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Spatial and energy distributions of the fragments resulting from the dissociation of swift molecular ions in solids

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Abstract

We have simulated the spatial evolution and energy loss of the fragments that result when swift molecular ions dissociate inside solid targets. In our calculations we have considered that these fragments undergo the following interactions: Coulomb repulsion (among like charged particles), stopping and wake forces (due to electronic excitations induced in the target), and nuclear scattering (with the target nuclei). We study the case of silicon targets irradiated with boron molecular or atomic ions; our results show that the main differences in the energy and spatial distributions of molecular fragments or atomic ions appear at shallow regions, and these tend to disappear at deeper depths. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: Stopping power; Energy loss; Molecular ions; Doping and ion implantation

1. Introduction

When swift projectiles penetrate through a solid, they interact with target atoms along their trajectories and lose energy through the excitation and ionization of the target atoms or transferring energy to the target nuclei. The knowledge of the projectile energy deposition becomes essential in studies of material science, such as particle penetration in solids, ion range distribution, impurity-atom implantation in solids, radiation damage, or radiation protection, among others [1–3].

It is known that when molecular (instead of atomic) beams interact with solids, there may appear effects associated with the correlated motion of the molecular constituents through the target [4–6], referred generically as vicinage effects. Many consequences of these effects have been studied so far in relation with the understanding of basic physics phenomena associated with the interaction of molecular ions with solids, in contraposition to the case of atomic ions.

The aim of the present work is to extend the analysis of vicinage effects to other situations of applied interest. We will study the energy deposition and main characteristics of the implanted region when molecular, instead of atomic, ions are used to irradiate a solid target. Specifically, we will examine the case of a silicon target irradiated with B_3^+ and B^+.

This work is organized as follows. In Section 2 we introduce the model we will use, in Section 3 we will discuss the results, and in Section 4 the main conclusions of this work will be presented.

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2. Model

Just after a swift molecular ion impinges on a solid, it dissociates in its constituents in the first atomic layers, becoming a set of atomic fragments in correlated motion [5]. Then each fragment interacts not only with the target components (through electronic excitations and atomic scattering), but also with its fragment partners (through wake forces and Coulomb repulsion).

A simulation code has been developed recently [7,8] that accounts for all these process in the interaction of molecular ions with solids. The electronic excitations created by each projectile in the solid give rise to a self retarding force acting on it (this is the well known stopping power), and to the wake force acting on its partner projectiles. We have also considered the statistical nature of the electronic interaction by including the energy loss straggling in our simulation. All the above mentioned magnitudes are calculated using the dielectric formalism, but taking into account the variation in the electronic charge state of the projectile as a function of its velocity.

When a projectile of atomic number Z and velocity v moves through a target, the stopping power, S_p, and the energy loss straggling per unit path length, Ω^2, are given in the dielectric formalism by

$$S_p = \frac{2e^2}{\pi v^2} \int_0^\infty \mathrm{d}k \, \frac{[Z-\rho(k)]^2}{k} \int_0^{kv} \mathrm{d}\omega \, \omega \, \mathrm{Im}\left[\frac{-1}{\epsilon(k,\omega)}\right] \tag{1}$$

and

$$\Omega^2 = \frac{2e^2\hbar}{\pi v^2} \int_0^\infty \mathrm{d}k \, \frac{[Z-\rho(k)]^2}{k} \int_0^{kv} \mathrm{d}\omega \, \omega^2 \, \mathrm{Im}\left[\frac{-1}{\epsilon(k,\omega)}\right], \tag{2}$$

where $\mathrm{Im}[-1/\epsilon(k,\omega)]$ is the energy loss function (ELF) of the target, which accounts for its electronic excitations with momentum $\hbar k$ and energy $\hbar\omega$; $\rho(k)$ is the Fourier transform of the projectile electronic density, e is the elementary charge and $\hbar$ is Planck's constant divided by 2π.

We model the ELF of real materials (silicon in the present work) according to the procedure explained in Refs. [9,10] where we use a combination of Mermin-type ELF to describe the outer electron excitations and the generalized oscillator strengths for the inner-shell electron excitations. $\rho(k)$ is described by means of the Brandt–Kitagawa (BK) model [11]:

$$\rho(k) = \langle N\rangle \left\{ 1 + (ka_0)^2 \left[\frac{0.23\langle N\rangle^{4/3}}{(Z-\langle N\rangle/7)^2} \right] \right\}^{-1}. \tag{3}$$

$\langle N\rangle$ is the average number of electrons bound to an atomic ion, whose dependence on the ion velocity inside the target is $\langle N\rangle = Z\exp(-0.92v_r/Z^{2/3})$, where v_r is the relative velocity of the projectile with respect to the valence electrons of the target [12]; $a_0 = 0.529$ Å is Bohr's radius.

Based in this procedure, we also calculate the wake forces as stated in Ref. [9], but now taking into account the average number of electrons bound to each projectile [12] and using the BK model [11] to describe these electrons. Note that for a given target, the self retarding force depends on the projectile velocity and charge, but the wake force depends also on the relative positions of the projectiles.

Fig. 1 shows, for a wide range of energies, the stopping power of silicon for boron atomic ions and also the corresponding energy loss straggling, as a function of the incident energy per atom E_0. The symbols represent the experimental data

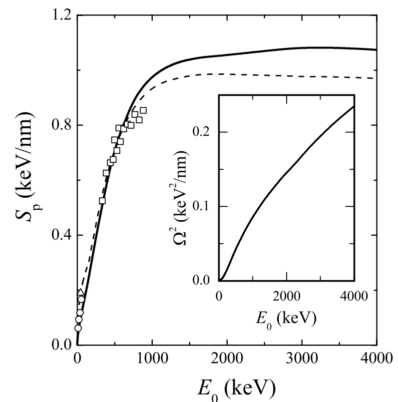

Fig. 1. Stopping power of silicon for boron ions. Lines correspond to present calculations (—) and results obtained with SRIM98 (- - -) [16]. Symbols represent experimental results: (□) [15], (○) [13], and (△) [14]. The inset shows the calculated energy loss straggling of silicon for boron ions.

[13–15] and the dashed line shows the result given by SRIM98 [16].

The mutual repulsion of the atomic ions dissociated from the molecule is described by a Coulombic interaction, whereas the scattering of these ions with the target atomic cores is accounted through a Monte Carlo model [17], where the universal potential cross-section [12] was used to calculate the scattering angles and the corresponding nuclear energy loss.

Using our simulation code [7,8], we take into account all these interactions in order to calculate the coordinates and velocities of each molecular fragment as they move through the target. With these magnitudes evaluated at different target depths, it is possible to characterize the spatial and energetic distributions of the projectiles.

3. Results and discussion

Using the procedure described in the previous section, we have studied both the cases in which B^+ and B_3^+ ions interact with silicon targets. We have considered the same incident energies for the molecular fragments and for the atomic ions.

Fig. 2 compares the lateral spatial distribution (i.e., perpendicular to the incident projectile direction) of boron fragments (dashed lines) and atomic ions (solid lines) for two incident energies ($E_0 = 68.75$ and 1100 keV) and for several depths D in the silicon target. It can be observed that for the shallow depths the distribution of atomic ions is narrower than the distribution of molecular fragments (probably due to the initial structure of the molecular ions and the subsequent Coulomb explosion), but these differences tend to disappear as the depth increases, due to the loss of correlation in the motion of the fragments, a situation that is reached faster the lower is the energy.

Fig. 3 compares the energy spectra of both type of projectiles (boron dissociated fragments and boron atomic ions), for the same cases than in Fig. 2. At high incident projectile energy the fragments show an energy distribution that begins with a structure that gradually tends to disappear as the target depth grows; in all the cases the mean energy of the fragments is smaller than that of the atomic ions. For the case of low incident projectile energy, both energy distributions (of fragments and atomic ions) are quite similar in structure, the mean energy of the former being larger than that of the latter. The structure developed in the energy distribution of the fragments can be understood as due mainly to the wake forces that tend to align the fragments behind the leading one [7,8]. The extinction of this structure is due to the scattering with the target nuclei, whose consequences appear immediately at shallow depths for the lower energies but that need a larger travel through the target for the higher projectile energies.

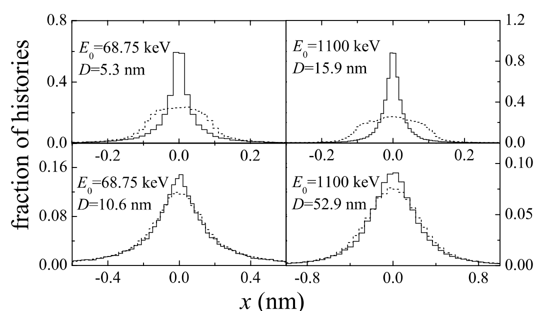

Fig. 2. Lateral distribution of boron fragments dissociated from B_3^+ (- - -) and boron atomic ions (—), at the indicated depths D in a silicon target. The incident energy (per atom) is $E_0 = 68.75$ keV for the left column, and $E_0 = 1100$ keV for the right column.

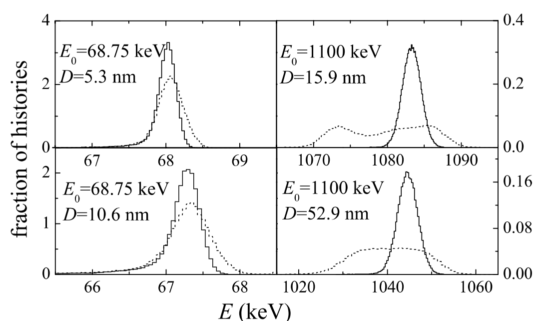

Fig. 3. Energy distribution of boron fragments dissociated from B_3^+ (- - -) and boron atomic ions (—), at the indicated depths D in a silicon target. The incident energy (per atom) is $E_0 = 68.75$ keV for the left column, and $E_0 = 1100$ keV for the right column.

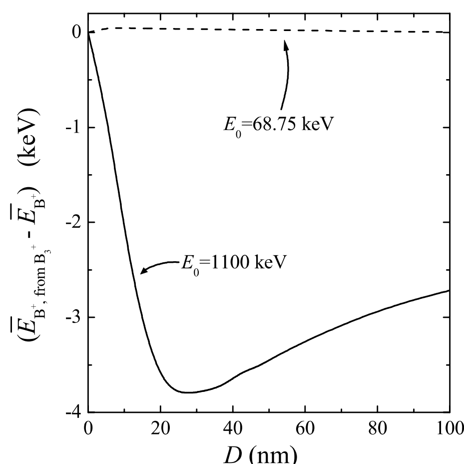

Fig. 4. Difference in the mean energies $\overline{E}$ of boron fragments compared to the case of atomic ions, as a function of the depth in a silicon target. Two incident energies are considered: $E_0 = 68.75$ keV (- - -) and $E_0 = 1100$ keV (—).

Finally, Fig. 4 depicts, as a function of the target depth, the differences in the mean energy corresponding to the energy distributions shown in Fig. 3 for boron fragments and atomic ions, respectively. It can be observed that for the low incident projectile energy, the mean energy of the boron fragments is scarcely larger than the one corresponding to the boron atomic ion. In the case of high incident projectile energy, the mean energy of the boron fragments is smaller than for the boron atomic ions, this feature being kept even for deeper target depths. The positive or negative differences between the mean energy of the boron fragments or atomic ions is easily understood in terms of the energy dependence of the wake force, which for low (high) energy tends to accelerate (decelerate) the fragments behind the leading one [7–9]. These vicinage effects due to the wake forces clearly disappear when the spatial correlation of the fragments is destroyed by the scattering with the target nuclei and Coulomb repulsion, which happens earlier (later) for low (high) projectile velocities.

4. Conclusions

We have compared the spatial and energy distributions of atomic ions with those of fragments dissociated from molecular ions, when they irradiate a solid target. In particular, we have studied the case of B_3^+ and B^+ incident on a silicon target, these elements being currently used for practical research in materials science.

Our analysis is based on the simulation of the trajectories of each projectile as they move through the target, taking into account the different interactions that they experience among them (Coulomb repulsion and wake forces) and with the target constituents (electrons and nuclei). Our results show that the spatial distributions of the molecular fragments and the atomic ions, both of the same energy, only differ in their widths for the shallow depths. The differences in the corresponding energy distributions affect both the width and the mean value, which again tend to disappear with increasing depths.

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