FIZIKA VOLUME 10 SUPPLEMENT 2, 1978
Proceedings of the VI Yugoslav Symposium of the Physics
of Condensed Matter, Kruševac, September, 18-22, 1978

DISPERSION AND LIFETIME EFFECTS ON THE STRENGTHS OF INTRINSIC PLASMON SATELLITES IN XPS

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Only recently, a systematic comparison of experimental data with theoretical predictions for plasmon satellite strengths in XPS from core levels has been made[1,2]. This comparison has shown that although the models[1,3] describe the behaviour of the loss spectra correctly, they somewhat overestimate the plasmon creation probability, especially the so-called "intrinsic" contribution[4].

In this paper we examine how the dispersion and finite lifetime of surface plasmons modify the strengths of plasmon lines in XPS from the core level of an adsorbed atom on a free electron metal[5]. We start from the results obtained for the case of a uniform-density, semi-infinite solid with a step function of electron density at the surface and dispersionless plasmons[3,4]. The strength of the n-th plasmon line (describing the excitation of n surface plasmons) relative to the no-loss line is given by[3]

$$R_n = \frac{1}{n!} Q_s^n \quad , \tag{1}$$

where

$$Q_s = \frac{1}{\hbar^2} \int_{|\vec{k}|<k_c} d^2k\,|Q^h+Q^e|^2 = \frac{1}{\hbar^2} \int_{|\vec{k}|<k_c} d^2k\{(Q^h)^2 + (Q^e)^2 + [(Q^h)^*Q^e + c.c.]\} \tag{2}$$

and the notation is the same as in Refs. 4 and 5. The so-called "intrinsic", "extrinsic" and "interference" contributions to the plasmon line strength can easily be identified

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from eq. (2).

In order to investigate the influence of plasmon dispersion and damping, we will again use eqs. (1-2) but will replace the free plasmon frequency by

$$\hbar\omega_s \to \hbar\omega_s(k) - i\Gamma(k) , \qquad (3)$$

where the dispersion relation $\omega_s(k)$ and the damping $\Gamma(k)$ are known functions of momentum, obtained independently, e.g. from experiment. One point should be stressed here. The case when the dispersion of surface plasmons is due to the geometry of the specimen, is exactly solvable. However, in this case it is assumed that in eq. (3) the dispersion and, additionally, the damping are a consequence of the interaction between plasmon modes and their decay into particle-hole excitation. Here we want to account for this effect.

In our calculation we use the following parameters for

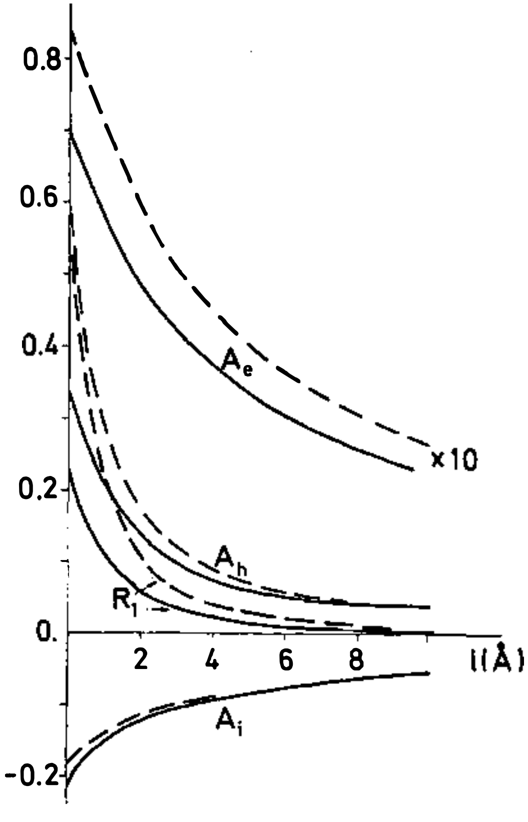

Fig.1. Contributions to the strength of the first plasmon peak.

the plasmon dispersion and damping in aluminium[6)]

$$\hbar\omega_s(k) = 10.7 + 1.1k + 2.2k^2$$

$$\Gamma(k) = 1.85 + 3k,$$

where the energy is measured in eV and k in Å^{-1}.

In Fig. 1, the contributions of the intrinsic (A_h), extrinsic (A_e) and interference (A_i) mechanisms to the strength of the first plasmon peak R_1 ($R_1=A_h+A_e+A_i$) are shown as a function of the distance of the excitation point above the surface. (The dashed line shows the results for a dispersionless, infinite-lifetime model). The kinetic energy of the photoelectron, emerging normally to the surface, is taken to be 967 eV.

As can be seen from Fig. 1, the intrinsic term is markedly reduced by plasmon dispersion and damping. Extrinsic and interference contributions are less affected. It is interesting to note that the absolute value of the interference term is increased (note that it is always negative). The net effect is a strong reduction of the total peak strength and, at the same time its behaviour becomes more extrinsic-like.

However, in spite of a considerable improvement in comparison with the free-plasmon model, the theory still overestimates intensities, especially for higher escape angles. This might be due to electron-refraction effects, surface roughness, or the unrealistic assumption of a step-function electron density.

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