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# Time-dependent induced potentials in convoy electron emission

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**Abstract**

We study the time-dependent induced potentials at the convoy electron position due to the self-interaction with a metal surface and to the shock wave created by the positive hole (vacancy) left. The time evolution of these potentials are calculated using the linear response theory. Results obtained are fitted with simple functions. We find that those two potentials nearly cancel each other in the first ten atomic units of time.


*Keywords:* Image potential; Convoy electron; Transient effects; Metal surface

## 1. Introduction

In grazing collisions of fast ions with metal surfaces, electrons from the inner shells are emitted while ions are specularly reflected. We are interested in the effect of the surface on the trajectory of those electrons following the ion with similar velocities; the so-called convoy electrons [1–6]. Besides the direct Coulomb interaction with the ion, convoy electrons feel other three induced potentials, namely:

– The potential induced by the interaction of the ion with the metal surface (projectile surface wake), $V^{\mathrm{p}}(\mathbf{r}_{\mathrm{p}})$.
– The self-interaction of the convoy electron due to the response of the metal surface (electron surface wake), $V^{\mathrm{e}}(\mathbf{r}_{\mathrm{e}}, t)$.
– The potential induced due to the interaction with the shock wave created by the positive hole left (inner vacancy) in the metal, $V^{\mathrm{h}}(\mathbf{r}_{\mathrm{h}}, t)$.

The coordinates $\mathbf{r}_{\mathrm{p}}$, $\mathbf{r}_{\mathrm{e}}$ and $\mathbf{r}_{\mathrm{h}}$ are taken with respect to the projectile, electron and hole respectively, and $t$ is the time. As it is considered in most cases, the ion moves with constant speed parallel to the surface $\mathbf{v}_0$ and the electron is supposed to travel near the projectile. Therefore, we will evaluate the interactions at $\mathbf{r}_{\mathrm{p}} \approx \mathbf{r}_{\mathrm{e}} \approx \mathbf{0}$ and $\mathbf{r}_{\mathrm{h}} \approx \mathbf{v}_0 t$ (see Fig. 1 for details). In this article we have simplified the calculations considering that the projectile, electron and hole are in the same line parallel to $\mathbf{v}_0$, and at the same distance from the surface $Z_0$ ($Z_0 > 0$ vacuum, $Z_0 = 0$ jellium border, and $Z_0 < 0$ bulk).

As the ion is moving with constant speed parallel to the surface, the projectile surface wake potential $V^{\mathrm{p}}(\mathbf{r}_{\mathrm{p}})$ can be treated in a stationary regime (time independent) within the projectile frame. But the other two, $V^{\mathrm{e}}(\mathbf{r}_{\mathrm{e}}, t)$ and $V^{\mathrm{h}}(\mathbf{r}_{\mathrm{h}}, t)$, strongly depend on the emission time and cannot be treated in the same way, but as transient processes. In this article we study the time-dependence of $V^{\mathrm{e}}(\mathbf{r}_{\mathrm{e}} \approx \mathbf{0}, t)$ and $V^{\mathrm{h}}(\mathbf{r}_{\mathrm{h}} \approx \mathbf{v}_0 t, t)$. The potential energy at the electron positions are then, $\phi^{\mathrm{p}} = -V^{\mathrm{p}}(\mathbf{0})$, $\phi^{\mathrm{e}}(t) = -(1/2)V^{\mathrm{e}}(\mathbf{0}, t)$, and $\phi^{\mathrm{h}}(t) = -V^{\mathrm{h}}(\mathbf{v}_0 t, t)$. Atomic units are used.

As it is well known, convoy electrons are accelerated by $\phi^{\mathrm{p}}$. It has been predicted by the simple image-charge model [7,5] and confirmed experimentally by Kimura

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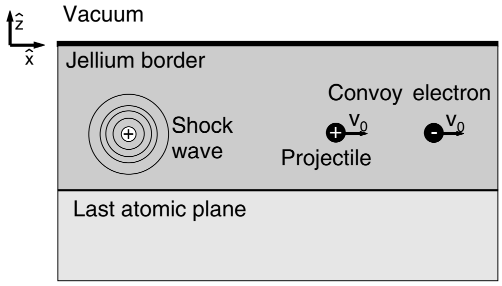


Fig. 1. Schematic diagram of the process.

and collaborators [4]. The acceleration of the convoy electrons was found to increase with the projectile Coulomb charge $Z_p$ [4]. The simplest way to deal with the interaction of point charges with surfaces is the stationary-image method [5]. In most of the works found in the literature, the electron trajectory is obtained in a time independent formalism, where the convoy electron self-interaction $\phi^e(t)$ is neglected [4,7,5], or is supposed to be created immediately, $\phi^e(t) = -(1/2)\phi^p/Z_p$ [8,9]. In all cases the shock wave created by the hole left, $\phi^h(t)$, was neglected. Kimura and collaborators [4] found a reasonable agreement of their experiments with the projectile surface wake model, i.e. in the presence of $\phi^p$ alone. A latter article confirmed that the experimental acceleration could be explained in the presence of only $\phi^p$ [10], neglecting $\phi^e(t)$. It is equivalent to stating that $\phi^e(t) = -(1/2)\phi^p/Z_p\Theta(t - T_e)$, and $T_e$ was supposed to be large for the cases considered.

The aim of this work is to answer two questions: first, how much time do the convoy electrons need to create their own image potential? Or mathematically, what is the time $T_e$ so that $\phi^e(t)$ reaches its stationary form $-(1/2)\phi^p/Z_p$? And second, can we really neglect the induced potential of the shock wave by the vacancy hole $\phi^h(t)$?

Our work will be developed within the framework of the time-dependent dielectric formalism. A useful approximation to describe the interaction of a charged particle with a metal surface is to use the specular reflectional model (SRM). The stationary potential induced by the ion has been extensively studied with this model [11,17]. Its extension to include a time-dependent formalism is very cumbersome from the numerical point of view; instead, we will use a recently proposed dielectric function derived from an axial model (AM) [19]. The AM dielectric response function is easier to evaluate and will make the calculation tractable. The AM model has proved to reproduce very well some parameters like the stopping, straggling and the inelastic mean free path obtained with the SRM.

The rearrangement of the electronic density has been long recognized as key concept in condensed matter physics. Screening plays a crucial role, for instance in photoexcitation [12]. Important theoretical developments in this field have being achieved by using the time-dependent density functional theory in two and three dimensions [13–15]. The time evolution of the Kohn–Sham orbitals within the independent particle picture yields an universal scaling of the charge depletion for short times.

This attempt follows previous works done by Canright [16], who calculated the time-dependent screening of a suddenly created point charge in an electron gas, and Alducin et al. [17] who obtained the surface wake potential induced once again by a point charge suddenly created in front of a metal surface.

## 2. Theory

The potential created by an external charge density due to the interaction with a metal surface, can be written in Fourier space as:

$$\widetilde{V}(\mathbf{k},\omega) = \frac{4\pi\widetilde{\rho}(\mathbf{k},\omega)}{k^2}\left(\frac{1}{\epsilon(\mathbf{k},\omega)} - 1\right), \tag{1}$$

where $\epsilon(\mathbf{k},\omega)$ is here the surface dielectric function and $\widetilde{\rho}(\mathbf{k},\omega)$ is the Fourier transform of the external charge density. All the variables: $\widetilde{V}$, $\widetilde{\rho}$ and $\epsilon$ depend parametrically on the distance of the projectile from the surface $Z_0$. The next steps are the derivations of $\phi^p$, $\phi^e$, and $\phi^h$.

### 2.1. Projectile surface wake potential

In grazing collisions the projectile path can be divided into subsequent segments parallel to the surface, therefore its charge density can be written as:

$$\rho^p(\mathbf{r},t) = Z_p\delta(y)\delta(x - v_0t)\delta(z - Z_0), \tag{2}$$

with $Z_p$ being the projectile charge, $v_0$ the parallel speed along the $\hat{x}$-axis at a distance $Z_0$ from the jellium border. See Fig. 1 for details. In the Fourier space this density is transformed into:

$$\widetilde{\rho^p}(\mathbf{k},\omega) = Z_p 2\pi e^{-ik_zZ_0}\delta(\omega - k_xv_0), \tag{3}$$

The induced potential is obtained by replacing Eq. (3) in (1) and anti-transforming Fourier. This leads us to:

$$V^p(\mathbf{r},t) = \frac{Z_p}{(2\pi)^2}\int\frac{d\mathbf{k}}{k^2}\int_{\infty}^{\infty} d\omega\delta(w - k_xv_0) \times \left[\frac{1}{\epsilon(\mathbf{k},\omega)} - 1\right]e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}. \tag{4}$$

This potential is time independent within the projectile reference frame. Typical plots of this potential can be found in Refs. [18,11]. In order to calculate the kinetic energy gained by the convoy electron (acceleration with respect to the projectile), this equation should be evaluated at the convoy electron position: $\phi^p = -V^p(\mathbf{0})$.

### 2.2. Convoy electron surface wake potential

In the case of the self-interaction of the convoy electrons, we consider that they are emitted at $t = 0$, following the projectile at the same distance $Z_0$ from the surface. We assume that the electron is assisted (pushed) by the projectile. The convoy electron charge density is then:

$$\rho^{\mathrm{e}}(\mathbf{r},t) = -\delta(y)\delta(x - v_0 t)\delta(z - Z_0)\Theta(t), \tag{5}$$

where $v_0$ is the convoy electron speed. The Fourier transformation of the last equation produces

$$\widetilde{\rho}^{\mathrm{e}}(\mathbf{k},\omega) = -\mathrm{i}\frac{\mathrm{e}^{-\mathrm{i}k_z Z_o}}{\omega - k_x v_0 + \mathrm{i}0^+}, \tag{6}$$

where $0^+$ represents a positive infinitesimal. Following the same procedure, the induced potential is obtained by combining Eq. (6) with Eq. (1), anti-transforming Fourier, and making $V^{\mathrm{e}}(t) = V^{\mathrm{e}}(\mathbf{0},t)$. Thus we obtain:

$$V^{\mathrm{e}}(t) = -\frac{2\mathrm{i}}{(2\pi)^3}\int\frac{\mathrm{d}\mathbf{k}}{k^2}\int_{\infty}^{\infty}\mathrm{d}\omega\left[\frac{1}{\epsilon(\mathbf{k},\omega)} - 1\right]\frac{\mathrm{e}^{\mathrm{i}(k_x v_0 t - \omega t)}}{\omega - k_x v_0 + \mathrm{i}0^+}. \tag{7}$$

Finally, the self energy $\phi^{\mathrm{e}}$ is calculated as half the induced potential evaluated at the convoy electron position $\phi^{\mathrm{e}}(t) = -(1/2)V^{\mathrm{e}}(t)$, One would expect that as $t \to \infty$, $\phi^{\mathrm{e}}(t) \to -(1/2)\phi^{\mathrm{p}}$.

### 2.3. Shock wave created by the hole

For the shock wave created by the hole left (inner shell vacancy), we consider that the vacancy is created again at $t = 0$, at the same distance $Z_0$ from the jellium border where which the electron has been emitted. Its charge density reads

$$\rho^{\mathrm{h}}(\mathbf{r},t) = \delta(y)\delta(x)\delta(z - Z_0)\Theta(t), \tag{8}$$

and in Fourier space,

$$\widetilde{\rho^{\mathrm{h}}}(\mathbf{k},\omega) = \mathrm{i}\frac{\mathrm{e}^{-\mathrm{i}k_z Z_0}}{\omega + \mathrm{i}0^+}, \tag{9}$$

The induced potential at the convoy electron position is calculated following the same procedure as in the previous cases to yield, $V^{\mathrm{h}}(t) = V^{\mathrm{h}}(\mathbf{v}_0 t, t)$,

$$V^{\mathrm{h}}(t) = \frac{2\mathrm{i}}{(2\pi)^3}\int\frac{\mathrm{d}\mathbf{k}}{k^2}\int_{\infty}^{\infty}\mathrm{d}\omega\left[\frac{1}{\epsilon(\mathbf{k},\omega)} - 1\right]\frac{\mathrm{e}^{\mathrm{i}(k_x v_0 t - \omega t)}}{\omega + \mathrm{i}0^+}. \tag{10}$$

and its potential energy is simply $\phi^{\mathrm{h}}(t) = -V^{\mathrm{h}}(t)$.

## 3. Numerical results

In this work, we report results for $\phi^{\mathrm{e}}(t)$ and $\phi^{\mathrm{h}}(t)$ considering protons colliding with aluminum surfaces (Fermi velocity $k_{\mathrm{F}} = 0.92$, lifetime $\gamma = 0.0375$). The AM was used to represent $\epsilon(\mathbf{k},\omega)$, as given by Eq. (8) of Ref. [19] with a minor change.[1] Three-dimensional integrals were required to obtain a value of $\phi^{\mathrm{e,h}}(t)$.

Fig. 2 displays the convoy electron potential energy $\phi^{\mathrm{e}}$ as a function of time, for distances from the jellium border $Z_0$ of 1, 0 and −1, and for $v_0 = 2$, 3, 4 and 5, as indicated. It should be mentioned that the last atomic plane of the Al (1 1 1) is placed at $Z_0 = -2.2$ a.u. The two limits are easily recognized: $\phi^{\mathrm{e}}(0) = 0$, and $\phi^{\mathrm{e}}(\infty) = -\frac{1}{2}\phi^{\mathrm{p}}/Z_{\mathrm{p}}$. To study the ranges of time, we have also included a fitting in solid line a function of the type:

$$\phi^{\mathrm{e}}(t) \propto 1 - \frac{(B\cos(\omega_{\mathrm{s}}t) + (1 - B)\cos(\omega_{\mathrm{b}}t))}{1 + t(1 - \mathrm{e}^{-t/T_{\mathrm{e}}})}. \tag{11}$$

which guarantees the two boundary limits. This fitting has a linear combination of oscillations, with $\omega_{\mathrm{s}} = 0.406$ the plasmon surface oscillation frequency, and $\omega_{\mathrm{b}} = 0.576$ the plasmon bulk frequency. The factor $B$ depends on $v$ and $Z_0$. For $Z_0 \geqslant 0$, $B = 1$, while for $Z_0 < 0$, $B$ tends slowly to zero depending on the velocity. For example, for $Z_0 = -1$, we have obtain the values $B = 0.67$, 0.77, 0.83, and 0.87, for $v = 2$, 3, 4 and 5, respectively.

We can identify two transients: one for $t < T_{\mathrm{e}}$, and the other for $t > T_{\mathrm{e}}$. The first transient falls off very rapidly (exponentially), while the second one for $t > T_{\mathrm{e}}$, $\phi^{\mathrm{e}}(t)$ tends slowly to the limit oscillating with an amplitude of $1/t$. In all cases, $T_{\mathrm{e}} \approx 5$; that is more than twice the estimated value $\pi/(4\omega_{\mathrm{b}})$ given in Ref. [10].

Similarly, Fig. 3 displays the hole shock-wave energy $\phi^{\mathrm{h}}$ for the same impact velocities and distances from the surface as a function of time. The two limits are obviously null here, i.e. $\phi^{\mathrm{h}}(0) = \phi^{\mathrm{h}}(\infty) = 0$.

The solid line represents a fitting of the type:

$$\phi^{\mathrm{h}}(t) \propto \frac{1 - \mathrm{e}^{-t/T_{\mathrm{h}}}(B\cos(\omega_{\mathrm{s}}t) + (1 - B)\cos(\omega_{\mathrm{b}}t))}{t}. \tag{12}$$

valid for $t \in \{0,80\}$. We obtain the same values for $B$ as in the previous case, while $T_{\mathrm{h}}$ is around 50 ($T_{\mathrm{h}} \gg T_{\mathrm{e}}$). Again we can identify two regimes; the first one, $t < T_{\mathrm{h}}$ which decays exponentially, corresponds to the hole shock wave and the second one, for $t > T_{\mathrm{h}}$.

It is very important to note that in the range $t \in \{0, 2T_{\mathrm{e}}\}$, it holds that $\phi^{\mathrm{h}}(t) \approx -\phi^{\mathrm{e}}(t)$. It means that, to some extent, both potentials cancel each other. One could roughly say that the total potential $\phi^{\mathrm{h}} + \phi^{\mathrm{e}}$ is small up to $t \approx 2T_{\mathrm{e}}(\phi^{\mathrm{h}} + \phi^{\mathrm{e}} = 0 + \mathcal{O}(t/T_{\mathrm{e}}))$. See Fig. 4 for details.

Qualitatively one could have predicted the cancellation of $\phi^{\mathrm{h}}$ and $\phi^{\mathrm{e}}$, as it is explained below. For small times, the newly created charges (electron and vacancy) are of different signs and are born at the same place. In this situation, the electron repels the electronic cloud, unlike the vacancy, which attracts one. Then a sort of cancellation should take place an the electronic cloud remains unaltered. As time proceeds, both charges separate, sampling different electronic regions and so the potentials decorrelate. As the electron escapes, captured into the continuum of the projectile, the hole is left far behind. Finally, the electron builds its own accompanying potential, thus

[1] The magnitude $q'_{\parallel}$ given by Eq. (9) of Ref. [19] was changed to $q'_{\parallel} = \sqrt{0.222q^2 + 0.778(\omega/v)^2}$. It can be proved that the potential so-defined satisfies the image charge limit as $v_0 \to 0$.

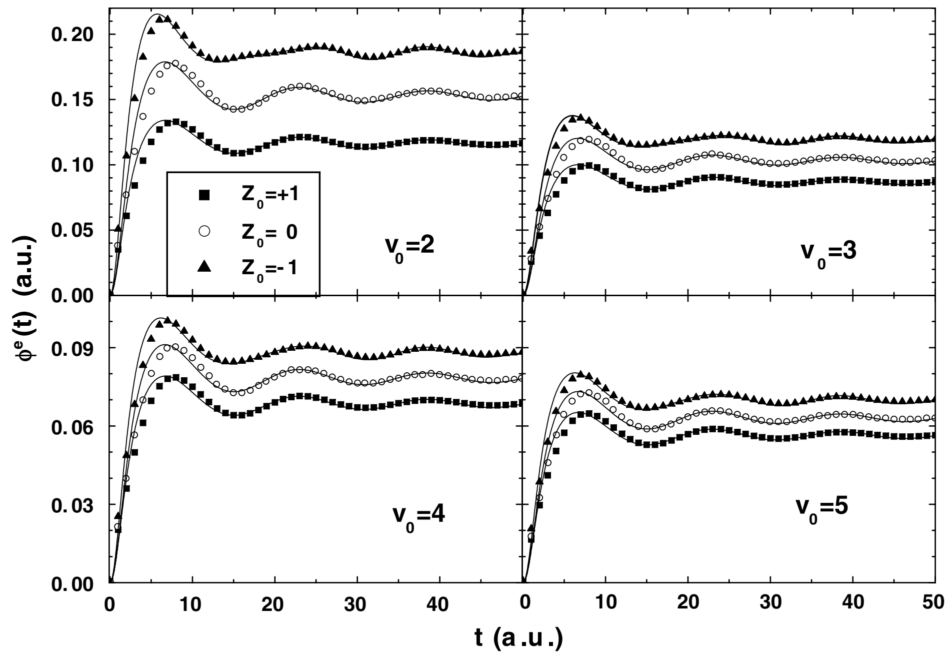


Fig. 2. Convoy electron self-interaction $\phi^{e}(t)$ on aluminum surface as a function of the time for different velocities and distances to the jellium border, as it is indicated. Solid line fitting given by Eq. (11).

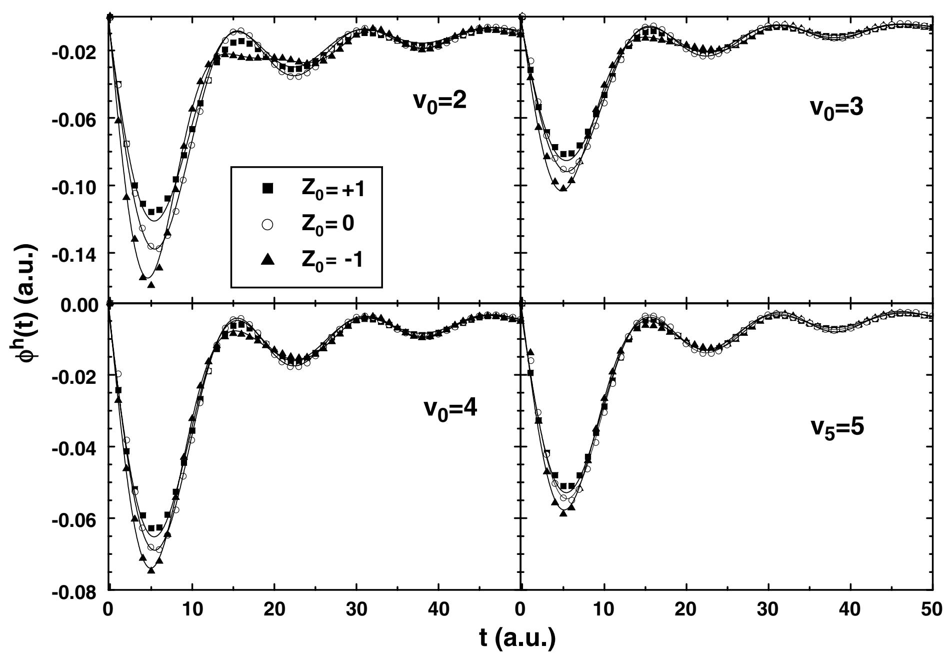


Fig. 3. Potential induced by the hole at the convoy electron position $\phi^{e}(h)$ on aluminum surface as a function of the time for different velocities and distances from the jellium border, as indicated. Solid line fitting given by Eq. (12).

reaching a stationary regime. It is quite possible that this behaviour at short times is a consequence of the scaling law mentioned in the introduction (see Appendix of Ref. [13]).

This is a very important conclusion of this work, because we could state that for times less than – say 10 a.u. – the only acceleration energy left is $\phi^{p}$. One can prove with a classical model that in this period of time the electron acquires a substantial part of the acceleration. According to this finding, it would be a good approximation to neglect the electron self-interaction; the explanation is that it has been cancelled by the shock wave created by the vacancy left.

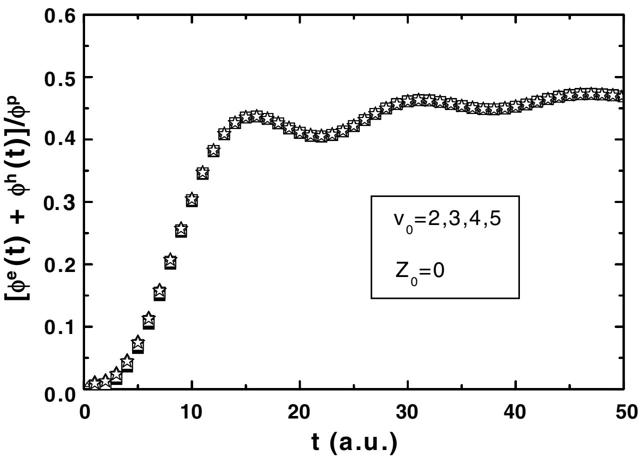


Fig. 4. Sum of the electron plus hole potentials induced at the convoy electron position divided by the one induced by the projectile as a function of time for different velocities and for $Z_0 = 0$.

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