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Sputtering of Metal Atoms by Surface Wake Potential

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Using the corona discharge example, the interaction of charged particles beam with a metal surface, which leads to the sputtering of the electrode substance, is considered. When a fast charged particle moves near and through the condensed state, fluctuations in the electron density of the metal electrode occur, which lead to the emergence of the surface wake potential (the surface plasmons). In this work, the cross-section expression was obtained for the electrode atoms sputtering under the influence of the surface wake potential excited by the movement of a charged particle near the electrode surface. It is shown that the sputtering result depends on the magnitude of the charge and energy of the incident particle. It is noted that surface plasmons excitations play an important role when the sliding angle of incident beams of charged particles on the metal surface becomes small. The sputtering coefficient value during the interaction of the electron beam with the silver surface is estimated.

Keywords: corona discharge, metallic surface, inelastic scattering, surface plasmons excitation, surface wake potential, metal sputtering.

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1. Formulation of the problem

To create nanoscale elements in modern technologies the processes are used, which are associated with electric discharges [1]. When obtaining objects with size of about fractions of nanometers the corona discharge is used [2,3]. During the corona discharge the electrode substance evaporation is observed, this is indicated by appearance of cavity at place plasma cord contact with the electrode surface [4–6]. It is easy to determine the nature of electrode atoms transition in gaseous state using the corona discharge [6] due to small energies (about tens of keV). This paper offers a theoretical metal sputtering model. It is shown that interaction of atoms of metal flat surface with surface wake potential [7–10] excited by incident charged particles of the corona discharge is the cause of abnormal atom emission.

Let's consider passage of fast charged particle through the interface vacuum-solid. During fast charged particle movement near and through the solid there are electron density fluctuations which generate the wake potential associated with passage of fast charged particle near the solid surface. When the corona discharge is implemented in air the electric field strength occurs (about several tens of kV/cm). Generally one of electrodes is made as needle,the second one is metal ring, this is shown schematically in Figure 1. At electric field strength E above some critical value the ambient air ionization starts. Particles of corona discharge (electrons or positive ions, depending on direction of the electric field applied to electrodes) bombard the needle surface. Note that bombarding particles fall at sliding angle to the needle surface.

The suggested model of the process includes the following. Due to Coulomb interaction of the incident charged particles of the corona discharge with electronic gas of metal needle these particle excite own oscillations of electronic gas density of electrode-emitter, both volume, and surface. Among them localized on surface oscillations — so called surface plasmons (SPs), bonded electron-photon modes (surface plasmon-polariton) [11–13], and volume oscillations of electronic gas (volume plasmons) [12,14], called wake potential (Figure 2). The charged particle bombarding the electrode due to the Coulomb interaction excites the surface wake potential (SWP) [12].

In paper [12] we consider the theory SWP excitation on metal surface with characteristic frequency ω_s. Let's consider closed loop Γ, containing part of metal surface (electrode-emitter) with electronic gas, it does not contain free charges (Figure 3).

Integral of electric offset vector $\vec{D}$ over closed loop Γ is equal to zero: $\oint D_n dS = 0$. Assuming in vacuum for normal component of electric offset vector $D_n = D_n^0$, and in metal $D_n = D_n^1$, we can write the following equality:

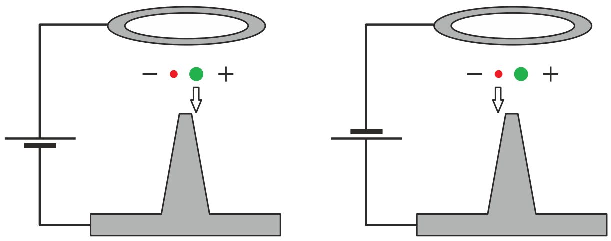

Figure 1. Schema of corona discharge.

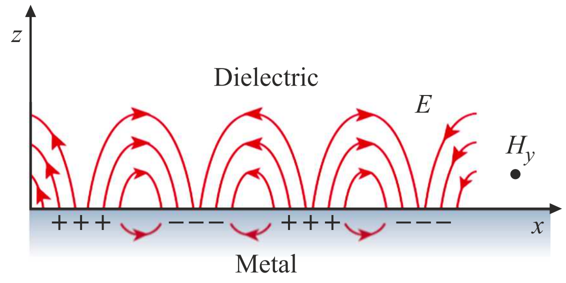

Figure 2. Surface plasmons on flat surface.

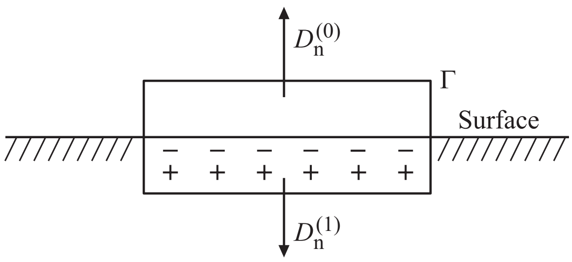

Figure 3. Continuity of vector of electrical offset on metal surface of electrode-emitter.

$D_n^0 + D_n^1 = 0$, or $\varepsilon_0 E_n + \varepsilon_1 E_n = 0$, where ε_0 — dielectric permittivity of vacuum $\varepsilon_0 = 1$ and $\varepsilon_1 = 1 - \omega_p^2/\omega_s^2$ (where ω_p — plasma frequency) — dielectric permittivity of metal [10]. Thus, we obtain

$$\varepsilon_0 + \varepsilon_1 = 0, \quad \text{or} \quad 1 + (1 - \omega_p^2/\omega_s^2) = 0.$$

From here we determine the natural oscillation frequency of surface potential: $\omega_s = \omega_p/\sqrt{2}$ [11]. SWPs interact with ion of crystal lattice of electrode-emitter. Our task is to evaluate the energy of such interaction, and show that it is sufficient to ejection of the ion from metal ($\hbar\omega_s > E_b$, where E_b — bond energy of ion in lattice of metal material).

2. Excitation of dynamic surface wake potential

In paper [12] the general formula for dynamic surface wake potential was obtained for the case when fast particle with charge e and mass m moves with speed $\vec{v}$ in relation to metal surface. Distribution Z_2 of external charges

$$\rho_{\text{ext}}(\vec{r}_2, t_2) = Z_2 e \cdot \delta(\vec{r}_2 - \vec{v}t_2),$$

located in point $\vec{r}_2$ at time moment t_2, leads to creation of potential $\varphi_{\text{eff}}(\vec{r}_1, t_1)$ in point $\vec{r}_1$ at time moment t_1:

$$\varphi_{\text{eff}}(\vec{r}_1, t_1) = \int d\vec{r}_2 \int dt_2 W(\vec{r}_1, \vec{r}_2; t_1 - t_2) \cdot \rho_{\text{ext}}(\vec{r}_2, t_2),$$

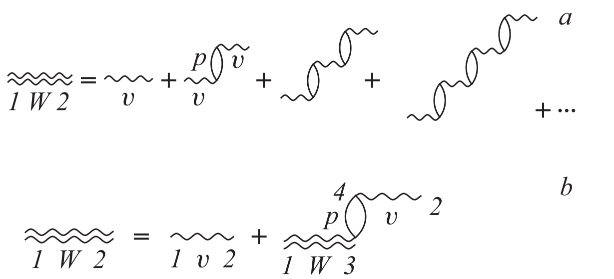

Figure 4. Diagram for calculating the response function W: *a*) equation for W in form of infinite series, *b*) equation for W in form of Dyson equation. Separate loop corresponds to single polarization (P), ordinary wavy line — to Coulomb potential (v), and double wave line —to response function (W). Number mark: *1* — initial, *2* — final, *3* and *4* — intermediate states.

where $W(\vec{r}_1, \vec{r}_2; t_1 - t_2)$ — response function complying with integral equation (Figure 4)

$$W(\vec{r}_1, \vec{r}_2; t_1 - t_2) = v(\vec{r}_1, \vec{r}_2; t_1 - t_2) + \int W(\vec{r}_1, \vec{r}_3; t_1 - t_3) P(\vec{r}_3, \vec{r}_4; t_3 - t_4) \times v(\vec{r}_4, \vec{r}_2; t_4 - t_2) \int d\vec{r}_3, dt_3 \int d\vec{r}_4, dt_4,$$

where the Coulomb potential $v(\vec{r}_1, \vec{r}_2; t_1 - t_2)$ has form

$$v(\vec{r}_1, \vec{r}_2; t_1 - t_2) = \frac{Z_2 e}{|\vec{r}_1 - \vec{r}_2|} \cdot \delta(t_1 - t_2),$$

and polarization function [13] $P(\vec{r}_1, \vec{r}_2; t_1 - t_2)$ is written as

$$P(\vec{q}_1, \vec{q}_2; \omega) = -\frac{\vec{q}_1 \vec{q}_2}{m\omega^2} \cdot n(q_1 + q_2).$$

here $n(q)$ — Fourier transform of electron density.

Assuming that electron density has step-like form — $n(\vec{r}) = n_0 \theta(z)$, where

$$\theta(z) = \left\{ \begin{array}{ll} 1 & \text{inside the metal volume} \, (z > 0) \\ 0 & \text{outside the volume of a solid} \, (z < 0) \end{array} \right\},$$

we can obtain solution of the integral equation for dynamic response function W [15]:

$$W(\vec{r}_1 - \vec{r}_2; t_1 - t_2) = \frac{Z_2 e}{[(\vec{\rho}_1 - \vec{\rho}_2)^2 + (z_1 - z_2)^2]^{1/2}} \delta(t_1 - t_2) \quad (1)$$

$$- \frac{Z_2 e}{[(\vec{\rho}_1 - \vec{\rho}_2)^2 + (z_1 - z_2)^2]^{1/2}} \times \omega_p \sin[\omega_p(t_1 - t_2)] \cdot \theta(t_1 - t_2)\theta(z_1) \quad (2)$$

$$+ \frac{Z_2 e}{[(\vec{\rho}_1 - \vec{\rho}_2)^2 + (|z_1| + |z_2|)^2]^{1/2}} \times \omega_p \sin[\omega_p(t_1 - t_2)]\theta(t_1 - t_2)\theta(z_1) \quad (3)$$

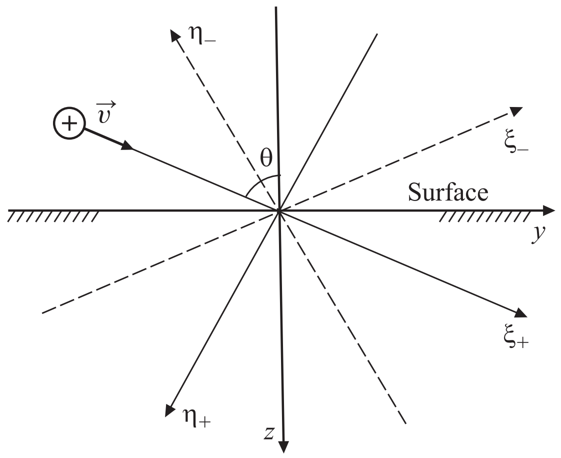

Figure 5. Location of coordinates. The charged particle moves in direction $\xi_+(\vec{v} \parallel O\xi_+)$.

$$-\frac{Z_2 e}{[(\vec{\rho}_1-\vec{\rho}_2)^2+(|z_1|+|z_2|)^2]^{1/2}} \times \omega_s \sin[\omega_s(t_1-t_2)]\theta(t_1-t_2), \qquad (4)$$

where $\vec{r}=(\vec{\rho}, z)$.

In obtained expression the first term (1) corresponds to Coulomb interaction, term (2) describes interaction due to excitation of intra-volume plasmons, term (3) determines interaction occurred during reflection of intra-volume plasmon from surface, term (4) corresponds to interaction occurred during excitation of the surface plasmon with energy $h\omega_s = h\omega_p/\sqrt{2}$. Substituting the obtained expression for the dynamic response $W(\vec{r}_1-\vec{r}_2; t_1-t_2)$ in equation

$$\varphi_{\text{eff}}(\vec{r}_1, t_1) = \int d\vec{r}_2 \int dt_2 W(\vec{r}_1, \vec{r}_2; t_1-t_2)\cdot\rho_{\text{ext}}(\vec{r}_2, t_2),$$

we can calculate the dynamic surface potential φ_{eff}.

Let's consider the case when charged particle contacts metal surface at angle θ to normal (Figure 5). At that we have

$$\rho_{\text{ext}}(\vec{r}_2, t_2) = Z_2 e\cdot\delta(\vec{r}_2 - v\vec{t}_2); \quad \vec{v} = (0, v\cdot\sin\theta, v\cdot\cos\theta).$$

Further cylindrical coordinates (ξ_+, ρ_+) and (ξ_-, ρ_-) are used, they are determined by expressions

$$\xi_+ = -z\cos\theta + y\sin\theta, \;\; \rho_+^2 = x^2+\eta_+^2,$$

where $\eta_+ = -z\cdot\sin\theta - y\cdot\cos\theta$;

$$\xi_- = -z\cos\theta - y\sin\theta, \;\; \rho_-^2 = x^2+\eta_-^2,$$

where $\eta_- = -z\cdot\sin\theta - y\cdot\cos\theta$.

Using cylindrical coordinates we can write explicit expression for the dynamic surface potential φ_{eff} as function of $(\xi_+, \rho_\pm)$. Let's write the expression for φ_{eff} as two parts: first part corresponds to surface plasmon created by charged particle before it penetrates into solid (in metal) $(t_2 < 0)$, and the second part corresponds to the surface plasmon created by a charged particle after it penetrates the solid (metal) $(t_2 > 0)$.

3. Potential of surface plasmon before the charged particle penetrates the solid

The surface potential of plasmon before the charged particle penetration to solid can be written as (for easy during writing the coordinates (ξ_{+1}, t_1) we omit index „1"):

$$\varphi_{\text{eff}} = -Z_2 e \int_0^{k_c} \frac{dk(\omega_s/v)^2}{k^2+(\omega_s/v)^2} J_0(k\rho_+)\cdot\exp(-k|\xi_+ - vt|) \qquad (5)$$

$$-2Z_2 e\cdot(\omega_s/v)\cdot\sin\omega_s(t-\xi_+/v)\int_0^{k_c}\frac{k\,dk}{k^2+(\omega_s/v)^2}J_0(k\rho_+), \qquad (6)$$

$(z > 0$, inside volume), where k_c — limit transmitted pulse. Term (6) corresponds to the wake potential formed by the surface plasmon („surface wake potential"). Note that contribution into φ_{eff} is provided by surface plasmons only, as the charged particle is beyond the volume of metal solid and does not excite the intravolume plasmons.

4. Metal ions sputtering by surface wake potential

Let's consider now interaction of surface wake potential with matrix ions of emitter metallic lattice. Doer incident charged particle of electron (ion) on metallic surface of electrode-emitter the potential of surface plasmon is described by the expression

$$\varphi_{\text{eff}} = -Z_2 e\int_0^{k_c}\frac{dk(\omega_s/v)^2}{k^2+(\omega_s/v)^2}\cdot J_0(k\rho_+)\exp(-k[\xi_+ - vt])$$

$$\times 2Z_2 e\cdot(\omega_s/v)\cdot\sin\omega_s(t-\xi_+/v)\int_0^{k_c}\frac{k\,dk}{k^2+(\omega_s/v)^2}\cdot(k\rho_+),$$

$(z > 0$, inside volume).

For ion of the target substance the transition probability per unit time (in unit of volume) to the first perturbation theory approximation [16] —

$$dP_{\text{fi}} = \frac{2\pi}{\hbar}\cdot|\langle\Phi_{\text{f}}^*|\varphi_{\text{eff}}|\Phi_{\text{i}}\rangle|^2\cdot\frac{mk_f\,d\Omega}{(2\pi\hbar)^3},$$

where the matrix element is defined by the integral

$$\langle\Phi_{\text{f}}^*|\varphi_{\text{eff}}|\Phi_{\text{i}}\rangle = \int\psi_{\text{f}}^*(\xi)\varphi_{\text{eff}}(\vec{r}, \xi)\psi_{\text{i}}(\xi)d\xi\;\exp(i(\vec{k}_i - \vec{k}_f)\vec{r})d^3\vec{r},$$

where

$$\varphi_{\text{eff}} = -Z_2 e\int_0^{k_c}\frac{dk(\omega_s/v)^2}{k^2+(\omega_s/v)^2}J_0(k\rho_+)\;\exp(-k[\xi_+ - v\xi]) \qquad (7)$$

$$-2Z_2e(\omega_s/v)\sin\omega_s(\xi-\xi_+/v)\int\limits_0^{k_c}\frac{k\,dk}{k^2+(\omega_s/v)^2}J_0(k\rho_+), \quad (8)$$

$\psi_f(\xi)$ and $\psi_i(\xi)$ — wave functions of finite and initial state of ion in lattice.

Integral of $d\xi$ has view

$$\int\limits_0^{\infty}\exp\Big(iE_b\xi+i\,\frac{p_i^2}{2m}\cdot\xi\Big)\cdot\exp\Big(-i\omega_s-i\cdot\frac{p_f^2}{2m}\cdot\xi\Big)d\xi$$

$$=1/2\delta\Big(\omega_s+\frac{p_f^2}{2m}-E_b+\frac{p_i^2}{2m}\Big).$$

Effective cross-section of (elastic and inelastic) scattering to the first Bohr approximation may be written as follows:

$$d\sigma_{fi}^{(\text{Bohr})}=\Big(\frac{m}{2\pi\hbar^2}\Big)^2\frac{p_f}{p_i}\,|\langle\Phi_f^*|\varphi_{\text{eff}}|\Phi_i\rangle|^2d\Omega,$$

where $p_f=\sqrt{p_i^2+2m(\hbar\omega_p-E_b)}$, Ω — solid angle.

For calculation of the total cross-section σ_{tot} use a quasiclassical expression for the optical theorem [17]:

$$\sigma_{\text{tot}}=4\pi\int\limits_0^{\infty}\rho d\rho\cdot\Big\{1-\cos\Big[\frac{1}{\hbar v}\int\limits_{-\infty}^{\infty}U\Big(\sqrt{\rho^2+\xi_+^2}\Big)d\xi_+\Big]\Big\}$$

$$\approx 2\pi\int\limits_0^{\infty}\rho d\rho\,\frac{1}{(\hbar v)^2}\cdot\Big[\int\limits_{-\infty}^{\infty}U\Big(\sqrt{\rho^2+\xi_+^2}\Big)d\xi_+\Big]^2.$$

Coordinate ξ_+ is directed along speed direction of bombarding particle $\vec{v}$ ($\vec{v}\parallel O\xi_+$, see Figure 5). Using the expression φ_{eff} for the interaction potential U,

$$U(\rho,\xi_+)=Z_1e\cdot\varphi_{\text{eff}}(\vec{r}_1,t_1)$$
$$=\int d\vec{r}_2\int dt_2W(\vec{r}_1,\vec{r}_2;t_1-t_2)\cdot\rho_{\text{ext}}(\vec{r}_2,t_2),$$

after introduction of dimensionless integration variables, we obtain

$$\sigma_{\text{tot}}\approx\frac{\pi}{2}\,\frac{\sin^2\theta}{\omega_s/v\varepsilon_b}$$
$$\times Z_1^2Z_2^2e^4\int\limits_0^{\infty}x\,dx\Big(\int\limits_0^{\infty}K_0\Big(\sqrt{x^2+\xi^2}\Big)\cdot\sin\xi d\xi\Big)^2,$$

where K_0 — Macdonald's function of zero order.

Thus, full cross-section is proportional to

$$\sigma_{\text{tot}}\propto\frac{\sin^2\theta}{\omega_s/vE_b}\,Z_1^2Z_2^2e^4\cdot\theta(\hbar\omega_s-E_b).$$

5. Discussion of results

The comparison of the results of bombardment with electrons and heavy ions shows that the result of sputtering does not depend on the sign of the charge of the incident particle (electron or ion). At same speeds of bombarding particles the cross-section depends only on charge of incident particle, and does not depend on its mass. Excitations of surface plasmons play important role when the sliding angle of incident beams of charged particles on crystal surface becomes low ($\theta\to\frac{\pi}{2}$).

$$\sigma_{\text{tot}}\propto\frac{\sin^2\theta}{\omega_s/vE_b}\,Z_1^2Z_2^2e^4.$$

The surface erosion during sputtering is characterized by sputtering coefficient Y, which is determined as average number of ions removed from surface of solid by one incident particle, i.e. under sputtering coefficient we understand the ratio of number of sputtered atoms of solid N_2 to number of bombarding particles (electrons or ions) N_1:

$$Y=\frac{dN_2}{dN_1}.$$

The beam of bombarding particles with density n_1 (number of particles per unit of volume) collides with ions of metallic lattice, their density is n_2. In near-surface layers of target (about path length L) collision of incident particles with target particles occurs, as per obtained expression for cross-section

$$\sigma_{\text{tot}}\propto\frac{\sin^2\theta}{\omega_s/vE_b}\,Z_1^2Z_2^2e^4.$$

Then number of collisions $d\nu$ in target volume with ejection of ion dN_2, during time period dt is

$$d\nu=n_1Sv_1dtn_2\sigma_{\text{tot}}L=dN_2,$$

where S — area of irradiated sample. Considering that $dN_1=n_1Sv_1dt$, we can obtain expression for the sputtering coefficient:

$$Y=\frac{\sin^2}{\omega_s/vE_b}\,Z_1^2Z_2^2e^4n_2L.$$

Therefore, (7) determines number of „evaporated" atoms. As you can easily see, for every 10^2-10^3 of approaching charged particles there is about one flying out atom [6].

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Conflict of interest

The author declares that he has no conflict of interest.

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