{2i}{ik_iz} e^{-\chi^2 z} e^{ik_iz} & z > 0 \end{cases} \]

Where \( k_i^2 = \frac{2m}{\hbar^2} E_i - k_\|^2 \), \( \chi^2 = \frac{2m}{\hbar^2} (V_0 - E_i) + k_\|^2 \), \( k_\| \) and \( r_\| \) are the components of \( k \) and \( r \) in the x-y plane i.e. the plane parallel to the surface.

Similarly for Kronig-Penney potential model, Schrodinger’s equation had been solved for the bulk, surface and vacuum regions by wavefunction matching. The initial state wavefunction for this case is given by

\[ \Psi_i(z) = \begin{cases} (1 - iPe^{-i\delta \sin \delta}) - (P - iPe^{i\delta \sin \delta})e^{-ik_i(z)} & z \leq 0 \\ 2ie^{i\delta \sin \delta}e^{-ik_iz} & z > 0 \end{cases} \]

where \( \chi^2 = \frac{2m}{\hbar^2} (V_0 - E_i) \) with \( V_0 \) being the step potential at the surface, \( P \) and \( T \) are reflection and transmission coefficients respectively. By wavefunction matching at the surface plane (\( z = 0 \)), we find that

\[ P = \frac{\chi^2 - (k_i - i\delta) e^{i\delta \sin \delta}}{\chi^2 + (k_i + i\delta) e^{i\delta \sin \delta}} \]

\[ T = \frac{2i(k_i \sin^2 + (k_i + i\delta) e^{i\delta \sin \delta}}{\chi^2 + (k_i + i\delta) e^{i\delta \sin \delta}} \]

For all these three cases, the final state wave function [6] is a plane wave which is

\[ \Psi_f(r) = \begin{cases} e^{ik_iz} + \frac{g-k_f}{g+k_f} e^{-gz} & z \leq 0 \\ \frac{2g}{g+k_f} e^{ik_iz}e^{ik_iz} & z > 0 \end{cases} \]

where \( k_f^2 = \frac{2m}{\hbar^2} E_f - k_\|^2 \), \( \chi^2 = \frac{2m}{\hbar^2} (E_f - V_0) - k_\|^2 \) and \( E_f = E_i + \hbar \omega \).

3. Results and discussions

We have calculated photocurrent for normal photoemission from the surface and bulk states of BP as a function of photon energy. For our calculations, we have taken work function \( \phi = 8.631 \) eV, potential energy \( V_0 = 15.95 \) eV, surface width \( a = 5.298 \) Å, angle of incident radiation \( \theta_i = 45^\circ \) and scattering factor \( \alpha = 0.35 \). The initial and final state energies are taken to be \( E_i = 6.098 \) eV and \( E_f = 7.319 \) eV. For electromagnetic field calculation which is related to vector potential, we have used the real and imaginary parts of dielectric constants calculated by using the full-potential linearized
augmented plane wave method implemented in Wien2k code [2] which is based on the density functional theory [8]. The value of vector potential had been used as a subroutine in the main FORTRAN program to calculate photocurrent.

![Figure 1. Plot of photocurrent in BP as a function of photon energy from the first two surface layers.](image1)

Plot of photocurrent as a function of photon energy ($\hbar \omega$) of the incident radiation for normal photoemission is shown in figure 1. In our calculations, the dielectric constants $\varepsilon_1$ and $\varepsilon_2$ were obtained using Wien2k code within generalized gradient approximation (GGA) [8]. The photocurrent increases with increase in photon energy. From the first surface layer, we found that there is small increase in photocurrent and a small bump at 29 eV photon energy. The trend of photocurrent from the second surface layer is different from that of photoemission from the first surface layer. Here, photocurrent shows a small peak at 18 eV and then decreases slightly after which it started increasing sharply giving a high peak at 30 eV. Beyond this, photocurrent then decreases with further increase in photon energy. The contribution of photocurrent from second surface layer showed similar trends as from the first layer, but occurrence of peaks are at different photon energies.

![Figure 2. Plot of photocurrent in BP as function of photon energy using free-electron model.](image2)

In the case of free-electron model, photocurrent increases with increase in photon energy showing a small peak at 15 eV as shown in figure 2. Photocurrent then decreases and reaches a minimum at 23 eV which is known as the plasmon energy after which increase variably and reaches a maxima at 30 eV photon energy. Beyond this photon energy, the photocurrent decreases gradually.
In figure 3, we studied the variation of photocurrent as a function of photon energy using Kronig-Penney model and the results are obtained using the dielectric functions as already used in the surface layer calculations. We found here that the photocurrent shows a small peak at 7 eV and then decreases. As found earlier in the cases of other metals like aluminium, iron, tungsten etc., there is a minimum at 9 eV photon energy. The current rises above the plasmon energy and we get another maximum at 16 eV of the incident radiation and decreases again. Thus, we can say that the surface variation of photon field is important in calculating the photocurrent cross-section also in the case of BAs. This fact has also been observed by Bagchi and Kar [5] in the case of tungsten. They have found that vector potential component in the surface region decreases greatly near the plasma frequency of the solids. The difference in the height of the peaks is due to change in the thickness of the surface.

Conclusions

The frequency dependence of the normal component of the photon field plays an important role in calculating the photoemission cross-section from the surface states of BP. The field component in the surface region normally increases with increase in photon energy and decreases greatly near the plasmon frequency of the metallic surface as seen in figures 1, 2 and 3 respectively. This explains the observed difference in normal photoemission from surface states near the plasmon frequency. We may thus state that the surface states play a very important role in the photoemission process.

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