Research Note

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Application of Mathieu potential to calculation of photocurrent from the surface of metals

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ABSTRACT

Mathieu potential have been used for the photoemission calculations from surfaces of ferromagnetic material, Fe (iron), and semiconductor, PbSe (lead selenide). This approach gives a qualitative characterization of surface state photoemission by considering only the surface contribution from the existing bulk-band structure calculations. In this paper, we present the calculations of photocurrent from Fe and PbSe by using the Mathieu potential which defines the crystal potential. The derived initial wave function was used and variation of photocurrent only by those contribution from the surface region defined was calculated. Photocurrent was calculated for values of z_0 = -2 a.u. and z_0 = -8 a.u. As the width of the surface is 10 a.u. in both the cases, z_0 = -2 a.u. is near the surface-vacuum interface and z_0 = -8 a.u. is towards the surface-bulk interface. We found that at low photon energy range, the metal and the semiconductor under study showed similar trend in the behaviour of photocurrent at a region nearer to edge of the surface.

Key words: Mathieu potential; photocurrent; surface states; wavefunctions.

INTRODUCTION

Mathieu potential is a sinusoidal type of potential which had been used by Davison and Levine[1] for surface band structure calculations. Pachuau *et al*.[2] had applied this approach for deriving the initial state wavefunctions for evaluation of the matrix element $\langle \psi_f | H' | \psi_i \rangle$ for calculating photocurrent. The photocurrent data as obtained by them in the ultra-violet photon energy range showed interesting features comparable to experimental results,[3] especially in the case of tungsten (W) and molybdenum (Mo).

However, the main drawback of the calculation for photocurrent is that the same initial state wavefunction is used both for the surface and the bulk regions of the metal. In this study, we used the derived[2] initial wavefunction and calculated the variation of photocurrent only by those contribution from the surface region defined.

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MATERIALS AND METHOD

The photocurrent density formula[4] from golden rule approximation can be written as

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

where ψ_i (ψ_f) refer to the initial (final) state wavefunctions and perturbation H′ can be written as

$$\mathrm{H}' = \frac{e}{2m_e c}\left(\boldsymbol{A}.\boldsymbol{p} + \boldsymbol{p}.\boldsymbol{A}\right) \quad (2)$$

In eq. (2), m_e is the mass of the electron, $\boldsymbol{p}$ the one-electron momentum operator and $\boldsymbol{A}$ the vector potential of the incident photon field. We assumed the z-direction to be perpendicular to the surface (which is chosen as z = 0 plane), and the surface region is defined by $-d = z = 0$ while the metal is assumed to occupy all the spaces to the left of z = 0 plane as shown in Figure 1.

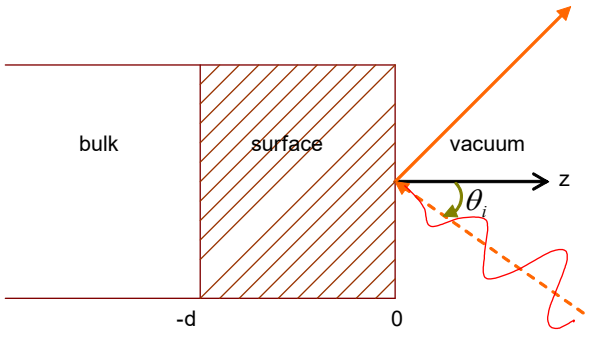

Figure 1. A model photoemission diagram.

We considered a *p*-polarised light to be incident on the surface plane making an angle θ_i with the z-axis. The vector potential $\tilde{A}_\omega(z)$ in the long wavelength limit $(\frac{\omega d}{c}) \to 0$ is given by

$$\tilde{A}_\omega(z) = \begin{cases} A_1\,, & z < -d \quad (bulk) \\ \dfrac{A_1.\varepsilon(\omega).d}{[1-\varepsilon(\omega)]z + d}, & -d \le z \le 0 \quad (surface) \\ A_1.\varepsilon(\omega), & z \ge 0. \quad (vacuum) \end{cases} \quad (3)$$

where A_1 is a constant depending on the dielectric function $\varepsilon(\omega)$, photon energy $\hbar\omega$ and angle of incidence θ_i. The final state wavefunction ψ_f used in eq. (1) is the scattering state of the step potential at the surface which is defined for surface region and is given by

$$\psi_f(z) = \left(\frac{1}{2\pi q_f}\right)^{\frac{1}{2}}.\frac{2q_f}{q_f + k_f}.e^{ik_f z}.e^{-\alpha|z|} \quad (4)$$

where $k_f^{\,2} = 2E_f$, $q_f^{\,2} = 2(E_f - V_0)$ and $E_f = E_i + \hbar\omega$.

The initial state wavefunction derived by using Mathieu potential is given[2] in atomic units (in one-dimension) by

$$\psi_i(z,q) = \begin{cases} \left(\dfrac{1}{4\pi k_i}\right)^{\frac{1}{2}}\left(1 - \dfrac{q}{16} + \dfrac{11}{640}q^2\right)e^{-\mu(z_0'-z)}, & surface\,(z \le 0) \\ (2\xi)^{\frac{1}{2}}\,e^{-\xi(z-z_0')}, & vacuum\,(z \ge 0) \end{cases} \quad (5)$$

Here, the various constants (in a.u.) used are as follows

$$q = 1$$
$$k_i^2 = 2E_i$$
$$\xi = 2 \qquad (6)$$
$$z_0' = \frac{\pi}{a} \cdot z_0$$

where z_0 is the location of the surface state wavefunction and a is the lattice constant which is taken as 6 unit.

We have calculated photocurrent for two locations of the initial state wavefunctions in the surface region, that is, at $z_0 = z_a$ and z_b, where z_a is closer to vacuum-surface interface and z_b is closer to bulk-surface interface.

The matrix element $\langle \psi_f | H' | \psi_i \rangle$ involved in eq. (1) can be expanded as follows

$$I = \langle \psi_f | H' | \psi_i \rangle = \int_{-\infty}^{\infty} \psi_f^* H' \psi_i \, dz =$$

$$\int_{-\infty}^{\infty} \psi_f^* \left(\tilde{A}_\omega(z) \frac{d}{dz} + \frac{1}{2} \frac{d}{dz} \tilde{A}_\omega(z) \right) \psi_i \, dz =$$

$$\int_{-\infty}^{-d} \psi_f^* \tilde{A}_\omega \psi_i \, dz + \int_{-d}^{0} \psi_f^* \tilde{A}_\omega \frac{d\psi_i}{dz} dz + \frac{1}{2} \int_{-d}^{0} \psi_f^* \frac{d\tilde{A}_\omega}{dz} \psi_i \, dz + \int_{0}^{\infty} \psi_f^* \tilde{A}_\omega \varepsilon(\omega) \frac{d\psi_i}{dz} dz \qquad (7)$$

Considering only the surface contribution, eq. (7) reduces to

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

Eq. (8) had been used to compute photocurrent from metal (Fe) and semiconductor (PbSe) and FORTRAN programmes were written to evaluate the above integrals.

Results

We dicuss here the results of photocurrent in the case of iron (Fe) and semiconductor lead selenide (PbSe). For Fe, we used the experimentally measured dielectric constants as given by Weaver,[5] whereas for semiconductor, the data as given by Edward.[6] Choice of parameter like initial state energy (E_i), magnitude of potential (V_0), Fermi level (E_F), were those pertaining to respective metal and semiconductor. However, angle of incidence was $\theta_i = 45°$ for p-polarised light under consideration in all the cases. Photocurrent was calculated for values of z_0 = -2 a.u. and z_0 = -8 a.u. As the width of the surface was 10 a.u. in both the cases, z_0 = -2 a.u. was near the surface-vacuum interface, and z_0 = -8 a.u. was toward the surface-bulk interface. We showed the plots of photocurrent which had been converted to normalized unity. This was done in order to avoid the large difference in numerical magnitude of the calculated photocurrent data in these two values of z_0.

1. Iron (Fe)

Figure 2 shows the behaviour of photocurrent in the case of Fe where we have shown the plot again for two locations of surface

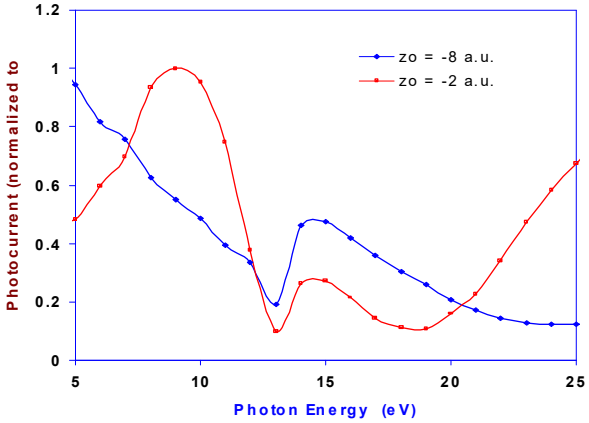

Figure 2. Plot of photocurrent against photon energy with ψ_i defined by Mathieu potential in the case of Fe.

states wavefunctions, that is, at z_0 = -2 a.u. and z_0 = -8 a.u. The observed value[6] of plasmon energy ($\hbar\omega_p$) of Fe was 15.8 eV. In the case of wavefunction located at z_0 = -2 a.u. plot of photocurrent showed a maxima at $\hbar\omega$ = 9 eV and it decreased to a minima at $\hbar\omega$ = 13 eV. A second peak of small magnitude in height was found at $\hbar\omega$ = 15 eV. The case of z_0 = -8 a.u. shows a different trend which decreases rapidly as the photon energy increases and having a minima also at $\hbar\omega$ = 13 eV. However, there was no proper peak in photocurrent near plasmon energy.

2. Lead selenide (PbSe)

In Figure 3 we show the plot of photocurrent against photon energy in the case of PbSe for z_0 = -2 a.u. and z_0 = -8 a.u. Photocurrent increases with the increase in $\hbar\omega$ for z_0 = -2 a.u. and reaches a maximum at $\hbar\omega$ = 7.5 eV. It decreases with the further increase in *žù* but showed a minimum at $\hbar\omega$ = 10 eV. A small peak in photocurrent is obtained at $\hbar\omega$ = 11 eV and photocurrent decreases with further increase in $\hbar\omega$. For the case of z_0 = -8 a.u., photocurrent goes on decreasing with the increase in $\hbar\omega$ and showed minimum at $\hbar\omega$ = 10 eV. Beyond $\hbar\omega$ = 10 eV, photocurrent showed similar behaviour as shown in the case of case z_0 = -2 a.u.

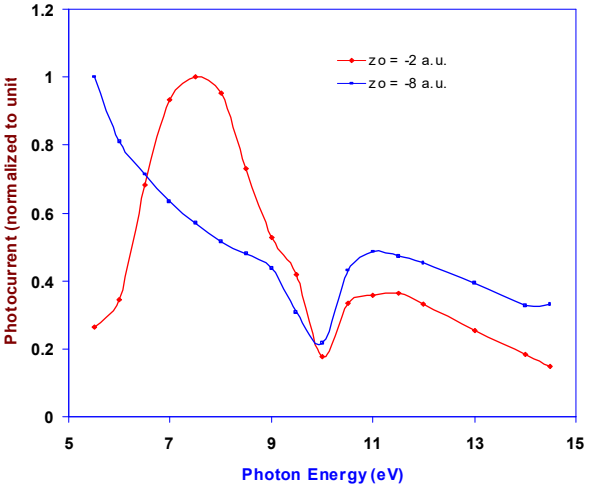

Figure 3. Plot of photocurrent against photon energy with Ψ_i defined by Mathieu potential for the case of PbSe.

Discussion

We find from our results that at low photon energy range the metal and the semiconductor under study showed similar trend in the behaviour of photocurrent at a region nearer to edge of the surface. For example in both cases, we see the occurrence of peak which is due to surface photoeffect and the decrease in photocurrent to minimum after the first peak which is due to loss of photon energy by excitation of bulk plasmons for z_0 = -2 a.u. The surface plasmon frequency (ω_p) is assumed to be the value of photon frequency at which photocurrent is maximum. As the incident photon approaches plasmon frequency, the component of electric field tends towards minimum which also causes the the photocurrent to be minimum Beyond the plasmon energy, a second peak in photocurrent was obtained whose height is smaller in magnitude than the first one at $\hbar\omega < \hbar\omega_p$. The reason for the occurrence of peak in photocurrent at $\hbar\omega < \hbar\omega_p$ is due to surface refraction effect where the z-component of electromagnetic field becomes maximum at $\hbar\omega < \hbar\omega_p / \sqrt{2}$. This had been also seen in the experimental[3] results of W and Mo.

We tried to see the effect of surface contribution only and excluded the bulk photoemission in Mathieu type of potential from metal and semiconductor surfaces. We find that at narrower surface width (z_0 = -2 a.u.) the photocurrent results from these element showed similar behaviour for as had been obtained by Zoliana *et al.*[7] and Thapa *et al.*[8] in the case of other metals and semiconductors.[9] As the initial state wavefunction approaches towards the

bulk-surface interface the photocurrent behaviour tend to deviate away from the qualitative behaviour.[9]

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