Contributed Paper

POTENTIAL ENERGY CALCULATIONS OF A CHARGED PARTICLE OUTSIDE A REAL METAL SURFACE

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Abstract. In this work we consider a more complex system with the point charge located between the real metal covered with thin dielectric film and multiply charged ion. In many cases, precise knowledge of the potential energy of a charge particle outside a real planar surface is very important for deep understanding many transfer processes. For metal-vacuum interface, the charge transfer play a significant role especially for photo and thermionic-emission and also in a different ion beam processes. Furthermore in electron diffraction and positron diffraction spectroscopy as well as in scanning tunneling microscopy, charge transfer between a metal and the vacuum is also involved.

1. LIMITATIONS OF THE CLASSICAL CHARGE-METAL SURFACE INTERACTION

The method of image charges is a basic problem-solving tool in electrostatics, see Jennings et al. 1988. The name originates from the replacement of certain elements in the original layout with imaginary charges, which replicates the boundary conditions of the problem.

Let's take a look at the potential energy of a point charge outside a planar surface. By using the method of mirror charges, we get the following expression for the potential energy of a charge q located at a distance d $(d > 0)$ from the metal vacuum interface:

$$V(d) = -\frac{q^2}{16\pi\varepsilon_0 d}. \tag{1}$$

There are several problems. From the above equation we will see that for $d \to 0$, classical image potential diverges to $-\infty$. This has no physical meaning since the potential energy inside a grounded metal is finite. That is obviously a huge problem because the description becomes unrealistic in the region which is very important for investigation of all surface processes. The use of appropriate models, like surface barrier model, is one of the ways to overcome the limitation of the classical approach.

Here we point out, that there is a big difference between short range electron-metal surface interaction and large ions-metal surface interaction, see Aumayr et al. 2011. Namely, large ions slowly approaching the metal surface interface feel the potential well because of the short range repulsion from the ion cores as the constituent elements

of the crystal lattice. Also, from the standpoint of classical physics, the precise determination of the metal surface position is not so important, but if we investigate for instance the charge transfer processes, knowledge about the position of the image plane relative to the layers of metal atoms, is of crucial importance. Moreover, we do not take into account electron-electron interaction, which means that we consider external electrons to be physically distinguishable from the electrons contained in metal under consideration. So, the classical electrodynamics can not specify which of the barrier models should be taken into account for appropriate interaction between incoming or outgoing charge with electrons in the considered metal. In that way, we need strict quantum mechanical calculations of interaction.
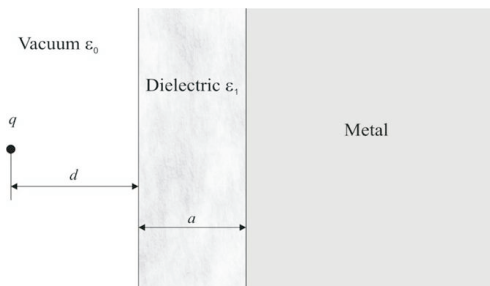

Figure 1: A point charged particle q at a distance d from the metal surface covered with a thin oxidized film. The thickness a reaches several nanometers.

2. THE METAL SURFACE COVERED WITH A THIN OXIDIZED FILM

Advantage of the image method is reflected in the fact that it can be applied not only in the case when we have a charge particle outside a metal or dielectric surface but also in the most realistic case of the interaction between a charged particles with real (oxidized) surface (see Fig. 1) effectively using analogy with optics. In this approach, after collision of the incident plane electromagnetic wave with real metal surface, the amplitude of the transmission and reflection coefficients are discussed.

For a point charged particle q positioned at a normal distance d from the metal covered by a very thin oxidized dielectric film with permittivity ε_1 (see Lake et al. 2011.), the potential energy can be expressed in the following form

$$V(d) \approx -\frac{q^2}{16\pi\varepsilon_0}\frac{1}{d+\frac{a}{\chi}}, \tag{2}$$

introducing dielectric constant of the thin oxidized film $\chi = \varepsilon_1/\varepsilon_0$ (under the condition $a \ll d$). The thickness a reaches several nanometers.

3. APPLICATION

As an illustrative example of the above analysis, we consider the population or partial neutralization of the Rydberg states of multiply charged ions interacting with

solid surfaces. That is, obviously, typical electron transfer process from solid structure to the ion. Considering the population of the Rydberg states ($n_A \gg 1$) of highly charged ions ($Z \gg 1$) interacting with solid surfaces, two aspects of the process can be analyzed. The first one is devoted to the intermediate stages of the population dynamics. These stages are characterized by the neutralization rates and the neutralization distances R_c^N, see Galijaš et al. 2019. The final population probabilities represent another important aspect of the process. Namely, from the population distributions one can recognize the Rydberg states $\mid n_A, l_A, m_A >$ with principal quantum number n_A and angular momentum quantum number l_A, that are dominantly populated. The both aspects of the population process have been considered in the last twenty years and still represent an open theoretical problem, see Nedeljković et al. 2012, Nedeljković et al. 2014. In order to find appropriate neutralization distances for example, or any other values which characterized the population process, we have to estimate the potential energy function, i.e., to estimate the electron potential energy at any point between real metal surfaces and approaching or outgoing ion subsystem (in our case in normal direction related to the metal surface).
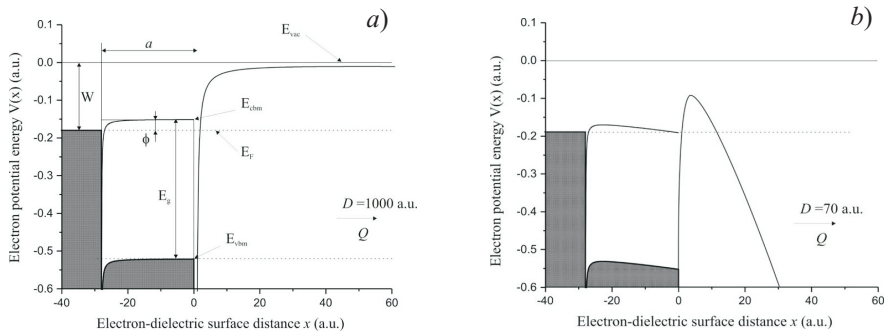

Figure 2: The electron potential energy inside metal Co, inside dielectric Al_2O_3 and between the dielectric surface and ion charge $Q = 44$ for a) $D = 1000$ a.u. and b) $D = 70$ a.u.

The potential energy V for an active charge q located in the region between the surface under consideration and the ion with charge Q is composed of three contributions: attraction between the charge q and its own image V_{qS}, direct interaction between the charge q and the ion V_{qQ} and interaction between the charge q and the ions self-image because of the existence of the metal-dielectric V_{qIQ}. If we restrict our consideration to the ionic states with large eccentricities, i.e. with low values of angular momentum quantum number, only a narrow cylindrical area around the ion trajectory participate in electron exchange process from real metal to ion during the neutralization process or in opposite way, during the reionization process. In that case we get

$$V \approx \frac{q^2}{16\pi\varepsilon_0} \left[\frac{-\eta}{d} + \frac{(1-\eta^2)}{\eta} \sum_{k=1}^{\infty} \frac{(-\eta)^k}{d+ka} \right] + \frac{1}{4\pi\varepsilon_0} \frac{qQ}{D-d}$$
$$+ \frac{qQ}{4\pi\varepsilon_0} \left[\frac{-\eta}{D+d} + \frac{(1-\eta^2)}{\eta} \sum_{k=1}^{\infty} \frac{(-\eta)^k}{D+d+ka} \right], \tag{3}$$

where $\eta = (\varepsilon_1 - \varepsilon_0/\varepsilon_1 + \varepsilon_0)$ denotes the dielectric function while the ion with charge Q is positioned at a normal distance D from the metal covered by dielectric film.

Inside the dielectric, the image potential V_{in} is screened by the dielectric media as ε^{-1}. Additionally, within the dielectric film, the reference energy becomes the conduction band E_{cbm} instead of the vacuum level. Along these lines, the potential energy of the point charge q inside the dielectric is given by

$$V_{in} = E_{cbm} - \frac{q^2}{16\pi\varepsilon_0\varepsilon(d + a)} + \frac{qQ}{4\pi\varepsilon_0\varepsilon(D - d)} - \frac{qQ}{4\pi\varepsilon_0\varepsilon(D + d + 2a)}. \tag{4}$$

The last two terms in Eq. (4) represent the additional contribution of the ion in our system.

4. DISCUSSION

In Fig. 2 we present the potential for an electron when an ion ($Q = 44$) is far away from dielectric surface at $D = 1000$ a.u. As an example we have considered Co, whose Fermi level is 5 eV (≈ 0.18 a.u.) below the vacuum level, covered with Al_2O_3. The dielectric layer has thickness $a = 1.5$ nm (≈ 28a.u.) with fixed band gap $E_g = 9.9$ eV (≈ 0.36a.u.) and dielectric permittivity $\varepsilon_1 = 9$ ($\eta = 0.8$). Electrons in the solid are restricted from entering the vacuum region by the barrier ϕ from $-a < x < 0$, and the work function W outside the dielectric. With E_{cbm} and E_{vbm} we denote the bottom of the conduction and the top of the valence band described through functions $V_{cbm}(x)$ and $V_{vbm}(x)$, respectively. E_F is Fermi level and E_{vac} is the vacuum level.

In the case when the ion charge Q comes close to the dielectric surface ($D = 70$a.u.), the potential curve changes in a way presented in Fig. 2b. Figs. 2a and 2b show the evolution of the barrier heights in the vacuum and in the dielectric regions as the ion (Q = 44) approaches the surface.

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