

## A simple study of photoemission from metals

B Zoliana<sup>a</sup>, Z Pachua<sup>a</sup>, P K Patra, S Srivastava, R C Tewari<sup>b</sup> and R K Thapa<sup>\*</sup>

<sup>a</sup> Department of Physics, Pachhunga University College, Aizawl 796 001, Mizoram

<sup>\*</sup> Department of Physics, Government Ziri Residential Science College, Aizawl 796 001, Mizoram

<sup>b</sup> Department of Physics, Government Serchhip College, Serchhip-796181 Mizoram

E-mail : ramkumar\_thapa@yahoo.com

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**Abstract** We have applied the Kronig-Penney model potential to calculate photocurrent from metals Mo and Cu. Spatially dependent vector potential had been used to evaluate the relevant matrix elements.

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In this note, a simple study of the behavior of photocurrent data is presented for molybdenum and copper metals in the low photon energy range. Photocurrent is calculated by using the golden rule formula [1]

$$\frac{dI}{d\omega} = \frac{2\pi}{\hbar} \sum |\langle \psi_f | H' | \psi_i \rangle|^2 \delta(E - E_f) \delta(E_f - E_i - \hbar\omega) \times f_0(E - \hbar\omega) [1 - f_0(E)], \quad (1)$$

where  $H'$  is the perturbation responsible for photoemission due to incident radiation of frequency  $\omega$ .  $|\psi_i\rangle$  ( $|\psi_f\rangle$ ) refers to the initial (final) state wavefunctions,  $E_i$  ( $E_f$ ) are initial (final) state energy,  $f_0(E)$  denotes the Fermi occupation function. We are considering the photoemission to take place along  $z$ -axis which is normal to the surface.  $H'$  can be written as

$$H' = \frac{e}{mc} \left[ \tilde{A}_\omega(z) \frac{d}{dz} + \frac{1}{2} \frac{d}{dz} \tilde{A}_\omega(z) \right], \quad (2)$$

where  $\tilde{A}_\omega(z) = \frac{A_\omega^z(z)}{A_0}$ , with  $A_\omega^z(z)$  as the component of vector potential along  $z$ -axis,  $A_0$  is the amplitude of the incident beam. We assume the  $z$ -direction to be perpendicular to the surface which is chosen as  $z = 0$ . The metal is assumed [2] to occupy all space to the left of the  $z = 0$  plane. The response of the electromagnetic field is bulk-like every where except in the

surface region defined by  $-a \leq z \leq 0$ . In this region, the model dielectric function is chosen to be a local one which interpolates linearly between the bulk value inside the metal and the vacuum value (unity) outside. The model frequency-dependent dielectric function used for calculating  $\tilde{A}_\omega(z)$  is given by

$$\epsilon(\omega) \equiv \epsilon_1(\omega) + i\epsilon_2(\omega) \quad \text{for } z < -a,$$

$$\epsilon(\omega, z) = 1 + [1 - \epsilon(\omega)] \frac{z}{a} \quad \text{for } -a \leq z \leq 0,$$

$$= 1 \quad \text{for } z > 0 \quad (3)$$

We consider [2] a  $p$ -polarised light to be incident on the surface plane making an angle  $\theta$ , with the  $z$ -axis. The vector potential of interest  $\tilde{A}_\omega(z)$  in the long wavelength ( $\omega a / c \rightarrow 0$ ) is given by

$$\tilde{A}_\omega(z) = \begin{cases} \sin 2\theta_i \\ \left[ \epsilon(\omega) - \sin^2 \theta_i \right]^{\frac{1}{2}} + \epsilon(\omega) \cos \theta_i, & \text{for } z < -a, \end{cases}$$

$$\frac{\sin 2\theta_i}{\left[ \epsilon(\omega) - \sin^2 \theta_i \right]^{\frac{1}{2}} + \epsilon(\omega) \cos \theta_i} \frac{a\epsilon(\omega)}{[1 - \epsilon(\omega)]z + a}$$

$$\text{for } -a \leq z \leq 0,$$

<sup>\*</sup> Corresponding Author

$$\frac{\epsilon(\omega) \sin 2\theta_i}{[\epsilon(\omega) - \sin^2 \theta_i]^{\frac{1}{2}} + \epsilon(\omega) \cos \theta_i} \quad \text{for } z > 0. \quad (4)$$

This initial state wavefunction  $\psi_i$  used in eq. (1) is the one deduced by Thapa and Kar [3] by employing Kronig – Penney potential model and had been applied to various cases [4-7]. Experimentally measured values of dielectric constants [8] were used for calculating the photon fields. Photocurrent was calculated from these metals for two values of the surface widths, namely  $a = 0$  (narrow surface width) and  $a = 10$  a.u. for the same values of surface state energy (10.24 eV), potential barrier height (14.99 eV) and  $\theta_i = 45^\circ$ . Figure 1 shows the plot of photocurrent as a function of photon energy ( $\hbar\omega$ ) in the case of Mo. We find that for  $a = 10$  a.u., a maximum in the value of photocurrent occurs at  $\hbar\omega = 10$  eV. With the further increase of photon energy, photocurrent decreases to a minimum value at  $\hbar\omega = 12$  eV and shows a small hump at  $\hbar\omega = 14$  eV. But for a narrow surface width ( $a = 0$ ), the behavior of photocurrent is quite different as shown in Figure 1. We do not find any peak for values of photon energy below and above 12 eV.

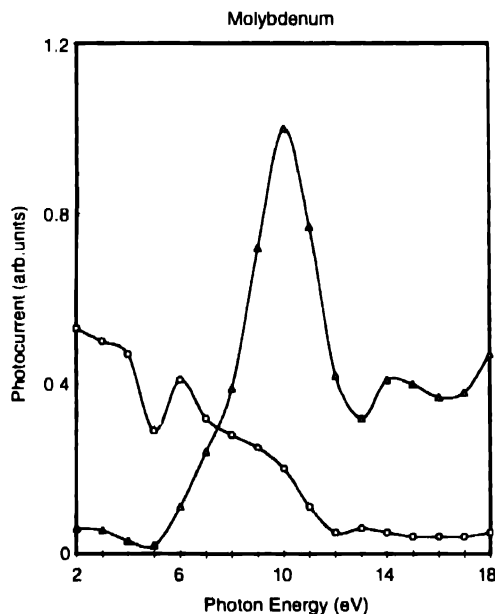


Figure 1. Plot of photocurrent from Mo as a function of photon energy (eV) for narrow surface width ( $a = 0$ ) (open circles) and surface width  $a = 10$  a.u. (triangle)

Figure 2 shows the plot of variation of photocurrent as a function of photon energy in the case of Cu. For the surface width  $a = 10$  a.u., the peak in the value of photocurrent occurs at  $\hbar\omega = 20$  eV and decreases to a minimum at 26 eV photon energy. A second peak is also seen in the case of Cu at  $\hbar\omega = 30$  eV. Copper shows totally different behavior for the narrow surface width ( $a = 0$ ) which is evident from Figure 2.

We find that both the metals Mo and Cu have shown atleast a qualitative agreement with the behavior of photocurrent as

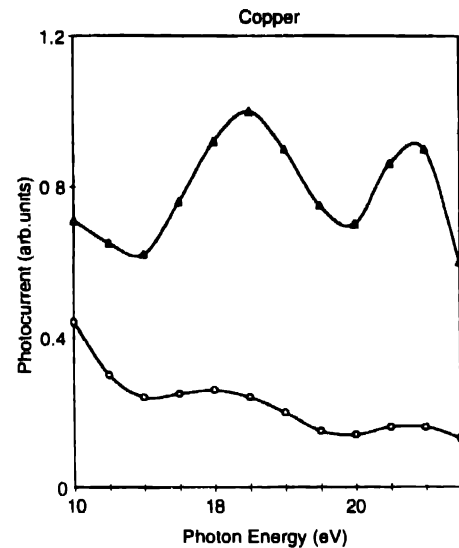


Figure 2. Plot of photocurrent from Cu as a function of photon energy (eV) for narrow surface width ( $a = 0$ ) (open circles) and surface width  $a = 10$  a.u. (triangle)

indicated also by other metals like Pd<sup>4</sup>, W<sup>5</sup>, Si<sup>5</sup> etc. in which we have also used the Kronig-Penney potential model. However we see that the model employed do not exactly reproduce the earlier reported results. For example, in the case of Mo, Weng *et al* [9] have shown that in the case of high lying surface state case, photoemission intensity which is maximum at a photon energy of 15 eV, tends towards a minimum at 25 eV photon energy followed by a hump at  $\hbar\omega = 30$  eV. It does show a minimum in photocurrent at plasmon energy of Mo *i.e.* 24.4 eV. The reasons for not exactly conforming to other models and the experimentally measured data [10] may be attributed to the fact that our model is a rather approximate one. For example, it does not consider the details of the band structure effects. Also the matrix element is mainly dependent on the variation of the vector potential as evidenced in previous cases [4,5]. In fact, it is the variation of the vector potential which mainly modulates the matrix element thereby bringing in the changes in photocurrent. This fact had been also argued by Weng *et al* [9] that the occurrence of a peak in photoemission intensity in the case of Mo is caused by the excitation of electrons by the  $A_2$  component of the vector potential. He further pointed out that the initial states with  $\Delta_1$  symmetry can only be photoexcited by the  $A_1$  component of the incident photon field. Though the model used here is simple, it gives first-hand information with regard to the effect of changes in surface width, as well as the location of initial state energy on photocurrent data.

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