Nuclear Instruments and Methods in Physics Research B 354 (2015) 197–199

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

In–out asymmetry in the interaction of a charged projectile traversing a vacuum–metal interface in an oblique trajectory

J.L. Gervasoni [a,b,*,1], S. Segui [a,1], R.O. Barrachina [a,b,1]

[a] Centro Atómico Bariloche (Comisión Nacional de Energía Atómica), R8402AGP S. C. de Bariloche, Río Negro, Argentina
[b] Instituto Balseiro (Universidad Nacional de Cuyo and Comisión Nacional de Energía Atómica), R8402AGP S. C. de Bariloche, Río Negro, Argentina

ARTICLE INFO

Article history:
Received 7 September 2014
Received in revised form 4 November 2014
Accepted 5 November 2014
Available online 2 December 2014

Keywords:
Plasmons
Energy loss
Interactions charged particle with condensed matter

ABSTRACT

In this work, we analyze the interaction of moving charged particles with plasmons in a semi-infinite material. For planar surfaces, and in the frame of a semiclassical dielectric formulation, we analyze the differences and similarities that arise when we compare incoming and outgoing trajectories in oblique incidence. We describe an oscillatory structure that only appears in the bulk contribution to the energy lost by an incoming projectile, and analyze how this in–out asymmetry depends of the angle of incidence.

1. Introduction

We study the excitation of plasmons by swift charged particles traversing the surface of a metal sample. These collective excitations are relevant in different spectroscopic techniques for studying surfaces, thin films and nanostructures, and their interest is maintained by the continuous improvements in high-resolution spectroscopic techniques [1,2].

The theoretical study of this kind of processes is usually based on quantized plasmon-field approaches or dielectric formulations, both providing valuable and complementary views of the quantum and semiclassical aspects of the problem [3]. However, here we are particularly interested in analyzing any difference that might appear for a projectile traversing a metal–vacuum planar interface in incoming or outgoing trajectories. To this end, we assume that the trajectory remains largely undisturbed by the plasmon excitation events. In particular, and except for the single scattering yielding the backscattered electrons, the effects of other elastic electron scattering are neglected. These approximations hold for sufficiently large kinetic energies, namely $mv^2/2 \gg \hbar\omega_p$, where m and v are the mass and velocity of the projectile, respectively, and ω_P is the plasmon frequency of the metal.

We employ the specular reflection model and extended pseudo-medium method [4–7] in order to analytically evaluate the induced potential and the energy dissipation rates due to plasmon excitations. Finally, we carry the present study not only for trajectories that remain perpendicular to the surface, as investigated in a previous article [8], but also for oblique trajectories, thus analyzing the dependence of the in–out asymmetry as a function of the incidence angle θ.

2. Induced potential and energy loss

We consider a particle of charge Z traversing the interface between vacuum and a medium of a given dielectric function $\epsilon(\mathbf{k},\omega)$ located in the semi-space $z<0$ in a rectilinear trajectory $\mathbf{v}t$. The electric potential reads,

$$\phi(\mathbf{r},t) = \phi_M(\mathbf{r},t)[1-\Theta(z)] + \phi_V(\mathbf{r},t)\Theta(z),$$

where $\Theta(z)$ is Heaviside step function, and (Atomic Units are used throughout this article)

$$\phi_M(\mathbf{r},t) = \frac{1}{(2\pi)^4}\int d\mathbf{k}\int d\omega\, e^{i(\mathbf{k}.\mathbf{r}-\omega t)}\phi_M(\mathbf{k},\omega),$$

$$\phi_V(\mathbf{r},t) = \frac{1}{(2\pi)^4}\int d\mathbf{k}\int d\omega\, e^{i(\mathbf{k}.\mathbf{r}-\omega t)}\phi_V(\mathbf{k},\omega).$$

The Fourier transformed potentials are obtained in terms of the charge densities through Poisson's equation,

* Corresponding author at: Centro Atómico Bariloche (Comisión Nacional de Energía Atómica), R8402AGP S. C. de Bariloche, Río Negro, Argentina.

[1] Also members of the Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Argentina.

http://dx.doi.org/10.1016/j.nimb.2014.11.010
0168-583X/

$$\phi_M(\mathbf{k},\omega) = \frac{4\pi}{k^2\varepsilon(k,\omega)}\rho_M(\mathbf{k},\omega),$$
$$\phi_V(\mathbf{k},\omega) = \frac{4\pi}{k^2}\rho_V(\mathbf{k},\omega).$$

According to the specular reflection model [4–7], here we are treating the metal (M) and the vacuum (V) separately as if they were infinite using symmetrized charged densities

$$\rho_M = Z[\delta(\mathbf{r}-\mathbf{v}t) + \delta(\mathbf{r}-2(\mathbf{r}.\hat{\mathbf{z}})\hat{\mathbf{z}}-\mathbf{v}t)][1-\Theta(z)] + \sigma(\mathbf{r},t)\delta(z),$$
$$\rho_V = Z[\delta(\mathbf{r}-\mathbf{v}t) + \delta(\mathbf{r}-2(\mathbf{r}.\hat{\mathbf{z}})\hat{\mathbf{z}}-\mathbf{v}t)]\Theta(z) - \sigma(\mathbf{r},t)\delta(z).$$

These expressions incorporate the specular image of the projectile and a surface-charge density σ that serves to match the potential at the interface. Variations of these expressions have been proposed by different authors [4,9–12]. Here we incorporate the Heaviside step functions in order to assure that the projectile would not interact directly with the semi-space that it does not occupies, but only through the surface charge density σ. This density σ is fixed by the continuity of the potential at the interface, i.e. $\phi_M(\mathbf{r},t)|_{z=0} = \phi_V(\mathbf{r},t)|_{z=0}$. Finally, we subtract the vacuum field of the projectile in order to obtain the induced potential $\phi^{\text{ind}}(\mathbf{r},t)$.

The potential $\phi_V^{\text{ind}}(\mathbf{r},t)$ induced in the vacuum is completely associated to the surface charge density σ. A similar surface (S) contribution can be singled out from the potential induced in the medium, so that the contribution that remains can be entirely associated to the interaction of the charge Z with the bulk (B). This bulk contribution is similar to the induced potential within an infinite material, except for the presence of the image charge, namely

$$\phi_B^{\text{ind}}(\mathbf{r},t) = \Theta(-z)\left[\tilde{\phi}_B^{\text{ind}}(\mathbf{r},t) - \tilde{\phi}_B^{\text{ind}}(\mathbf{r}-2z\hat{\mathbf{z}},t)\right].$$

Thus, we see that the induced potential $\phi_B^{\text{ind}}(\mathbf{r},t)$ is made up of two contributions. One reaching the point $\mathbf{r}$ directly from the projectile, and another one (with a phaseshift of π) through a reflection on the surface [8]. In particular, deep inside the material (i.e. for $z \ll 0$), the direct contribution $\tilde{\phi}_B^{\text{ind}}(\mathbf{r},t)$ approaches the potential induced in an infinite medium.

Finally, we evaluate the energy loss rate as

$$\frac{\mathrm{d}W}{\mathrm{d}t} = Z\frac{\partial\phi^{\text{ind}}(\mathbf{r},t)}{\partial t}\bigg|_{\mathbf{r}=\mathbf{v}t},$$

and again separate it into surface (S) and bulk (B) contributions.

For the calculation of these induced potentials and energy loss rates, it is customary to extended to infinity the limits of integration over the component of $\mathbf{k}$ perpendicular to the surface (see e.g. [7], and references therein), keeping the usual cutoff [13,14] of the plasma response function only in the parallel component of k, namely $k_{\|} \leqslant k_c$ with

$$k_c = \omega_P\sqrt{\frac{1}{v_F^2}-\frac{1}{v^2}},$$

where v_F is the Fermi velocity. Here, however, we are interested in studying oblique trajectories, where this approximation fails, Note that there is no physical reason to cut the integral in $\mathbf{k}$ only in one direction and not in the other [7,13], and that by doing so a spurious spatial asymmetry is introduced that might lead to unrealistic results. For instance, it produces a dependence of the energy loss on the incidence angle at asymptotic distances from the surface, as explained in the following section. For this reason, in this article we avoid this standard approximation, and keep the cutoff symmetrically in all the directions of $\mathbf{k}$, i.e. $k \leqslant k_c$. This generalization singles out our results from previous calculations (see e.g. [3,7,8], and references therein).

3. Particle traversing a vacuum–metal interface with oblique incidence

Since we are particularly interested in analyzing any difference that might appear in incoming or outgoing trajectories due to plasmon excitations processes, we apply the previous results to the particular case of a classical frequency – dependent dielectric function $\epsilon(\omega) = 1 - \omega_P^2/\omega(\omega + i\gamma)$ [15]. Here, ω_P and γ are the plasma frequency and damping rate of the metal, respectively.

It is assumed that the surface contribution to the energy loss is the same for incoming and outgoing trajectories [8,16], and thus it will not be considered any further in this article. Let us only mention that this in–out symmetry of the surface plasmon production occurs within the limitations of the present model, and that more comprehensive descriptions [11,12] might lead to the appearance of similar effects as the ones shown here for bulk plasmons.

In Figs. 1–3 we show the bulk contribution to the energy loss rate as a function of the distance to the surface $z = v_\perp t$ of an incoming ($v_\perp < 0$) or outgoing ($v_\perp > 0$) projectile for different incidence angles θ, measured with respect to the surface's normal. In particular, notice that the results for normal trajectories ($\theta = 0°$),

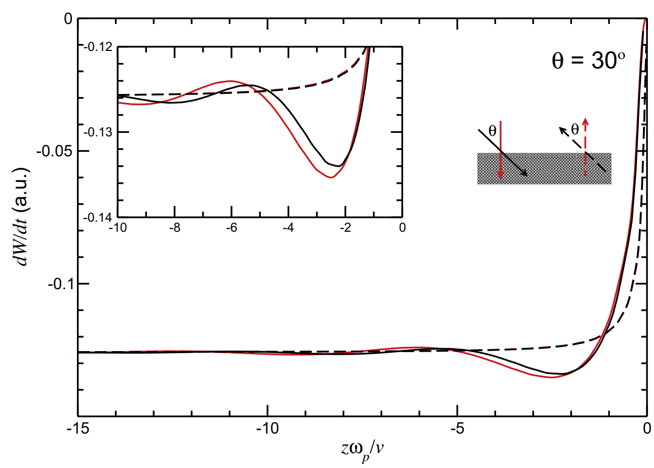

Fig. 1. Bulk contribution to the energy lost per time unit by a projectile of charge Z traversing the interface of an aluminum sample (located at $z < 0$) with velocity $v = 10$ au and angle $\theta = 30°$. Continuous black line: incoming trajectory; dashed black line: outgoing trajectory. Continuous gray (red in on-line version) line: incoming perpendicular trajectory ($\theta = 0°$), dashed gray (red in on-line version) line: outgoing perpendicular trajectory ($\theta = 0°$), included for reference.

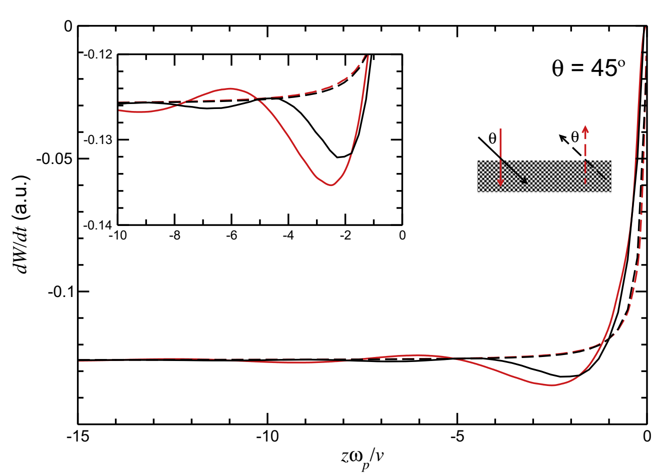

Fig. 2. Same as Fig. 1 with $\theta = 45°$.

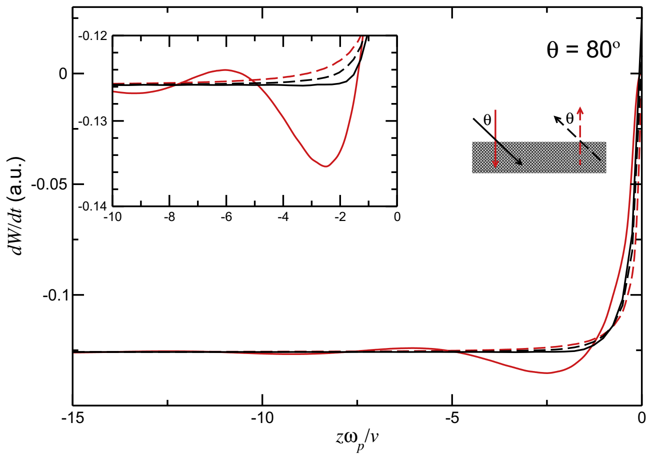

Fig. 3. Same as Fig. 1 with $\theta = 80°$.

included in the plots for reference, are almost identical to those obtained previously with the standard cutoff $k_{||} \leqslant k_c$ [3,8].

Both for incoming and outgoing trajectories, dW_B/dt deep within the solid tends to a constant value that is independent of the angle θ (and equal to that within an infinite medium). Note that this result differs from that of previous articles [3], where the asymptotic limit $z \to -\infty$ showed a spurious dependence on the incidence angle due to the use of the standard cutoff of the plasma response function.

The bulk contribution to the energy loss becomes zero for $z > 0$, as expected, since the induced potential cannot act on the projectile when it is outside the material. Furthermore, the *begrenzung* effect, by which dW_B/dt is drastically reduced in the vicinity of the surface interior, is also clearly observed.

In spite of these similarities, we see that the energy lost by incoming projectiles is very different from the outgoing case. In fact, it shows an oscillatory contribution that is not present for outgoing trajectories, and is still clearly visible for angles as large as 45°, as shown in Fig. 2. However this oscillation fades away with increasing angles θ. For instance, at $\theta = 80°$ it is negligible, and the energy loss rates for incoming and outgoing trajectories have become similar to each other, as shown in Fig. 3.

4. Conclusions

By means of a semiclassical dielectric formulation and by using the specular reflection model and the extended pseudo-medium method, we have found that the energy lost by a charged projectile traversing the planar surface of a semi-infinite material at an oblique trajectory is essentially different for outgoing and incoming trajectories. While for the former the bulk plasmon production is almost identical to that within an infinite medium, an oscillatory structure is observed when the projectile penetrates the material. Even though the begrenzung effect is present in both cases, the oscillations are only observed for incoming trajectories.

This effect was already studied in a previous article [8], but only for perpendicular trajectories ($\theta = 0°$), and with an anisotropic response function within the medium. Here we have removed this approximation and extended the calculation to oblique trajectories. By doing so we found that deep inside the solid semi-space, the bulk contribution to the energy loss rate is independent of the angle θ, and equal to that within an infinite medium, as expected. This result differs from previous calculations that showed a spurious dependence on θ. On the other hand, we found that the oscillations that were observed for incoming perpendicular trajectories persist for oblique incidence, even though they fade away for very large values of θ.

Finally, let us point out that even though we have employed a Drude-type approximation for $\epsilon(\mathbf{k}, \omega)$, the present discussion still applies when allowance is made for spatial dispersion, provided that the projectile moves faster than the group velocity in the medium [3].

Acknowledgments

This work was supported by the Consejo Nacional de Investigaciones Científicas y Técnicas (Grant PIP 11220120100374) and Universidad Nacional de Cuyo (Grant Nos. 06/C416 and 06/C435). The authors are also members of the Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Argentina.

References

[1] R. Raether, Excitations of Plasmons and Interband Transitions by Electrons, Springer Tracts in Modern Physics 88, Springer, Berlin, 1980.
[2] R.F. Egerton, Electron Energy-Loss Spectroscopy in the Electron Microscope, Springer-Verlag, Berlin, 1996.
[3] C.D. Denton, J.L. Gervasoni, R.O. Barrachina, N.R. Arista, Phys. Rev. A 57 (1998) 4498.
[4] R.H. Ritchie, A.L. Marusak, Surf. Sci. 4 (1966) 234.
[5] F. García Moliner, F. Flores, Introduction to the Theory of Solid Surfaces, Cambridge University Press, Cambridge, 1978.
[6] F. Flores, F. Garcia-Moliner, J. Phys. C: Solid State Phys. 12 (1979) 907.
[7] J.L. Gervasoni, N.R. Arista, Surf. Sci. 260 (1992) 329.
[8] J.L. Gervasoni, S. Seguí, R.O. Barrachina, W. Werner, Surf. Interface Anal. 45 (2013) 1849.
[9] J.L. Gervasoni, Interacción de partćulas en movimiento con la materia (Ph.D. Thesis), Instituto Balseiro, Bariloche, 1992.
[10] Y.F. Chen, C.M. Kwei, Surf. Sci. 364 (1996) 131.
[11] F. Salvat-Pujol, Secondary-electron emission from solids: coincidence experiments and dielectric formalism (Dissertation), Technische Universität Wien, Vienna, 2012.
[12] F. Salvat-Pujol, W.S.M. Werner, Surf. Interface Anal. 45 (2013) 873.
[13] G.D. Mahan, Phys. Status Solidi B 55 (1973) 703.
[14] G.D. Mahan, in: L. Fiermans, J. Venik, W. Dekeyser (Eds.), Electron and Ion Spectroscopy of Solids, Plenum Press, New York, 1978.
[15] J. Lindhard, Kgl. Danske Videnslab. Selskab, Mat-Fys. Medd. 28 (1954) 1.
[16] C.M. Kwei, C.Y. Wang, C.J. Jung, Surf. Interface Anal. 26 (1998) 682.