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EMISSION OF SHORT-WAVE RADIATION DURING ION IMPACT ON SOLID SURFACES

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The possibility of short-wave photon emission during surface scattering of positive ions is investigated by selection of the type of charge-exchange process (one- or two-electron processes), through the calculation of the neutralization probabilities and the charge-transfer cross sections. These probabilities are calculated statically as a function of distance between the incident ion and the surface, and dynamically as a function of the ion velocity. The model is applied to real systems such as He^+/semiconductor (silicon and germanium), taking into account the difference in the physical constants of the two systems. We found that emitted photons have short wavelengths, lying in the ultraviolet range of the electromagnetic spectrum of the helium emission spectrum.

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Keywords: impact of He^+ on surfaces, charge transfer process, neutralization probabilities, short-wave emission

1. Introduction

The interaction of an ion with a solid surface is a dynamic, many-body processes which encompass the trajectory evolution of the ion above the surface, the electron exchange between the solid and the ion, and the excitation of both the ion and the surface [1 − 3]. The charge-exchange scattering of ions at solid surfaces has been intensively studied both theoretically and experimentally, due to the fact that the charge exchange process provides valuable informations on the properties of the solid materials. In particular, slow ions are a suitable tool for probing the surface properties of solids, as the interaction processes take place at the vacuum-solid interface.

The charge-transfer process, which takes place between a slow, multiply charged ion and a solid surface, can be classified in four major types: (a) one-electron resonant transition, in which an electron is captured resonantly into an atomic level (resonant neutralization (RN)) or transferred into an empty surface state (resonant ionization (RI)), Fig. 1a ; (b) Auger transitions, two-electron interaction, so that the first electron decays to a deeper-lying level and the excess energy is carried away by another, Fig. 1b; (c) radiative transitions, when the energy difference between the initial and final states is carried away by a photon of short electromagnetic wavelength, Fig. 1c, and the polarization of the light emitted by the excited projectiles after scattering from the surface can be used to probe long-range surface magnetization; and (d) collective excitations, in which a conduction band electron is transferred into low-lying levels of the incoming ion, while the energy difference is used to excite a plasmon. The energy of the plasmon is provided by the potential energy released by the neutralization of the ion. As no electrons are emitted during this process, the creation of a plasmon shows up as a dip in the energy distribution of secondary electrons emitted during ion bombardment of the surface, Fig. 1d.

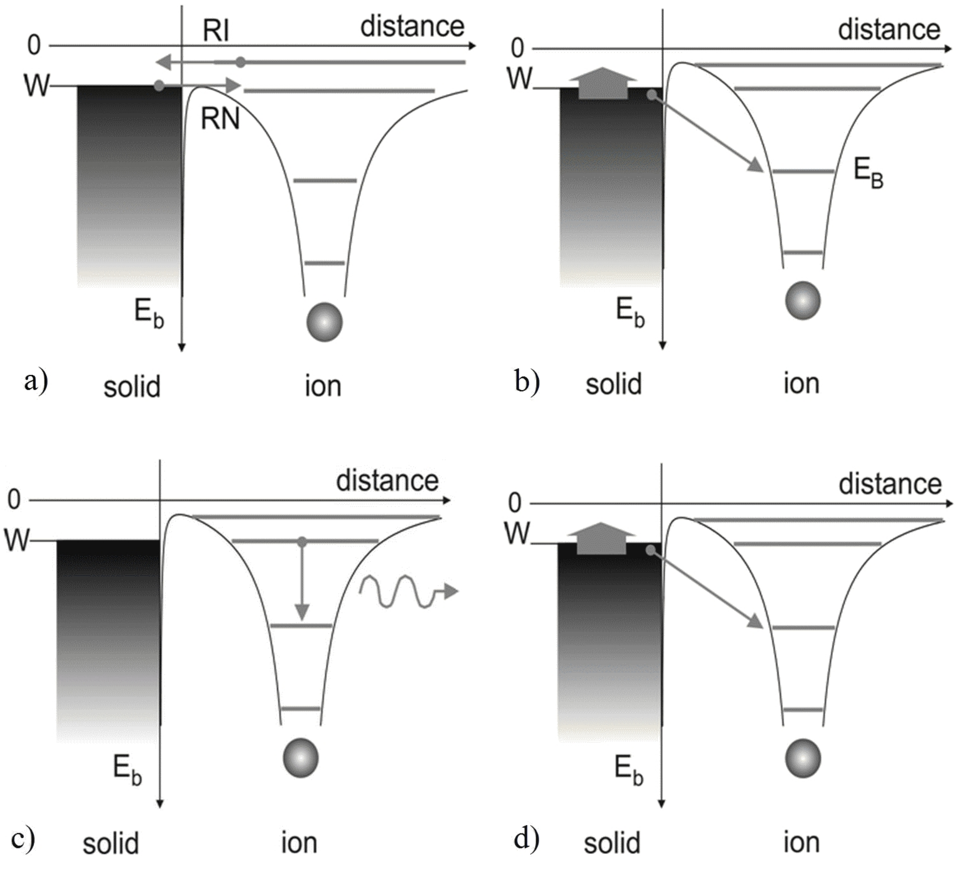

Fig. 1. The charge-transfer processes which take place between a slow, charged ion and solid surface. (a) One electron resonance transition; (b) Auger neutralization process (AN); (c) Radiative transition; (d) Collective excitation.

Observation of electromagnetic-wave emission from laser-produced plasmas suggests a possibility of utilizing surface processes to induce charge exchange in the solid [4 – 6] such as adsorption, desorption, dissociation and migration. On the other hand, some of the charge-exchange processes between the ion and the solid may serve as a means of achieving population inversion to obtain a short-wavelength laser.

Most of the theoretical investigations focused on the possibility of using ion – surface charge exchange process to obtain coherent short-wavelengths were introduced by T. George [7], H. W. Lee [8] and J. S. Helman [9].

The main purpose of this study is to extend many-electron theory, which has been applied to resonance charge transfer only [10 – 11], to include the Auger charge-transfer process too, and the situation in which the two processes can occur together at the same time.

Since the theoretical treatment of the problem is quite complex, the present model is a mixture of classical and quantum-mechanical concepts to describe the ion-surface interaction. The model calculates the electron charge exchange probability and the related electromagnetic wavelengths for a positive helium ion (He^+) scattered from different surfaces (metals and semiconductors).

2. *Theoretical considerations*

The two mechanisms by which the neutralization may proceed are the Auger and the resonance charge-transfer processes. The two processes are responsible for the charge transfer, which arises when an ion (atom) is scattered from a surface (metal or semiconductor).

In such processes, it is sufficiently accurate to follow a classical trajectory (following the assumption given by Tully [12]). So, the total Hamiltonian for the system is reduced to electronic motion only.

2.1. *The time development determined by solving Schrödinger equation*

Following the theoretical consideration given by Amos et al. [13], the neutralization probabilities for both resonance and Auger processes are calculated.

We define the wave function $\psi(\boldsymbol{r}, t)$ describing electronic motion and satisfying the time dependent Schrödinger equation,

$$\mathrm{i}\,\frac{\mathrm{d}\psi(\boldsymbol{r}, t)}{\mathrm{d}t} = H_e(\boldsymbol{r}, t)\psi(\boldsymbol{r}, t)\,. \tag{1}$$

$H_e(\boldsymbol{r}, t)$ represents the total energy operator of the electron at point $\boldsymbol{r}$, and under the assumption that the nuclei follow classical trajectory, hence the electronic Hamiltonian becomes time-dependent operator $H_e(\boldsymbol{r}, t)$.

The simplest model given to the solution of the time dependent Schrödinger equation allowing for both Auger and resonance charge-transfer processes at the same time, is represented by the wave function [13]

$$\psi(t)=a_o\psi_o+\sum_i b_i\psi_i+\sum_{j,A^*}C_{jjA^*}\psi_{jjA^*}+\sum_{j<k.A^*}\left(d^1_{jkA^*}\psi^1_{jkA^*}+d^2_{jkA^*}\psi^2_{jkA^*}\right)\times\exp(-\mathrm{i}\epsilon_o t), \tag{2}$$

where ϵ_o is the energy of ψ_o and a_o, b_i, C_{jjA^*}, ...etc. are time-dependent coefficients, k is the first electronic state for the Auger process in the solid surface, A^* is the excited state of the incoming ion, j is the second electron for Auger process and o is the valence orbital of the incoming ion.

The coefficients a_o, b_i, C_{jjA^*}, ...etc. allow the calculation of the ion survival probability, P_+, resonance and Auger charge-transfer probabilities, P_{R} and P_{A}, respectively,

$$P_{\mathrm{su}}=|a_o(\infty)|^2, \qquad P_{\mathrm{R}}=\sum_i|b_i(\infty)|^2\,.$$

The probability of Auger charge transfer can be calculated in terms of C_{jjA^*} and d_{jkA^*}. As the probability sum equals unity, then

$$P_A=1-P_+-P_{\mathrm{R}}\,.$$

Substituting $\psi(t)$ in the time-dependent Schrödinger equation and integrating over all space, we introduce a set of equations for the above coefficients,

$$\mathrm{i}\,\dot{a}_0=\sum_i\langle\phi_i|H_e|\phi_o\rangle b_i+\sum_{j,A^*}C\big[j_o,jA^*\big]C_{j,A^*}+\sum_{j<K,A^*}\left(V^1_{jKA^*}d^1_{jKA^*}+V^2_{jKA^*}d^2_{jKA^*}\right), \tag{3}$$

$$\mathrm{i}\,\dot{b}_i=\epsilon b_i+\langle\phi_o|H_e|\phi_i\rangle a_o\,, \tag{4}$$

$$\mathrm{i}\,\dot{C}_{jjA^*}=\epsilon_{jjA^*}C_{jjA^*}+C^*\big[j_o;JA^*\big]a_o\,, \tag{5}$$

$$\mathrm{i}\,\dot{d}^{1,2}_{jKA^*}=\epsilon_{jKA^*}d^{1,2}_{jKA^*}+V^{1,2}_{jKA^*}a_o\,. \tag{6}$$

By integrating Eqs. (4) to (6) to express b_i, C_{jjA^*} and $d^{1,2}_{jKA^*}$ in terms of the integrals involving a_o and substituting into Eq. (3) lead to the integro-differential equation for a_o,

$$\dot{a}_o(t)=-\sum_i\langle\phi_i|H_e|\phi_o\rangle\int_{-\infty}^{t}\langle\phi_o|H_e|\phi_i\rangle\exp\big[-\mathrm{i}\epsilon_j(t-t')\big]a_o(t')\mathrm{d}t'-\sum_{j<k.A}2C\big[jo,kA^*\big]$$

$$-C\big[ko,jA^*\big]\times\int_{-\infty}^{t}C^*\big[jo,kA^*\big]\times\exp\big[-\mathrm{i}\,\epsilon_{jkA^*}(t-t')\big]a_o(t')\mathrm{d}t'. \tag{7}$$

The matrix elements in this equation depend on the ion-surface distance and on time. Equation (7) includes two terms. The first term is expressing the resonance neutralization process, with the integrals equal $V_i u(t)$, V_i depending on ϕ_i and $u(t)$ is the part of the wave function depending on time.

It has been shown that for a wide band, the first term on the right hand side of Eq. (7) can be replaced by $\omega(t)a_o(t)$ [13, 3, 4, 18], where

$$\omega(t) = \frac{\pi}{W} u^2(t)\,. \tag{8}$$

W is the band width and $u(t)$ is a part of the wave equation that depends on time.

By applying a local-time approximation, $C^*[jo; kA^*]$ and $a_o(t')$ are taken outside the integral as a function of t and inside function of t', so the last two terms of Eq. (7) are reduced to $\gamma(t)a_o(t)$ which represent the Auger charge-transfer rate, where

$$\gamma(t) = \pi \sum_{j,k,A} \big\{2C[jo; kA^*] - C[ko; kA^*]\big\} \times C^*[jo; kA^*]\delta(\epsilon_{jkA^*})\,, \tag{9}$$

where $\delta(\epsilon_{jkA^*})$ is the energy conservation condition for the Auger charge-transfer processes.

So, the combination of these approximations for both neutralization processes in Eq. (7) reads

$$\dot{a}_o = -\big[\omega(t) + \gamma(t)\big]a_o(t)\,. \tag{10}$$

The solution of this equation gives the wave amplitude as a function of time,

$$a_o(t) = \exp\left[-\frac{1}{2}(\Omega(t) + \Gamma(t))\right], \tag{11}$$

where $\Omega(t)$ and $\Gamma(t)$ are functions that increase with time and have the definitions [13]

$$\Omega(t) = 2\int_{-\infty}^{t} \omega(t')\mathrm{d}t', \tag{12}$$

$$\Gamma(t) = 2\int_{-\infty}^{t} \gamma(t')\mathrm{d}t'. \tag{13}$$

Using the simple exponential approximation given in Ref. [13] for $\gamma(t)$ and $\omega(t)$,

$$\omega(t) = A\mathrm{e}^{-\alpha\nu|t|}, \qquad \gamma(t) = B\mathrm{e}^{-\beta\nu|t|},$$

Eq. (12) is resolved to

$$\Omega(t) = 2A \int_{-\infty}^{0} \mathrm{e}^{-\alpha\nu|t'|}\mathrm{d}t' + 2A \int_{0}^{t} \mathrm{e}^{-\alpha\nu|t'|}\mathrm{d}t'.$$

Then

$$\Omega(t) = \frac{4A}{\alpha\nu} - \frac{2A}{\alpha\nu}\exp(-\alpha\nu|t|)\,, \tag{14}$$

Using the same calculation for $\Gamma(t)$, Eq. (13) becomes

$$\Gamma(t) = \frac{4B}{\beta\nu} - \frac{2B}{\beta\nu}\exp(-\beta\nu|t|)\,. \tag{15}$$

The parameters α and β are important, they determine how rapidly the ion – surface interaction declines with the distance. Their reciprocals are used to determine the ion – surface distance over which a specific interaction is strong.

Making use of Eq. (11), the probability of RCT (P_R) is

$$P_R = \int_{-\infty}^{\infty} \frac{\mathrm{d}\Omega}{\mathrm{d}t}\exp\big[-(\Omega+\Gamma)\big]\mathrm{d}t, \tag{16}$$

and the probability of ACT (P_A)

$$P_A = \int_{-\infty}^{\infty} \frac{\mathrm{d}\Gamma}{\mathrm{d}t}\exp\big[-(\Omega+\Gamma)\big]\mathrm{d}t. \tag{17}$$

The sum of all probabilities equals one, so the survival probability is given by

$$P_+ = 1 - P_R - P_A. \tag{18}$$

2.2. Charge-exchange cross section

The charge-exchange cross section (σ) can be estimated by calculating the neutralization probability [16]

$$\sigma = \pi z_0^2 P, \tag{19}$$

where P represents the resonance or Auger charge-exchange probabilities and z_o is the closest distance of the ion from the surface at which the electron capture occurs.

3. Short-wave emission

We are interested in our work in the possibility of using ion – surface charge-exchange processes to obtain short-wavelength photons. So we make use of results of Ref. [17] and we consider the gain (g) of a Doppler-broadening medium given by the expression

$$g = \sqrt{\pi \ln 2}\, \frac{\lambda^2}{8\pi}\, \frac{\Delta N}{\tau_{\rm spon}\Delta\nu}\,, \tag{20}$$

where $\Delta\nu$ and λ are the linewidth and wavelength of the transition (that we calculate here), ΔN is the population inversion and τ is the spontaneous lifetime. It has been suggested that $g \geq 10$/cm to get a good population inversion and a short wavelength.

$$\Delta N = N_{\rm ion} N_e \sigma v \tau_{\rm spon}\,, \tag{21}$$

where $N_{\rm ion}$ and N_e are the number densities of the incident ions and surface electrons, respectively and v is the ion velocity. So the wavelength of emitted d-photon can be represented by

$$\lambda = \left[\frac{8g\Delta\nu}{\sqrt{\pi \ln(2)} N_{\rm ion} N_e v Z_o^2\, {}^*P} \right]^{1/2}, \tag{22}$$

or, if we take P in terms of the ion velocity, then

$$\lambda = \left[\frac{8g\Delta\nu}{\sqrt{\pi \ln(2)} N_{\rm ion} N_e v Z_o^2 \left[1 - \exp\left\{ -(4/v) \int\limits_0^\infty \Gamma(Z) {\rm d}Z \right\} \right]} \right]^{1/2}.$$

4. Calculation and discussion

We consider an electron-capture process of a positive He^+ ion with incident energy $E_{\rm i} = 24.45$ eV, in it's ground state ($n = 1$) with electron binding energy $\epsilon_a^* = -54.4$ eV, or in it's first excited state ($n = 2$) with electron binding energy $\epsilon_{a2}^* = -13.6$ eV, or in it's second excited state ($n = 3$) with electron binding energy $\epsilon_{a3}^* = -6.0$ eV, scattered from silicon (111) surface with the energy gap $\epsilon_g = -1.1$ eV, $\phi_g = -4.6$ eV, $E_F \approx -(\phi - 0.5\epsilon_g)$, and the bottom of the conduction band $\epsilon_o = -12$ eV.

The energy level structures of He^+ and the silicon surface are illustrated in Fig. 2. The energy gap ϵ_g can be included in the work function ϕ of the surface.

The interesting point in such a system is the simplicity of getting excited states after neutralization such as

$$\mathrm{He}^+ + \mathrm{Si} \to \mathrm{He}^* + \mathrm{Si}^+(111) \to \mathrm{He} + \mathrm{Si}^+ + h\nu\,.$$

$\Omega(t)$ and $\Gamma(t)$ for resonance and Auger charge transfer are increasing functions with time, but according to the term $\exp[-\Gamma(t)]$ (Eq. (16)), P_R decreases with time. A reversed behavior is expected for P_A.

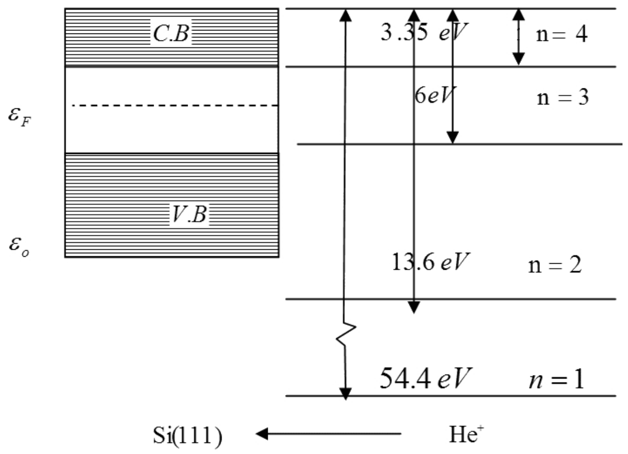

Fig. 2. Energy level diagram for He$^+$/Si(111)*. The valence and conduction bands are labeled by V.C. and C.B., and ϵ_o is the bottom of the valence band.*

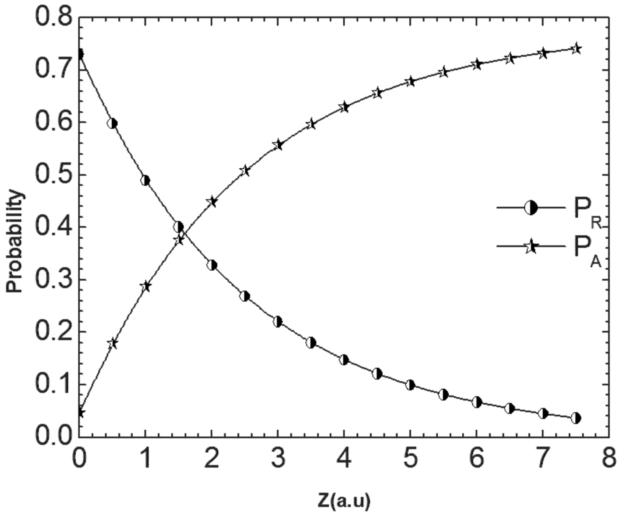

Fig. 3. Competition probabilities for Auger and resonance processes as functions of the ion distance.

In Fig. 3, we present our numerical results for P_R and P_A as functions of the distance z between the incoming ion and the semiconductor surface, in the case when both processes act together.

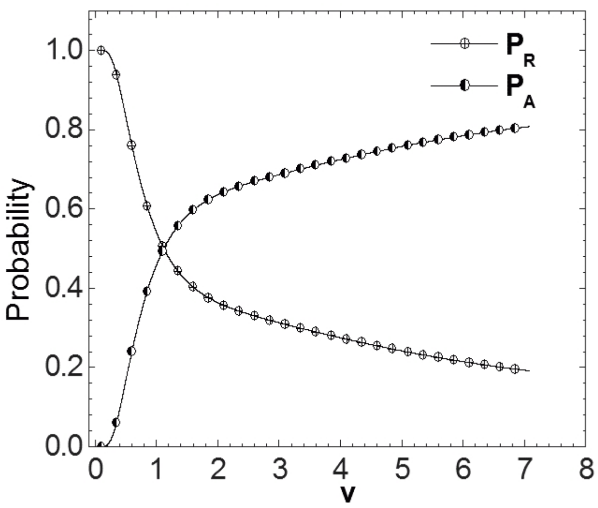

Fig. 4. Competition probabilities for Auger and resonance processes as functions of the ion velocity in (a.u.).

Figure 4 shows these probabilities as a function of the ion velocity (slow ions). For our particular choice of the dependence of $\gamma(t)$ and $\omega(t)$ on the ion velocity, we have $P_R \to 1$ and $P_A \to 0$ as $v \to 0$, while $P_R \to \Omega(\infty)$ and $P_A \to \Gamma(\infty)$ asymptotically as $v \to \infty$. So, we may say that the two neutralization processes are independent of each other at very large ion velocity.

From Fig. 3 follows that the resonant charge transfer (RCT) has a larger neutralizing range than Auger charge transfer (ACT) at small velocities, so the RCT dominates in this range of velocities. By increasing the ion velocity, the two curves cross. This behavior is in a good agreement with that found by Amos et al. [13]. He used the parameters $A = 0.4$, $B = 1.2$ and $\beta = 2\alpha$.

With these figures, and making use of Eq. (21) we calculated the wavelengths emitted for the He^+/Si(111) and He^+/Ge(111) systems. So, in Fig. (5) we give the calculated wavelengths as a function of the resonance charge transfer probability P_R.

In Table 1, we give our results for P, σ and λ calculated for slow ions ($v = 0.24$ a.u.), and they are compared with the results of Lee [8]. The difference in λ between these results and those calculated by Lee is due to our approximation in taking the Fermi level to be equal to the surface work function $E_F = -\phi$.

Table 2 gives a comparison between the resonance neutralization (RN) and Auger neutralization (AN), in calculating P, σ and Λ for the He^+/Si(111) system.

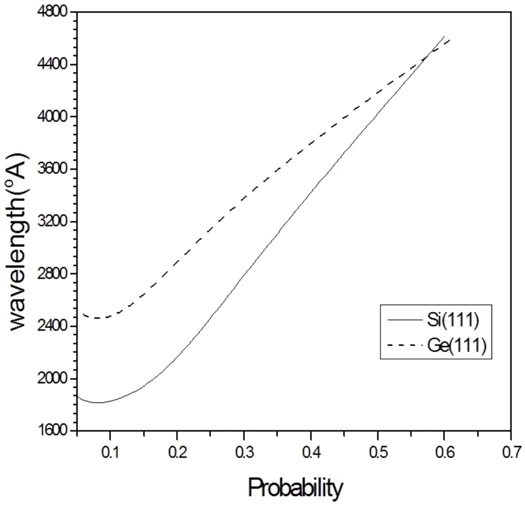

Fig. 5. The wavelength of emitted radiation as a function of the resonance charge-transfer probability P_R.

TABLE 1. Calculated values of P, σ and λ for the He^+/Si(111) *system.*

	Lee calculation [8]	Our calculation, $v = 0.24$ a.u.
P	0.097	0.097
σ (Å^2)	4.19	4.19
λ (Å)	1460	2320

TABLE 2. Calculated values of P, σ and λ at the distance between the incoming ion and the Si(111) surface of $z = 0.24$ (a.u.).

	RN	AN
P	0.488	0.289
σ (Å^2)	5.2	1.7
λ (Å)	1458.4	2541.7

From the calculations, we conclude that the spectrum of the emitted wavelength has short wavelengths lying in the ultraviolet range of the electromagnetic spectrum (helium spectrum). But in normal conditions, the intensity of the emitted radiation is too weak to be considered for laser effects.

5. *Conclusion*

In this work, we study the emission of short-wave-length radiation from charge-exchange processes (one- or two-electron processes) during positive-ion – surface scattering, through the calculation of the neutralization probabilities and the charge transfer cross section, when the two charge-transfer processes are treated on an equal footing.

These probabilities are calculated statistically as a function of the distance between incident ion and the surface (Fig. 3) and also dynamically as a function of ion velocity (Fig. 4). For slow ions, the dominating process is the one with the longer range of interaction.

Our model is applied to real systems such as He^+/Si and He^+/Ge systems, taking into account all physical constants related to the systems. It is clear, particularly from Fig. 5, that the emitted waves have short wave lengths, laying in ultraviolet range of the electromagnetic spectrum.

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EMISIJA KRATKOVALNOG ZRAČENJA TIJEKOM UDARA IONA O ČVRSTU POVRŠINU

Istražujemo mogućnost emisije kratkovalnih fotona tijekom udara iona o čvrstu površinu odabirom procesa izmjene naboja (jedno i dvoelektronski procesi) i računanjem vjerojatnosti neutralizacije i udarnog presjeka za prijenos naboja. Te vjerojatnosti računamo statički kao funkcije udaljenosti upadnog iona i površine, i dinamički kao funkcije brzine iona. Model primjenjujemo stvarnim sustavima kao što su poluvodiči silicij i germanij, uzimajući u obzir razlike fizičkih svojstava dvaju sustava. Nalazimo da fotoni imaju kratke valne duljine, u području elektromagnetskog spektra helija.