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External electron emission near nanocylinders

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A B S T R A C T

In this work we investigate in detail the effects due to the interaction between an electron and a stationary positive ion (or atomic hole) in the neighbourhood of a nanostructured surface. In particular, we study how a positive charge, located near to the surface of a nanostructured (cylindrically shaped) body, can influence the probability of the surface plasmon excitations and consequently the energy loss of the emerging electron. We deal with simple nanostructured systems of Al, having a strong plasmon peak in its electron energy loss spectra. The method described here is useful for understanding the electron spectra excited from these nanostructures (different from those of the same bulk material).

1. Introduction

In the last years the studies of nanostructures have gained a great and increasing relevance. As surface effects are very important in the case of nanostructures, the applicability of conventional surface analytical methods, such as X-ray Photoelectron Spectroscopy (XPS) [1] and Auger Electron Spectroscopy (AES) [2], two of the most well known methods, for investigation of new nanostructures represents a significant issue.

Recent work [3,4] as well as earlier papers [1,5] call our attention to the fact that surface effects may become stronger when the creation of the electron-hole pair occurs close to the surface.

The creation of the hole in a core level of an atom (and the associated electron-hole pair production) leads to intrinsic plasmon excitation, while the excited photoelectron, through inelastic scattering, induces extrinsic plasmon excitations. The interference between these two kinds of effects (extrinsic and intrinsic plasmon excitations lead to the same energy loss of the emitted photoelectron) makes it difficult to identify and properly describe them.

Both techniques (XPS and AES) provide the possibility for observing both intrinsic and extrinsic plasmon structures [6], recognising and identifying these two effects under certain experimental situation, basically for planar surfaces.

In the case of nanostructures, neither the three step model [7] (electron-hole creation, electron transport in the bulk solid and electron emission crossing the surface) nor the assumption on the two separable mode of excitations (extrinsic –during electron transport– and intrinsic –due to the sudden appearance of the positive hole) as independent processes are valid and applicable anymore.

In this work we study the plasmon generation made from an electron and an atomic hole in first approximation, without taking into account the mentioned effects of interference, and assuming the hole contribution as coming from a planar surface.

2. Plasmon excitation

The excitation of collective bulk and surface modes, known as plasmons, was studied earlier extensively in the case of planar surfaces [6,8–10]. More recently, several works have been dealing with the excitation of plasmons in materials with different shapes and sizes going from macro to nanostructures [13–15].

In the case of electron emission, the presence of a hole or electron-vacancy/deficiency alters considerably the process of plasmon excitation by the emitted electron. This influence was widely studied for the case of planar surfaces [3,4,6,11,12]. With the development of nanostructured materials, it becomes necessary to apply the previous techniques to these new materials.

Based on our previous theoretical work, where we considered the plasmon excitations in nanocylinders due to the presence of one external charged particle [13,14], we will extend our calculations to the plasmon excitations due to the presence of both particles: the external electron, plus the hole.

In a first approximation, and with the idea of following in detail the different contribution as long as we can, we analyze the excitation of surface plasmons in an Al cylinder (wire or capillary), induced by an electron moving parallel to its axis, in the presence of

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a hole (see Fig. 1), without assuming that the electron-hole pair was suddenly created (This is another source of plasmon excitations, but we will not take it into account in this approximation).

2.1. Surface modes

We will focus our attention on the case of the external emission from the surface (it means, that the electron emission takes place outside the material as opposed as internal emission which means that the electron emission takes place inside the material) and for a trajectory of the electron parallel to the axis of the cylinder, in order to excite only the surface plasmons.

According to our previous work [13–15], and following its formalisms, the electron induces a potential in the material as it moves next to the surface. This induced potential in cylindrical coordinates is given by:

$$\Phi_{tot} = 2Ze\sum\int_0^{\infty} dk e^{im(\phi-\phi_0)} A_m I_m(k\rho) \times \left[e^{ikz}\delta(\omega-kv)+e^{-ikz}\delta(\omega+kv)\right]$$

for $\rho < a$, and

$$\Phi_{tot} = \Phi_0 + 2Ze\sum\int_0^{\infty} dk e^{im(\phi-\phi_0)} B_m K_m(k\rho) \times \left[e^{ikz}\delta(\omega-kv)+e^{-ikz}\delta(\omega+kv)\right]$$

for $\rho > a$, where Φ_0 is the potential generated by the external charged particle:

$$\Phi_0 = 2Ze\sum\int_0^{\infty} dk e^{im(\phi-\phi_0)} I_m(k\rho_<) K_m(k\rho_>) \times \left[e^{ikz}\delta(\omega-kv)+e^{-ikz}\delta(\omega+kv)\right]$$

In the previous equations: I_m and K_m are the modified Bessel functions of first and second kind of m-order, respectively. We define: $\rho_< = \min\{\rho, \rho_0\}$ and $\rho_> = \max\{\rho, \rho_0\}$, being ρ_0 the radial coordinate of the electron, which is moving parallel to the cylinder axis with speed v.

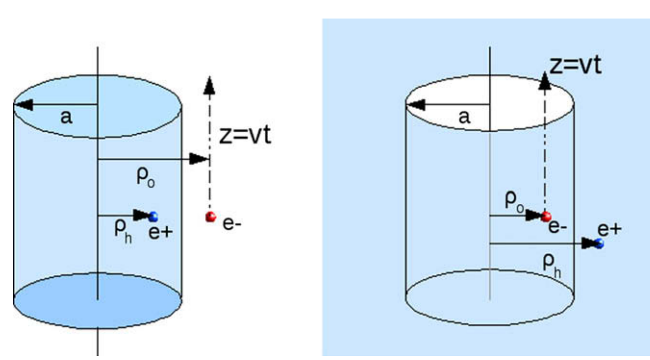

Fig. 1. Scheme of the system. Left: A stationary positive atomic hole is created near a cylindrical wire of radius a (nanowire) at a distance ρ_h from the axis, and an electron is moving parallel to this axis at a distance ρ_0, outside the cylinder. Right: A stationary positive atomic hole is created near the cylindrical cavity of radius a (nanocapillary) at a distance ρ_h from the axis, and an electron is moving parallel to this axis at a distance ρ_0, inside the cylindrical cavity. In both cases, the electron runs outside the material (external emission).

The coefficients A_m and B_m are determined by imposing boundary conditions at the surface ($\rho_0 = a$). Then the stopping force on the particle, obtained in terms of the induced potential, is:

$$F_z = \sum F_{z,m} = -Ze\frac{\partial\Phi_{ind}}{\partial z}$$

from which we get the average number of plasmons in the m-mode:

$$Q_m = \frac{L|F_{z,m}|}{\hbar\omega_{k,m}},$$

where L is the length of the cylinder and $\omega_{k,m}$ is the plasmon surface mode frequency.

Then the average number of surface plasmons excited when an electron passes externally parallel to the cylinder axis with a velocity v is (see Fig. 2):

$$Q^{(e)\,\mathrm{wire}}_m = \frac{L}{\hbar\omega_{k,m}}\frac{(Ze\omega_p)^2}{v^2} x I'_m(x) I_m(x)[K_m(k\rho_o)]^2. \quad (1)$$

We define the scaled variables: $x = \omega_{k,m}a/v$ and $k\rho_0 = x\rho_0/a$. (See details in ref. [13]).

Complementarily, we obtain the average number of surface plasmons excited when an electron passes internally parallel to a capillary (cylindrical cavity) axis with a velocity v:

$$Q^{(e)\,\mathrm{capillary}}_m = \frac{L}{\hbar\omega_{k,m}}\frac{(Ze\omega_p)^2}{v^2} x K'_m(x) K_m(x)[I_m(k\rho_o)]^2. \quad (2)$$

(See Fig. 3 and details of the calculation in ref. [14]).

2.2. Presence of the residual hole

In addition, in the XPS and AES processes, the presence of a hole (ion) is another source of plasmon excitations. For calculating its influence, we assume that the hole remains static in front of the cylindrical surface and is created in an adiabatic way. This assumption is not the real one for electron emission, but represents a reasonable first approach to this process. The contribution to plasmon excitations due to the hole must be added to $Q^{(e)}_m$.

We can approximate such a contribution making the supposition that the cylinder surface can be assumed as planar, which is

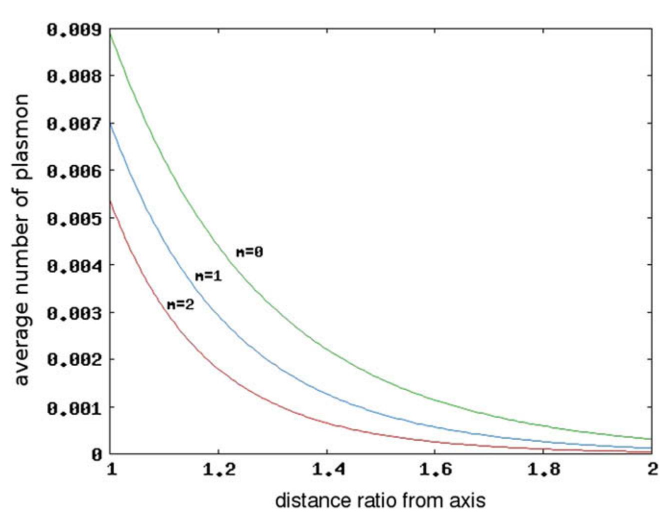

Fig. 2. Wire. Contribution over unit length $Q^{(e)}_m/L$ from the moving electron ($v = 4$ au) to the total number of surface plasmons for the modes $m = 0,1,2$, for an aluminium ($k_c = 0.626$ au, $\omega_P = 0.58$ au) cylinder ($a = 20$ au, $L = 200$ au), vs. distance ratio ρ_0/a.