Coulomb heating of channeled C^+ and C_2^+ molecules in Si

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Si x-ray and backscattering yields have been measured as a function of the C^+ and C_2^+ entrance angle along the Si ⟨100⟩ channel in an energy interval between 900 and 2200 keV/atom. A significant enhancement of the x-ray production has been observed for the well-aligned C_2^+ beam in comparison with the monoatomic case. It is shown that this effect results from the Coulomb explosion of the molecule during the channeling motion. By combining the Rutherford backscattering channeling (RBS-C) and the x-ray results we were able to determine the value of the transverse energy transfer as a function of the beam energy due to the break up process (Coulomb heating). This energy increases monotonically from 14 eV for 900 keV/atom up to 30 eV for 2200 keV/atom. In addition, we were able to predict the theoretical Coulomb heating values by combining calculations and simulations, the theoretical-experimental agreement, within the experimental errors, being quite reasonable.

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I. INTRODUCTION

It is well established that the effects of a molecular beam clearly deviate from those related with its individual components [1,2]. Significant coherent effects such as the vicinage one have been predicted theoretically and found experimentally [3,4]. Other effects related to the coherent motion of cluster atoms such as enhanced sputtering yields [5–7] and electron emission [8] have also been reported and reviewed in recent publications. In particular, the study of the Coulomb explosion of molecules [9,10] is a clear example where the cluster cannot be described as a simple sum of the constituents ions motions.

In a channeling motion, molecules undergo a break up process, since they lose their bonding electrons due to ionization in the first monolayers of the crystal. The break up and the subsequent mutual nuclei repulsion is known as *Coulomb explosion*. The combination of these two motions, that is, the channeling one and the Coulomb explosion of the molecule lead to the so-called transverse *Coulomb heating*. First studies of this Coulomb heating have been performed in transmission experiments [9,11]. Furthermore, by studying the behavior of H, H_2, and H_3 beams in backscattering geometry the group of Tombrello was able to deduce the dynamics of the Coulomb break-up during the channeling trajectory in a Si crystal. However, they did not quantify the transversal energy contribution due to the Coulomb explosion [10]. On the other hand, by studying the dechanneling profiles of the same hydrogen clusters (H, H_2, and H_3) Khodyrev *et al.* [12] have obtained values for the Coulomb heating. However, the computer simulations strongly overestimated the experimental results.

More recently Fadanelli *et al.* [13] by using the x-ray yields produced by the H ion and H_2 and H_3 molecules at 150 keV/amu induced by a scanning around the Si⟨100⟩ channel together with a modeling of the corresponding Rutherford backscattering channeling (RBS-C) spectra were able to determine in a quantitative way the values of the H_2 and H_3 Coulomb heating energies. The obtained experimental values were 2.3 ± 0.4 and 4.5 ± 0.8 eV, respectively, in good agreement with the theoretical predictions [13].

The scenario described above shows a clear progress in the study of the cluster-matter interaction for hydrogen molecules. Although many questions still remain to be answered, hydrogen molecules are relatively simple when compared with heavier multielectrons clusters. Then, the main objective of the present work is to investigate if the experimental-theoretical approach described in Ref. [13] is valid for heavier clusters.

To this end we have undertaken the present work where we studied the Coulomb heating produced by a C_2 molecular beam. We followed the same procedure as in Ref. [13]. That is, we have made an angular scan around the Si ⟨100⟩ channel recording at each step simultaneously the x-ray yield and RBS-C spectrum induced by C^+ and C_2^+ beams. At variance with the experiment of Ref. [13] we have varied the ion and molecule energy between 900 and 2200 keV/atom and for each energy we have determined the Coulomb heating values. Finally, the heating experimental results were compared with theoretical estimations, and it was found a reasonable theoretical-experimental agreement.

II. EXPERIMENTAL PROCEDURES

The experiments were carried out at the Ion-Implantation Laboratory of the Federal University of Rio Grande do Sul. The 3 MV Tandetron has delivered C^+ and C_2^+ beams with energies ranging between 900 and 2200 keV/atom with average currents of 40 and 20 nA for C^+ and C_2^+, respectively. In order to ensure identical conditions we kept the same C^+ and C_2^+ flux hitting the target.

The Si ⟨100⟩ samples were mounted on a four axis goniometer inside a chamber that was kept in a vacuum better than 10^{-6} mbar. The Si ⟨100⟩ channel of the target was determined by using a 1.2 MeV alpha beam, in order to minimize the radiation damage induced by C^+ or C_2^+ impinging beams on the target, as well as on the solid state detectors.

The full azimuthal average procedure was avoided because it would be time consuming and could lead to severe

damage of the sample. Instead, following the procedure recommended in Ref. [14], we have first determined the position of the {100} plane and then fixed the azimuthal angle at $\phi=12°$ relative to the plane. Further, by changing the other two angles we have determined the position of the Si ⟨100⟩ channel.

Subsequently the position of the sample was changed by using the vertical axis of the goniometer in order to get a fresh spot not damaged by the alpha beam. Following, we have changed to a C^+ beam and performed the angular scan around the Si ⟨100⟩ axis. The 1.74 keV Kα x rays emitted from the Si target were detected by a high purity Si(Li) detector with an energy resolution of 200 eV (at 5.6 keV). After performing the whole sweep around the center of the channel going from −3° up to 3° in 0.2° steps and recording at each step the x-ray yield, we have changed to a C_2^+ beam. On this occasion we moved the sample to another fresh target spot free of damage and we have subsequently repeated the above-described procedure.

As can be observed from the mentioned description extreme care has been taken in order to avoid or minimize the damage induced by the incoming beam during the scanning procedure. After each scan we have checked the $\chi_{\min}$ with an alpha beam and in all the cases we have obtained a 5% value or less, a feature that indicated that the C^+ or C_2^+ beam did not damage significantly the crystal. These precautions have been taken because the x-ray emission is very sensitive to damage or amorphization produced inside the channel.

In addition and simultaneously with the x-ray detection, for each position of the goniometer the corresponding C^+ and C_2^+ RBS-C spectra were recorded. The backscattered particles were detected by a Si surface detector, positioned at 165° with respect to the incoming beam. The overall Si detector and electronic system resolution (full width at half maximum) was around 30 keV. For each beam energy, the x-ray yields as well as the RBS-C spectra were obtained as an average from five (or six, depending on the involved cross sections) independent measurements performed under the same conditions of energy and C ion flux. The uncertainties were calculated taking into account the independent measurements as well as the fittings to the spectra.

III. EXPERIMENTAL RESULTS

As mentioned in the Introduction, our main objective that motivated the present work was to verify if the theoretical-experimental approach used in Ref. [13] for H_n^+ molecules can be applied to more complex molecules such as the C_2^+ ones.

The results for x-ray emission induced by C^+ and C_2^+ beams around the Si⟨100⟩ channel at 2200 keV/atom are shown in Fig. 1. Here, large angles correspond to nearly random direction. Two features can be clearly observed: First, at zero or near zero polar angle (see inset of Fig. 1) there is a small but significant difference in the x-ray yield (about 15%) induced by C^+ ions or C_2^+ molecules. In addition, in Figs. 2(a) and 2(b) we show a similar effect for C and C_2 beam energies of 900 and 1500 keV, respectively. Therefore it is clear that the Coulomb explosion effect is indeed

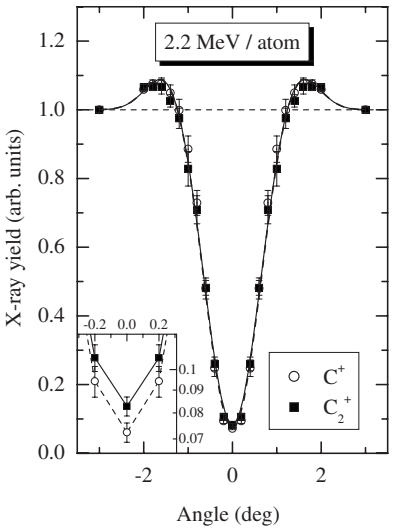

FIG. 1. C and C_2 x-ray yields as a function of the tilt angle with respect to the Si ⟨100⟩ direction at an energy of 2.2 MeV/atom. In the main panel is shown the whole scan between −3° and +3°. The lines are drawn only to guide the eye. In the inset it is shown the difference between x-ray yields for C and C_2 at around 0°.

present in the x-ray experiments and the difference is, without doubt, out of the experimental errors. This feature is a clear signature of the heating of the transverse motion due to the Coulomb explosion. Second, for large angles there are no differences in the x-ray yield induced by the C^+ and C_2^+ beams. This feature indicates that the vicinage effect does not play a significant role in the Coulomb heating mechanism. This behavior is expected, since the C_2^+ internuclear distance (about 1.5 Å) is larger than the characteristic x-ray and backscattering impact parameters [15]. Finally, the apparent inversion of the points corresponding to the C and C_2

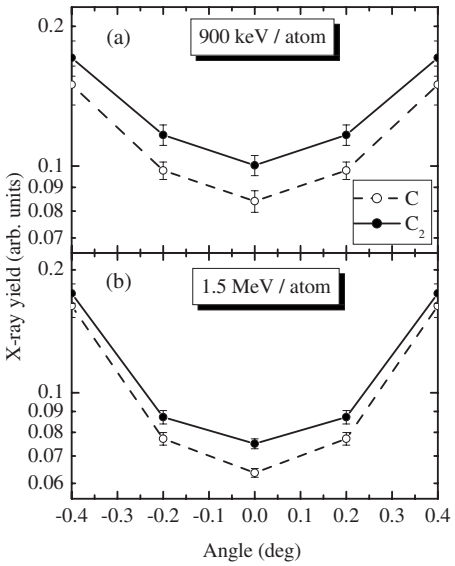

FIG. 2. C and C_2 x-ray yields near the Si ⟨100⟩ direction as a function of the tilt angle at an energy of 900 keV/atom (a) and 1.5 MeV/atom (b). The increase in the x-ray yields for C_2 is a clear signature of the Coulomb heating effect.

x-ray yields for larger angles (if well within the experimental errors) is justified by the Lindhard's angular compensation rule [16].

In order to obtain quantitative results from the experiments for the Coulomb heating, it is necessary to find the dechanneling rate as a function of the tilt angle, $\alpha(\psi)$. In order to extract the experimental values for the Coulomb heating, we have used the two-beam model [16,17], which has been successfully used in previous works [13,18]. The two-beam model is, in fact, a particular case of the discontinuous model used to solve the master equation for the transverse-energy distribution [17]. In this model, the beam is considered as a sum of two beam fractions distinguished by their transverse energies range: the fraction of ions with transverse energy below a critical value [17] is called "channeled." The remaining fraction is called "dechanneled." Under the restiction of a perfect or nearly perfect crystal, and disregarding the transitions from the dechanneled to the channeled fraction (since these transitions have low probability), we have that the dechanneled fraction $\chi(z)$ is given by:

$$\frac{d\chi}{dz} = \alpha[1 - \chi(z)], \tag{1}$$

where z is the depth inside the target and $[1-\chi(z)]$ is the channeled fraction, which, as well as $\chi(z)$, are both functions of the penetration depth z. For C^+ ions, the dechanneling rate α was chosen to be independent of z [18]. In fact, in Ref. [17], α was taken as a weak function of the depth z. In practice $\alpha(z)$ is almost constant for the first 1500 Å, and then have a feeble dependence on z. In the present work as well as in Refs. [13,18], α was assumed to be constant over all the analyzed depth (4000 Å). We have calculated that in this zero-order approximation the final error on the Coulomb heating values is less than 5%. The α value was determined, for each incident angle ψ, from the fitting of the C^+ RBS-C spectra. For this analysis we have used the electronic stopping to convert the energy loss in depth z as well as the Rutherford cross section to determine the backscattering yield [19] and each spectrum has been convoluted with the experimental resolution and energy loss straggling.

In order to determine the C_2^+ corresponding α parameters the RBS-C fittings were obtained following the same procedure as described above. Figure 3 shows two of the well-channeled C^+ and C_2^+ RBS-C spectra. It can be clearly seen that the C_2^+ RBS-C spectra shows an increasingly larger dechanneling (for lower backscattering energies) than the corresponding C^+ one. In this type of experiment, the dechanneling due to the Coulomb explosion seen in RBS spectra is more striking than the effect seen in the x-ray experiment. This happens because, as shown later in the present work, there is a delay in the Coulomb explosion effect. Consequently, the dechanneling feature is also a clear signature of the Coulomb heating effect. In the same figure is shown the fitting for the aligned C_2^+ spectrum (dashed line) assuming that the Coulomb explosion occurs at the surface ($z=0$).

However, this last assumption is not correct since there might be a delay time before the Coulomb explosion process

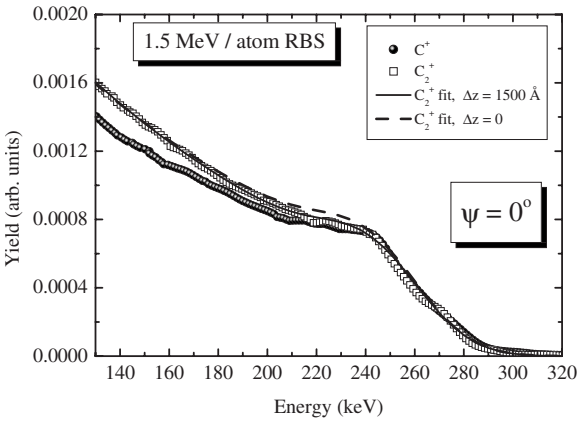

FIG. 3. RBS-C for 1.5 MeV/atom obtained with C^+ and C_2^+ beams, under channeling conditions, for $\psi=0°$. The dashed line represents the calculated fit assuming that the Coulomb explosion occurs at the near surface. The continuous line is a fit assuming that the explosion starts at around 1500 Å.

starts effectively. In fact, there are two reasons to consider an explosion delay. First, in the H_2^+ molecular experiment [13], it was shown that there is a Coulomb explosion delay (denoted as Δz) of the order of 400 Å. Second, the C_2^+ fit (dashed line) tends to overestimate the experimental values. The molecular breakup begins soon after the C_2 molecular ions penetrate a few monolayers in the target, however, the Coulomb explosion usually takes several hundreds of angstroms of ion penetration to change the ion flux and thus the transverse energy distribution. Although the flux change is a continuous process, for simplicity we assume in the fittings that the C_2^+ ion flux before Δz is the same one for the monoatomic ions and that all changes in flux due to the explosion are complete after Δz. Consequently, the obtained Δz values are a first-order estimation of the heating delay.

In this sense, in order to obtain a good fit, we have assumed $\Delta z \neq 0$. However, we have obtained several possible pairs ($\alpha(\psi)$, Δz) yielding a reasonable fit for the C_2^+ spectra. Then, we fitted the x-ray yields as well (not shown in Fig. 1), to ensure that a correct pair is chosen. The two-beam model function was modified to take into account the adequate K-shell ionization cross sections. Finally, a unique pair ($\alpha(\psi)$, Δz) that fits simultaneously the x-ray yields and the RBS-C spectra was found. An example of this procedure is given in Fig. 3 where the full line is a fitting of a 1.5 MeV/atom for a C_2 molecule assuming that $\Delta z=1500$ Å. This procedure was repeated for all the beam energies and Table I shows the obtained Δz results.

Once all $\alpha(\psi)$ are known, we can find the Coulomb heating energy through the Hamiltonian of the transverse ion motion which, for small ψ angles, reads

$$H_\perp = E_0\psi^2 + V(\vec{r}_\perp), \tag{2}$$

where E_0 is the beam energy per atom and $V(\vec{r}_\perp)$ is the channel potential. We consider the z direction of motion (parallel to the channel) as cyclic. In order to estimate the value of heating or enhancement of the transversal energy, we estimated that the time of the Coulomb explosion process

TABLE I. In the first column are quoted the energies of the C_2 clusters. In the second one, ΔE_c stands for the Coulomb heating experimental values. In the third one, Δz stands for the determined distances from the surface where the Coulomb explosion begins. The typical error is around 300 Å. The fourth one represents the molecular fragments equilibrium charge states obtained for each energy from Ref. [24].

Beam energy (keV/atom)	ΔE_c (eV)	Δz (Å)	Z_{eq} (e)
900	13.8 ± 3.8	1200	2.27
1200	19.3 ± 3.5	1200	2.57
1500	23.2 ± 3.5	1500	2.81
1600	25.0 ± 3.5	1500	2.88
2200	30.0 ± 3.5	2500	3.24

(about 10^{-15} s) is much shorter than the typical time for a single particle to get channeled (typically the period of an oscillation inside the channel, about 10^{-14} s). Under this assumption, the Coulomb explosion acts like an initial beam divergence or "astigmatic lens" [20] and increases the initial transversal energy by an effective Coulomb-heating energy ΔE_c. Since the initial transversal energy $H_\perp$ depends on the incident entrance angle (through the Hamiltonian), the additional Coulomb energy component ΔE_c will be equivalent to a tilt offset ($\psi \rightarrow \sqrt{\psi + \Delta E_c / E_0}$). Therefore we can finally find ΔE_c by using the equation

$$\alpha_{mol}(\psi = 0) = \alpha_{atom}(\psi = \sqrt{\Delta E_c / E_0}). \tag{3}$$

In Fig. 4, we show a direct application of Eq. (3) for the particular case of RBS at 900 keV/atom. There are displayed the α_{atom} of the C^+ ion for two different angles and the $\alpha_{mol}(0)$ corresponding to C_2^+. From a simple interpolation (displayed in the figure as a dashed line) we have obtained the corresponding $\Delta\psi$ and consequently the Coulomb heating value, since $\Delta\psi = \sqrt{\Delta E_c E_0}$.

In Fig. 5 and in Table I we displayed the experimental transverse heating values, the corresponding Δz as a function

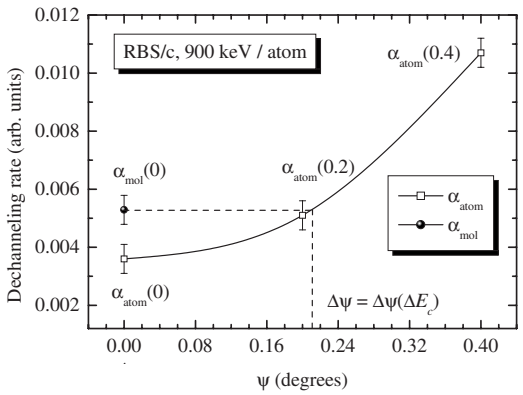

FIG. 4. Two-beam model dechanneling factor α as a function of the tilt angle obtained from the 900 keV/atom experiment. The numbers in parentheses stand for the tilt angles in degrees—see text.

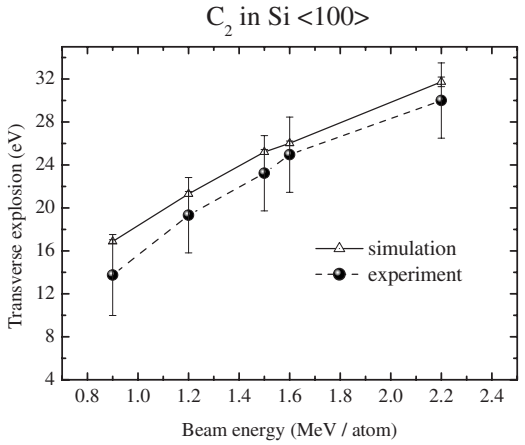

FIG. 5. Transverse explosion as a function of the C_2^+ incident energy per atom. The circles stand for the experimental results, while the triangles represent the theoretical calculations.

of the beam energy. Other effects, such as the position-dependent screening by the targer electrons, close-collisions with target electrons and nuclei, and projectile electon capture and loss can lead to heating or cooling effects (not related to the Coulomb explosion) [21]. However, we expect that these mechanisms change the channeled C and C_2 ion fluxes nearly in the same way. Therefore the Coulomb heating values quoted in Table I should be mainly due to the Coulomb explosion.

As can be observed from an inspection of Table I, the heating values change from 14 eV (for 900 keV/atom beams) up to 30 eV (for 2.2 MeV/atom) and seem to reflect the variation of the equilibrium charge (Z_{eq}) of the molecular fragments as a function of the beam energy.

IV. THEORETICAL CONSIDERATIONS

In order to obtain the theoretical Coulomb heating values, a Monte Carlo simulation was developed for both C^+ and C_2^+ ions channeling along the Si ⟨100⟩ direction. Several assumptions were used in order to describe the ion motions in a simple way. The main idea is to simulate how the ion flux in the Si ⟨100⟩ channel behaves for the monatomic as well as the molecular beams. To that end, the Si ⟨100⟩ channel is described using the string potential model [16,22], and Newton's equations are solved in order to describe the motion of an ensemble of ions or molecules impinging on the channel under a given tilt angle Ψ (and internal angles in the case of molecules). In order to describe the interaction between the ions and the target nuclei, we used the Molière interatomic potential. A slightly better ion motion description near the strings was performed by including thermal vibrations effects [23]. The angle between the molecular axis and the motion direction, as well as the initial position of the projectile impinging the channel, are chosen randomly. The ion charge state is chosen randomly from a Gaussian distribution centered in the equilibrium charge value with known width Δq [24]. Due to the relatively small amount of experimental information about C equilibrium charge states under channeling conditions in our energy range, we have selected those

of Ref. [24] which corresponds to the ones obtained for amorphous Si—see Table I. This choice is not far from reality. In fact Jiang *et al.* [25] have investigated equilibrium charge states for different ions impinging on Si films under channeling and random conditions. In particular he found that for N at energies similar to the present ones or higher, the equilibrium charge states were achieved and are independent on the channeling or random conditions of the target film. Therefore as an initial guess, it seems reasonable to adopt the present procedure [26].

The charge state is kept constant along all considered ion paths and the Molière potential screening parameter for a given ion path is evaluated accordingly. It is important to point out that, in this way, charge changing effects along each ion motion were not taken into account in our simulations. The energy loss was taken into account by the use of the unitary convolution approximation [27,28] that gives the energy loss of an ion as a function of the impact-parameter $Q(b)$. The energy loss is then evaluated at chosen depths (as a function of the Si lattice parameter). In this way, the energy loss is strongly dependent on the transverse ion energy and then on the ion trajectory. In this procedure we assume that some of the electrons from the impinging C_2^+ molecule are suddenly removed along the first monolayers and, consequently, the molecule undergoes a breakup process. We assume that each atom reaches its own equilibrium charge state as soon as the breakup process begins. In this way, our simplified simulation does not take into account a more detailed molecular fragmentation description. In fact, orientation, velocity, and position-dependent effects on the molecule breakup (as, for instance, wake effects [1]) not included here are expected to decrease the obtained theoretical values for the Coulomb heating. The interaction between the C_2^+ molecule fragments is modeled using an analytical fitting to the Dirac-Hartree-Fock-Slater calculations for the screened ion potential [28–30] between each C nuclei and the electron clouds, which takes into account the chosen charge state for C ions in the target. No further screening due to the target was assumed, as indicated by results observed in Ref. [31]. In order to study the explosion effects on the ion flux, the simulations were carried out only along the first 4000 Å. There are two reasons for this depth choice. First, at 4000 Å, it is safe to assume that the potential energy stored in the molecule is nearly completely transferred to the molecular fragments motion. Thus no further increase on the transverse energy can be expected from the Coulomb explosion after that depth. Second, a significant amount of ions is still channeled. Then, it is possible to compare the monoatomic beam and the molecular beam flux peakings.

Figure 6 shows the ion flux for both C and C_2 beams averaged along the depth (4000 Å). The ion flux for the C^+ beam displays the well-known flux peaking, i.e., a strong enhancement of the flux near the center of the channel. The C_2^+ beam still shows the flux peaking effect. However, as presented in Fig. 6, this effect is considerably damped for the molecular beam due to the Coulomb explosion, which enhances the transverse energy of the molecule fragments and, consequently, produces higher ion fluxes far from the channel center.

In order to evaluate the average transverse explosion energy transfer to the molecule fragments, we considered, for each beam energy, the distributions of transversal energies at 4000 Å depth in the target, far after the Coulomb explosion process. One of these distributions, as obtained from our simulations, is shown in Fig. 7 which corresponds to 2.2 MeV/atom C and C_2 beams. As can be observed for the same yield, the transversal energy distributions for the molecular ions are shifted to higher energies, a consequence of the Coulomb-heating process. The theoretical values of the Coulomb heating were then obtained by shifting (dashed curve) the atomic distribution in Fig. 7 to agree with the molecular one at higher transversal energies. This is because only higher transverse energies ions have a high probability of undergoing close encounter events that yield x-ray emission and backscattering. The obtained theoretical values are displayed as triangles in Fig. 5. An observation of Fig. 5 shows that the theoretical curve overestimates the experimental values but it follows the tendency of the experimental results, the agreement, within the experimental errors, being quite reasonable. In fact with the exception of the lowest energy point the difference between the theoretical and experimental values is less than 10%. Based on both observations we can conclude that the main objective of the present work has been achieved. First, using the same experimental method as for the H_n molecules and the same data analysis [13] we

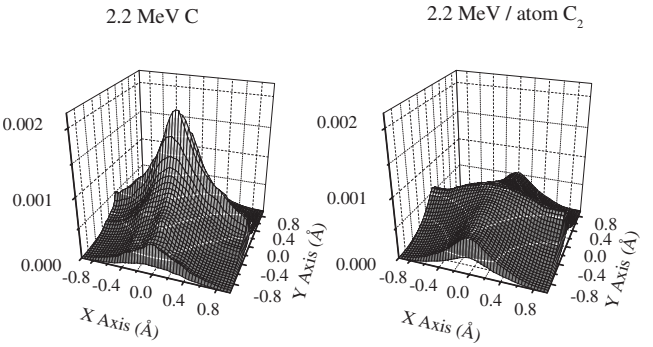

FIG. 6. C and C_2 fluxes inside the ⟨100⟩ Si channel obtained via simulation of aligned 2.2 MeV/atom C and C_2 beams—see text. The flux peaking is clearly seen for both beams, however, it is heavily damped for the C_2 beam due to the Coulomb explosion.

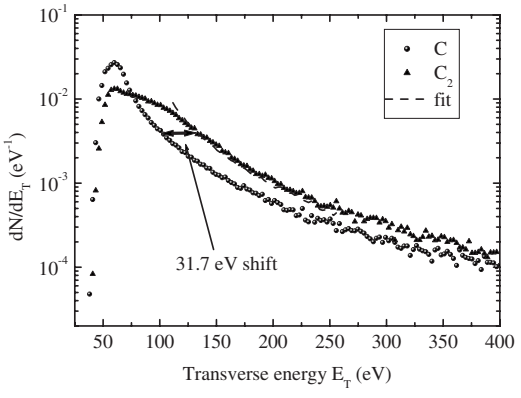

FIG. 7. Simulated transversal-energy distribution for 2.2 MeV/atom C and C_2 beams. An energy of 31.7 eV is necessary in order to match the C_2 and C distributions at transverse energies above 150 eV—see text.

were able to obtain the Coulomb heating values for more complex molecules like C_2. Second, the simple model used in H_n molecules [13] still can be used for first estimatives in the present case. However, we cannot disregard the systematic theoretical-experimental difference observed in Fig. 5. This feature indicates that the present simulation should be refined. It is possible that the introduction of (a) possible new experimental equilibrium charge state values under channeling conditions, (b) the dissociation cross section of the molecule, (c) a full three-dimensional molecular fragmentation description, and (d) position-dependent charge exchange effects (taking into account the local electronic and atomic densities inside the crystal channel) can improve the theoretical-experimental agreement.

V. SUMMARY

In the present work, we have determined quantitatively the effect of the C_2 Coulomb explosion on the transverse energy distribution in a Si ⟨100⟩ channel. This was done by combining the Si x-ray yield as a function of the tilt angle and the corresponding C and C_2 RBS+channeling spectra. This study was performed in a wide beam energy range, between 900 and 2200 keV/atom and it was found that the Coulomb heating ranges between 14 and 30 eV. This behavior could be, in essence, attributed to the fact that the molecules initially have different velocities and consequently the fragments have different equilibrium charge states, leading to different average transverse energies added by the Coulomb explosion. Finally we should mention that the simple theoretical model used in Ref. [13] for H_n molecules still can be used for more complex molecules like the C_2 ones for a first-order estimation. In the present work we have obtained a satisfactory theoretical-experimental agreement. However, the theoretical tendency to overestimate the experimental values (but still within the experimental errors) is a clear indication that the model used in the simulations needs to be refined in order to get a better agreement.

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