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Electromagnetic fields near surfaces in a simple model : the case of aluminium

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In angle resolved photoemission, the photon field responsible for photoemission may play an important role especially when the spatial symmetries of the initial and final states are known. If the photoemission cross section is measured as a function of photon energy then the behaviour of the photon field may become crucial for explaining the experimental data. One example is the photoemission from the surface state of the tungsten (100) surface. The data of Weng *et al* (1977) for p-polarised light showed a pronounced dip near the plasmon energy which was interpreted in terms of refraction effects by Bagchi and Kar (1978) using a simple model. The calculation of electromagnetic fields in the presence of real metal surfaces is a formidable problem. However, *ab initio* calculations have been done for jellium (Feibelman 1975a, b, Mukhopadhyay and Lundqvist 1977). Levinson *et al* (1979) used these results for jellium for comparison with the experimental data for aluminium and showed that the variation of the photon field in the surface region is extremly important for the explanation of the variation of photo-current as a function of photon energy. However, the *ab initio* calculations have been performed only for jellium and even this is an extremly complex computational procedure. The standard methods for calculation of photo-current, for example, that of Pendry and Hopkinson (1978) neglected the variation of the photon field in the surface region. The model of Bagchi and Kar (1978) which involves a linear interpolation in the surface region between the experimentally measured frequency-dependent bulk value of the dielectric constant and its vacuum value is relatively easy and can be used for both metals and semiconductors. It was shown to be successful in explaining the qualitative behaviour of the photo-emission cross section for the surface states of tungsten. We propose to use the model for bulk states also. As a first step, we show that for aluminium the use of this model indicates that the photon field near the surface shows qualitatively the same behaviour as that obtained from the photo-current measurements.

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The model used by Bagchi and Kar (1978) is a fairly simple one. The z-direction is taken to be the normal to the nominal surface plane which is chosen to be the $z=0$ plane. The metal is assumed to occupy all the space to the left of the $z=0$ plane. It is assumed that the response of the metal to an electromagnetic fields is bulk-like every where except in a surface region which extends over $-a/2 \leqslant z \leqslant a/2$. In this region, the model dielectric constant is chosen to be a local function which interpolates linearly between the bulk value inside the metal and the vacuum value (unity) outside. The model frequency-dependent dielectric function is, therefore the following :

$$\epsilon(\omega, Z) = \begin{cases} \epsilon(\omega)=\epsilon_1(\omega)+i\epsilon_2(\omega), & z \leqslant -a/2 \\ \frac{1}{2}[1+\epsilon(\omega)]+[1-\epsilon(\omega)]\cdot\frac{z}{a}, & -a/2 \leqslant z \leqslant a/2 \\ 1, & z \geqslant a/2 \end{cases}$$

For the complex dielectric function of aluminium, we use the experimental values given by Weaver (1987-88). For p-polarised light, the magnetic field $B(z)=B(\vec{Q}, \omega ; z)$, (where $Q=\omega/c \sin\theta_i$ is small) is in the y-direction and obeys the following equation (Landau and Lifshitz 1960) with $\epsilon=\epsilon(\omega, z)$,

$$\frac{d}{dz}\left(\frac{1}{\epsilon}\frac{dB}{dz}\right)+\left(\frac{\omega^2}{c^2}-\frac{Q^2}{\epsilon}\right)B=0.$$

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

$$E^x(\vec{Q}, \omega ; z)=\frac{c}{i\omega\epsilon}\frac{dB}{dz},$$

$$E^z(\vec{Q}, \omega ; z)=-\frac{\sin\theta_i}{\epsilon}B.$$

The solution of the above equation leads to the following long wave length result (Bagchi and Kar 1978) ($\omega a/c \to 0$),

$$\frac{E^z(Q\to 0, \omega, z)}{E_0} = \begin{cases} \dfrac{\sin 2\theta_i}{[\epsilon(\omega)-\sin^2\theta_i]^{1/2}+\epsilon(\omega)\cos\theta_i}, & z \leqslant -a/2 \\ \dfrac{\sin 2\theta_i}{z/a+\frac{1}{2}[1+\epsilon(\omega)]/[1-\epsilon(\omega)]} \cdot \dfrac{\epsilon(\omega)/[1-\epsilon(\omega)]}{[\epsilon(\omega)-\sin^2\theta_i]^{1/2}+\epsilon(\omega)\cos\theta_i}, & -a/2 \leqslant z \leqslant a/2 \\ \dfrac{\sin 2\theta_i \epsilon(\omega)}{[\epsilon(\omega)-\sin^2\theta_i]^{1/2}+\epsilon(\omega)\cos\theta_i}, & z \geqslant a/2 \end{cases}$$

We are interested in the z-component of the electric field because in normal photoemission E^z is the component which will give a non-vanishing matrix element if the initial and final states are symmetric. We have computed

$\tilde{A}_\omega(z) = E^z(Q \to 0, \omega, z)$ as a function of ω for various values of z using the experimental values of $\epsilon(\omega)$. The plots for $z/a = 0.5$, 0.0 and $+0.5$ are shown in the Figure 1. The curves for $z/a = 0.0$ and $z/a = 0.5$ both exhibit a minimum around 15 eV (The plasmon energy for aluminium is 15.75 eV). Further, the plot of $\tilde{A}_\omega(z)$

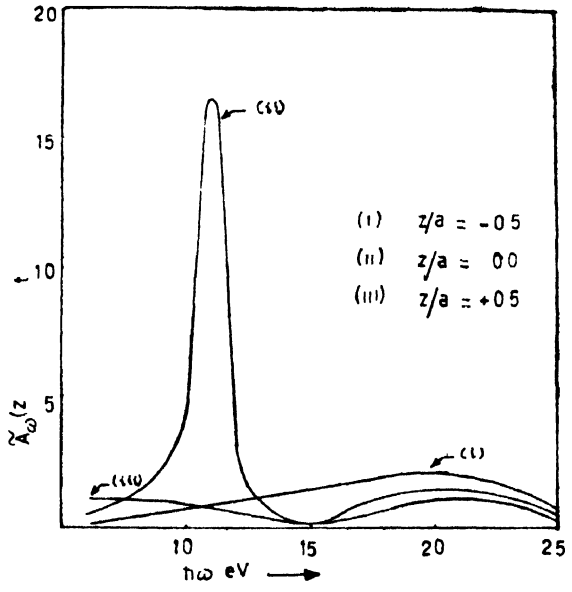

Figure 1. Variation of vector potential $\tilde{A}_\omega(z)$ in aluminium for $z/a = -0.5$, 0.0 and + 0.5 with respect to the change in incident photon energy $\hbar\omega$ (eV).

for $z/a = 0.0$ shows a strong peak at around 12 eV. These facts lead us to correlate the experimentally observed minimum at 15 eV and a peak at 12 eV for both the state at Fermi level and the surface state at Γ (Levinson et *al* 1979) with refraction effects. Preliminary calculations for the photoemission cross section with a simple model seem to confirm this. We note that these conclusions were reached by Levinson et *al* (1979) using a much more sophisticated calculation of the photon field but their calculation was restricted to jellium. We have used this much simpler model for tungsten with some success and now see that the results for aluminium also agree qualitatively with experiments. We are going to incorporate this model for photoemission cross section calculations and will be using it for cases where results obtained for jellium would not be applicable.

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