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Surface photoeffect with non specular surface scattering of electrons

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Résumé. — On argumente (a) que la diffusion non spéculaire des électrons à la surface augmente le rendement photoélectrique et (b) que, en désaccord avec la notion généralement acceptée, il y a des diverses situations où il est aussi important de retenir une description non locale de la réponse diélectrique transversale.

Abstract. — It is argued that (a) diffuse surface scattering of electrons enhances the internal photoyield and (b) contrary to the commonly held view, non locality in the transverse dielectric response also plays an important role in many situations.

Photoemission and the electronic properties of surfaces are receiving a great deal of current interest [1]. Effects associated with the electromagnetic field near the surface [2, 3], surface potential [4] and surface wavefunctions [5] have been discussed by various authors. Others [6-8] have hinted that the non specular scattering of electrons from the surface might have an appreciable influence on the photoyield. The purpose of this note is to provide an explicit discussion of the effect of non specular scattering on the internal photoyield.

For this we follow Kliewer's approach [7], based on a semiclassical infinite barrier model. This amounts to a loss of accuracy as compared with a more detailed quantum mechanical analysis [4], but allows us to isolate the problem of non specularity and to focus on its effect. The calculation of the photoyield, avoiding the complicated problem of the escape probability for electrons with different energies, is based on the formula

\[ Y = \frac{4 \pi}{C \cos \theta} \int_0^{\infty} e^{-z/\delta} \text{Re} \left[ J(z) \cdot E^*(z) \right] \, dz. \]  

(2)

As in Kliewer's calculation [7] we study P-polarized incident light. The analysis is based on the method of extended pseudomedia [9, 11], which has been used [11] to study in the same way the total absorption, the limiting case \( \delta \to \infty \) of the problem studied here. As in [9, 11] we use simplified dispersive dielectric functions \( \varepsilon_L(k, \omega) \) and \( \varepsilon_T(k, \omega) \). These model dielectric functions are chosen so that they incorporate the main features of spatial dispersion while being sufficiently simple that the problem is amenable to analytical study. This avoids the mathematical complications which arise when one uses elaborate dielectric functions [12, 13], in which case one must soon resort to heavy numerical computation. Previous experience has shown that the use of these simplified dielectric functions gives very satisfactory results in the calculation of reflectivity [11] and surface plasmon dispersion relation [9]. It will be seen here that they also produce results for the photoyield which compare quite well with the results obtained with more elaborate calculations in the cases in which such calculations have been performed. The form of \( \varepsilon_L \) is like that of the hydrodynamic model, but the approximation pro-
ducing $\varepsilon_k$ and $\varepsilon_T$ is different [10] in one important respect, namely, that spatial dispersion is also included in the transverse response. We stress that the analysis of [7] was based on a very elaborate (essentially RPA) $\varepsilon_k$ and a local $\varepsilon_T$. The point of this paper is that including dispersion in $\varepsilon_T$ is important for non specular surfaces.

Now, when the excitations near the surface are important one might expect that the dominant role that diffuse surface scattering plays in determining the decay of collective excitations [9, 11] may enhance incoherent excitations and therefore the photoyield. In order to formulate this qualitative idea we use the analysis of [9-11] in which the strength of diffuse surface scattering is represented by the phenomenological parameter $p$ ($0 \leq p \leq 1$). This parameter has a statistical meaning. It represents the fraction of incoming electrons which are specularly reflected from the surface. This phenomenological model has been widely used in the theory of surface transport and radio frequency size effects in metals [14] and also in the previous studies of electrodynamic [9, 11, 15] and optical properties of non ideal surfaces performed on the basis of the approach used here to study the photoyield.

The outline of the calculation is as follows: we put $k = (k, q, 0)$, so that $k$ is the component of $k$ parallel to the surface and the $\Omega x$ axis is chosen as the direction of $k$. For given $(k, ; \omega)$ we consider the root $L(k, ; \omega)$ of

$$e_k(k, ; \omega) \equiv \frac{(q^2 + L^2)}{(q^2 + l^2)} = 0$$

and the two roots $R(k, ; \omega)$ and $r(k, ; \omega)$ of

$$k^2 - \frac{\omega^2}{C^2} \varepsilon_T(k, ; \omega) \equiv \frac{(q^2 + R^2)(q^2 + r^2)}{(q^2 + l^2)} = 0.$$  

$L$, $R$, and $r$ are determined by the model dielectric functions

$$\varepsilon_i = 1 - \frac{\omega_p^2}{\omega^2 - \beta_i q^2 + i\gamma} ; \quad i = L, T ;$$

$$\beta_L = \sqrt{3} \gamma F; \quad \beta_T = \sqrt{3} \gamma F.$$  

The field inside the metal ($z > 0$) is obtained in the form

$$E(z) = E_L e^{-lz} + E_R e^{-rz} + E_e e^{-rz}.$$  

As regards the transverse field, the mode $q = + iR$ can be approximately obtained by taking

$$e_T = 1 - \frac{\omega_T^2}{\omega^2}$$

and represents the normal EM mode propagating in the metal, while the mode $q = ir$ is a polariton-like vibration associated to the electronic transverse mode given by $\varepsilon_T \rightarrow \infty$. 

The method of extended pseudomedia [9, 10] yields the longitudinal ($E_L$) and transverse ($E_R, E_e$) amplitudes as functions of $p$. The current is likewise obtained in the form

$$J(z) = J_L e^{-Lz} + J_R e^{-rz} + J_e e^{-rz}$$

and with this one can evaluate (2) carrying through the effects of $p$. We shall concentrate on the extreme cases $p = 0$ and $p = 1$. In the specular limit ($p = 1$) we should make contact with [7]. All the calculations have been done with same input parameters as in [7]: $\omega_p = 10^3$ and the sodium density.

In order to see the effect of accounting for spatial dispersion in $\varepsilon_T$, figure 1a shows the differential absorptance $dA/dz$ as a function of $z$ for $\theta = 45^o$. Simplified non local $\varepsilon_k$ and $\varepsilon_T$. Full line : $p = 1$, dashed line : $p = 0$. a) $\Omega = 0.33$, b) $\Omega = 1.1$. 

![Fig. 1. — Differential absorptance as a function of $z$ for $\theta = 45^o$. Simplified non local $\varepsilon_k$ and $\varepsilon_T$. Full line : $p = 1$, dashed line : $p = 0$. a) $\Omega = 0.33$, b) $\Omega = 1.1$.](image-url)
physical terms by noting that surface scattering strongly affects the transverse current density fluctuations near the surface [17]. In our case, the polariton-like transverse mode has an energy essentially associated with transverse electron vibrations, while the normal EM mode is associated to a propagation of an EM energy. This explains why electron surface scattering predominantly affects to the polariton-like mode.

When the plasmon threshold is reached, the longitudinal mode $L$ begins to play an increasingly important role. Figure 1b ($\Omega = 1.1$) shows that this mode dominates if $p = 1$. In this case the periodicity in the oscillations of $dA/dz$ is $2 \pi/\Omega \approx 13 \, \text{Å}$. However, for $p = 0$ the situation is still dominated by the transverse mode $r$. At this frequency $2 \pi/\Omega \approx 3 \, \text{Å}$, which is the periodicity of the oscillations of $dA/dz$. As $\omega$ increases the situation changes and is increasingly dominated by the longitudinal mode. The difference between the results for $p = 0$ and $p = 1$ decreases and this is why the resulting photoyield for $\Omega = 1.5$ is almost the same, as is seen in figures 2 and 3. Notice that large differences in $dA/dz$ result in large differences in the photoyield only for small values of $\delta$. As $\delta$ increases the details of $dA/dz$ tend to wash out in the integral (1).

It is also interesting to remark that if one assumes a literal hydrodynamic model for $\varepsilon_L(k, \omega)$, and consequently a local $\varepsilon_r(\omega)$, then no assumption about reflection of the free electrons at the surface is necessary. It turns out that in this case standard electromagnetic matching conditions and current conservation at $z = +0$ suffice to determine the problem [16]. In this model the fields and currents near the surface do not depend on $p$. The situation changes entirely if $\varepsilon_r$ is non local. In this case [15] the field inside contains a non vanishing amplitude of the $r$ mode and the full determination of the solution requires an extra condition at the surface. As discussed in [9, 10] this amounts to a model for the scattering of the quasiparticles at the inner surface of the medium. It is this model that is represented by the phenomenological parameter $p$ in the case of metals.

Figure 2 shows the calculated photoyield vs. reduced frequency $\Omega = \omega_0/\omega_p$. The results with a simplified $\varepsilon_L$ are in excellent agreement with those obtained [7] with an elaborate $\varepsilon_L$ for $\Omega > 1$, when the plasmon excitation dominates. Of course there is a loss of accuracy for $\Omega < 1$, where single particle excitations dominates and this is just the structure which is lacking in our simplified $\varepsilon_L$. This is not important in the calculation of the total absorptance, even down to very low $\Omega$ [11], but figure 2, with $\delta = 2 \, \text{Å}$ (a really extreme case), weights very heavily the differential absorption for very short distances and this is already sensitive to the details of $\varepsilon_L$. However, we can now see what happens when diffuse surface scattering is switched on. The result (dashed line) is a very considerable enhancement of the photoyield for $\Omega < 1$. The case $\delta = 2 \, \text{Å}$ is only shown for illustrative purposes. A more plausible value could be $\delta \approx 20 \, \text{Å}$ (actually $21.2 \, \text{Å}$, to compare with [7]). The results are shown in figure 3. There is no doubt that the effect of diffuse surface scattering is far more important than that of single particle structure for $\Omega < 1$. For $\Omega > 1$ the photoyield tends to be insensitive to the value of $p = 0$, has we have just seen.

A complementary view is obtained by fixing $\Omega$ and studying $Y$ vs. $\theta$. Figure 4 shows the results for $\Omega = 1.01$, when plasmon excitation is already sufficiently important, although at this frequency it is appreciably damped. There is no need to compare with reference [7], as the results for $p = 1$ would be indistinguishable. We can now see the effects of diffuse
surface scattering for all angles and these are everywhere significant even for $\delta = 20 \text{Å}$. The minimum difference between $p = 1$ and $p = 0$ appears (for any $\delta$) at the peak, which corresponds to the critical angle for total external reflection, when the transmitted light wave runs parallel to the surface. This residual, but not negligible, difference is due to the dominant role of the transverse part of the transmitted wave. A local $\varepsilon_T$ and $p = 0$ would give in this case a poor approximation.

The role of $\varepsilon_T$, which is usually treated in a local approximation, can be more explicitly discussed in the light of figure 5, which shows the calculated photoyield for normal incidence and $\delta = 20 \text{Å}$. The difference between $p = 1$ and $p = 0$ is again quite considerable (in fact at all frequencies). In this case $E_s = 0$ and there is no longitudinal excitation. Moreover, for $p = 1$ the analysis shows that the power absorption associated with transverse waves is negligible, and using a local $\varepsilon_T$ is a good approximation. However, this changes drastically for $p = 0$. The large enhancement of the photoyield is then due to the transverse transmitted waves and it is here that $E_s$ is important. In this case the Fourier amplitude of $E_s(z)$ inside the metal turns out be

$$
E_s(q) = \frac{-i 4 \pi}{\omega} \left\{ \frac{\omega^2}{C^2} J_s^M \frac{q(\varepsilon_T \phi + \varepsilon)}{q^2 - \varepsilon_T(k; \omega) \omega^2/C^2} + \frac{\omega}{C} \frac{\Gamma_s^M}{q^2 - \varepsilon_T(k; \omega) \omega^2/C^2} \right\}
$$

where $J_s^M, \Gamma_s^M, f_2$ and $f_3$ are $\kappa$ and $\omega$ dependent parameters which are eventually eliminated [9, 10].

The resulting $E_s(z)$ is then very sensitive to the details of $\varepsilon_T(k; \omega)$. These features remain for small angles of incidence. The case $\theta = 0$ serves also to make contact with the case of S-polarization and shows that keeping a dispersive $\varepsilon_T$ is important for the study of the photoyield $Y_s$ with S-polarized light. This is important because the experimental information is usually given as the ratio $Y_p/Y_s$, which is very convenient for the theoretical interpretation. Assuming that the passage through the surface barrier is indifferent to the polarization of the light which has produced the excitations, one can compare directly experimental data with calculations of internal photoyield, but it is important to have equivalent theories for both $Y_p$ and $Y_s$.

In conclusion we find: (i) The non specular surface scattering of electrons enhances the photoyield. (ii) While a local $\varepsilon_T$ is a good approximation for $p = 1$, inclusion of non specularity requires the use of a dispersive $\varepsilon_T$. A detailed analysis shows that this can be important in a variety of cases, contrary to the commonly held view that only the use of a dispersive $\varepsilon_T$ matters.

Furthermore, in connection with other related phenomena it is worth stressing that [11]: (i) The reflectivity, unlike the photoyield, is very insensitive to the value of $p$. (ii) The total absorptance, corresponding to $\delta \rightarrow \infty$ in (1), does depend on $p$ a little more than the reflectivity, but considerably less than the photoyield for a typical representative escape length of $20 \text{Å}$. 

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Fig. 4. — Fixed $Q = 1.01$. Photoyield vs. $\theta$ for $\delta = 2 \text{Å}$ and $\delta = 20 \text{Å}$. Full line : $p = 1$. Dashed : $p = 0$.

Fig. 5. — Normal incidence. Photoyield vs. $\Omega$. Full line : $p = 1$. Dashed : $p = 0$. 

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