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# Molecular dynamics simulations of Coulomb explosion

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## Abstract

A swift ion creates a track of electronic excitations in the target material. A net repulsion inside the track can cause a “Coulomb explosion” (CE), which can lead to damage and sputtering of the material. Here we report results from molecular dynamics simulations of CEs for cylindrical tracks as a function of charge density and neutralization/quenching time,  $\tau$ . Screening by the free electrons is accounted for using a screened Coulomb potential for the interaction among charges. The yield exhibits a prompt component from the track core and a component from the heated region produced, which dominates at higher excitation density. For the cases studied, the number of atoms ejected per incident ion, i.e. the sputtering yield  $Y$ , is quadratic with charge density along the track as suggested by simple models.  $Y$  does not depend greatly on  $\tau$  for  $\tau \gtrsim \tau_D$  (one Debye period), and even  $Y$  ( $\tau = 0.2\tau_D$ ) is still nearly 20% of the yield when there is no neutralization ( $\tau \rightarrow \infty$ ). The connections between ‘CEs’, thermal spikes and measurements of electronic sputtering are discussed.

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## 1. Introduction

When a solid is bombarded by a fast ion, a track of excitations is formed [1]. The incident ion promotes atoms to excited states, and also creates electron–hole pairs. Some electrons are expelled from the track as fast delta electrons, creating other electron–hole pairs in a time scale of  $10^{-17}$ – $10^{-16}$  s. They gradually thermalize, screening the holes, and finally recombine with the holes in times which vary from  $\sim 10^{-16}$  to  $10^{-6}$  s depending on the material. If hole mobility is low and recombination

slow, the holes can repel each other leading to a “Coulomb explosion” (CE), in which the charges acquire large velocities and transfer energy to neighbors. CE has been suggested to produce track amorphization, material damage [1–3], surface modification [4], and particle ejection (sputtering) [5–7]. However, it is not clear whether or not the Coulomb repulsion in the track core lasts long enough to produce significant effects and whether or not it can quantitatively describe the energy deposition in the track core.

Although CE has been thought to play a role in many experiments on swift ion bombardment, there are few direct simulations of this process. In a recent paper [8], we presented molecular dynamics (MD) simulations of CE focusing on the

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comparison of CE and “thermal spike” (TS) models. Here we explain our simulations in more detail and present some new results. We first review some existing models of CE, then give the details of our model computer simulation, which includes screening and neutralization/quenching effects, and finally present our results.

### 1.1. Models of Coulomb explosion

In 1965 Fleischer, Price and Walker (FPW) developed their now well-known “ion explosion model” to account for track registration in solids [1]. In this model the large positive charge density in the track core leads to a transformation of the electrostatic potential energy into kinetic energy (KE) of the charged atoms. These in turn transfer KE to neighboring atoms. This model appeared to successfully predict when ion tracks could be “registered”, but was not used to describe surface effects. Damage in the track was related to the ionization per unit path length,  $dJ/dx$ , rather than to the energy loss per unit path length,  $dE/dx$ . FPW showed that analytic TS models [9] could not explain track registration data. These TS models were overly simplified [10–12] and the experimental data were not comprehensive. Models and experiments [3] appear to suggest that even in metals, where screening by the conduction electrons is rapid, CE can deposit enough energy in the lattice to produce a shock wave which produces defects.

Haff [6] first used the ion explosion concept to estimate a sputtering yield,  $Y$ , suggesting that  $Y \propto (dJ/dx)^2$ . Subsequently, Tombrello and co-workers developed a “thermalized ion explosion model” [13]. In this model the CE leads to a localized high temperature region, and sputtering was then calculated using an analytic spike model. This gave  $Y \propto (dJ/dx)^4$  when the radius of the spike,  $r_{\text{cyl}}$ , was such that  $r_{\text{cyl}} \propto dJ/dx$ . This model appeared to fit certain data over a limited range of  $dJ/dx$  [13]. Ritchie and Claussen [14] suggested that the secondary electrons from the ion track heated the neutrals by collisions. Later, Ritchie et al. [15] developed a numerical model to track all charged particles, including electrons, assuming complete ionization within a certain time-varying radius. A class of models which are a variation on

the CE model [16,17] assume that the escape of the electrons from the track changes the effective potential among atoms. This leads to an instability which increases the KE of the atoms in the track. Ejection may then be direct or due to the resulting TS. Such a model has been used to explain recent gigantic sputtering data for GaAs [7]. A CE model of sputtering, applied to ionic crystals, was also presented by Bitenski et al. [18], where the value of the yield depended on a fitting parameter and on the value of the neutralization time for the charges.

### 1.2. Coulomb explosion simulations

We use MD simulations to follow the evolution of the “ionized track” in a Lennard-Jones (LJ) fcc solid. Details of the MD code have been described elsewhere [8,10]. Because the cohesive energy and spatial dimensions scale with the LJ parameters, results for other solids can be obtained using the appropriate number density  $n$  and cohesive energy  $U$ . The Debye period,  $\tau_D$ , gives a characteristic time scale for phonons and also scales with  $n$  and  $U$ . MD simulations of CE have been performed for small clusters [19], and there have also been other simulations where the initial velocity of the atoms induced by Coulomb repulsion was assumed to be known and the motion of atoms was then followed [20,21]. CE in LiF due to two neighbor holes has been reported [22], but the first MD simulations of CE in the solid phase with more than two charges [23] were carried out only for small 2-D samples. Cheng and co-workers [24] have reported large-scale 3-D simulations for CE in Si, with a charge configuration that extended a few layers below the surface, such as produced by a slow, highly charged projectile. In this work we deal with different initial conditions. For a swift ion the track length is much larger than the other relevant sizes. Not all atoms inside the track are ionized by the passage of the ion, and the number of ionizations changes with the stopping power of the incoming ion. Finally, the charges in the track can have a lifetime that can be much shorter than the simulation time, so neutralization is included.

In order to simulate the CE process within an ion track, a specified number of atoms within a

cylinder of radius  $r_{\text{tr}}$  were given a net charge at time  $t_0$ . Atoms were chosen randomly for each simulation, giving a mean number of charges per layer  $N_{\text{ch}}$ , which is proportional to  $dJ/dx$ ,  $l_s dJ/dx = N_{\text{ch}}$ , where  $l_s$  is the layer spacing. Most simulations are performed for  $r_{\text{tr}} \sim l_s$ , which gives a maximum of two charges per layer. Runs for  $r_{\text{tr}} \sim 2.5l_s$  show the same behavior at early times. Here we simulate an ‘ionization track’ in which the holes have low mobility and are not fully screened during the time atomic displacements occur. Even if the holes are neutralized, a track of excited atoms will have overlapping charge clouds that act repulsively [5,16,17]. Therefore, we do not distinguish between closely spaced, partially screened holes or interacting excited atoms. We describe the repulsion between such excited (‘ionized’) atoms using a screened Coulomb potential in addition to the LJ potential. The screening function was chosen to be an exponential, giving the Yukawa form for the potential  $V = (e^2/r) \exp(-r/a)$ , where  $a$  is an average screening constant. This interaction has a large cut-off at  $r_{\text{cut-Coul}} = 7a$  in order to provide energy conservation. Coulomb interactions in polar insulators, such as water, are typically neglected due to the high dielectric constant. In non-polar materials, screening is small when there are no excited (‘free’) electrons. For our simulations we assume that the produced ‘free’ electrons screen the ions in the track, creating a very hot plasma [14].  $a$  can be taken to be the Debye screening length [25], which depends on the local electron density,  $n_e$ , and electron thermal velocity,  $v_T$ ,  $a = \lambda_D = v_T/\omega_p = \sqrt{\epsilon k_B T/n_e e^2}$ , where  $\epsilon$  is the dielectric constant. A Yukawa potential with Debye screening has been used to calculate the screening among atoms of  $\text{C}_{60}$  clusters which ‘Coulomb-explodes’ on penetrating a solid [26]. The classical Debye length should be replaced by the Thomas–Fermi length,  $a_{\text{TF}}$ , for certain densities/temperatures of the electrons [25] but, for the cases considered here,  $\lambda_D$  is more appropriate. Using  $n_e = 0.01/\text{\AA}^3$  and  $k_B T = 10$  eV gives  $\lambda_D \sim l_s \sim 3a_{\text{TF}}$ . The screening in fact varies with time, due to the cooling of the electrons to the lattice, and depends on the local environment. Recombination models (for instance Auger [27], columnar [28], or geminate recombination [29]), that predict the changes of the electronic density could

be included in future studies. If the screening length does *not* change significantly during the time scale at which CE occurs, then MD simulations with a constant value of  $a$  can be carried out. Monte Carlo simulations of a track of holes and electrons in amorphous solid Ar by Vidal and Ferrón [30] show that the electron density is roughly a Gaussian by  $t \sim 1$  fs, and that it does not change significantly during several fs, when the simulation stops. In molecular solids, the electrons will suffer significant inelastic collisions, leading to an even narrower spatial distribution around the initial track. Neutralization may also change the distribution of electrons before CE is effective. In order to test the validity of using a constant screening length,  $a$ , track simulations including inelastic energy loss have been performed and it was found that the density did not change significantly for times of the order of  $\tau_D$  and energy losses appropriate for ice [8,31].

Neutralization in the track core during sputtering should be taken into account. To evaluate its effect on the sputtering yield, we allow the number of charges within the track to decrease exponentially with a quenching/neutralization time  $\tau$ , as  $\exp[-(t - t_0)/\tau]$ . Screening and neutralization are closely related. That is, a large electron density which heavily screens the charges is similar to electrons which neutralize the charges. At large electron densities hole neutralization is initially fast, but the resulting reduction in the screening rapidly slows the process [8,31]. Estimates of neutralization times vary by orders of magnitude. Ion-induced electron emission spectra can give insight into the magnitude of the neutralization times [32,33].

The interaction of the charged atoms with the neutral atoms was left unchanged in our simulations. The neutrals, of course, contribute to the screening, but in test simulations the effect of the polarization of the neutrals on lattice heating was small. Particles are counted as sputtered if they cross a plane  $2r_{\text{cut}}^{\text{Coul}}$  above the surface. The number of atoms ejected per run is called the yield. Only results for the (001) surface are shown. The samples had an open top surface to allow for sputtering. Sample sizes ( $3 \times 10^{4-5}$  atoms) and simulation times (15–80 ps) were adjusted

according to the size of  $a$  and  $dJ/dx$ , so that the dynamic region was accommodated. Extending times by tens of picoseconds, doubling the thickness, or changing the boundary conditions did not change these results. Sample depth was chosen to be at least twice the cut-off radius for the Yukawa potential. Yields from individual simulations were averaged over  $\sim 10$ – $100$  ‘ionization’ distributions because the spread in the size of the yield is broad, especially for small  $(dJ/dx)$  where sputtering only occurs when two excitations are produced close together at the surface [5,6].

## 2. Results

We find that the sputtering yield,  $Y$ , for a given screening constant,  $a$ , and for a given neutralization time,  $\tau$ , is roughly given by

$$Y(\tau = \infty) \approx 14.1 \ln[1.3a/r_{tr}] [l_s(dJ/dx)]^2, \\ Y(\tau \lesssim 50T_D) \approx Y(\tau = \infty) \times \exp[-0.75(-\tau_D/\tau)^{0.50}], \quad (1)$$

$Y(\tau = \infty)$  indicates the yield obtained with static screening but no neutralization. The quadratic dependence with  $(dJ/dx)$  predicted by several models is only valid if the screening length  $a$  is assumed to be constant for different values of  $(dJ/dx)$ . Fig. 1 shows the sputtering yield as a function of  $a$ , for  $a$  in the range  $l_s$  to  $5l_s$ . Values of the screening constant  $a$  smaller than the nearest neighbor distance give very small yields since the repulsion between excited species is negligible. The logarithmic dependence on  $a$  in Eq. (1), seen in Fig. 1, agrees with analytic predictions [5]. Fig. 2 shows the yield from MD simulations as a function of  $\tau$  together with the fit from Eq. (1) for a number of cases. For  $\tau = 0.2\tau_D$  the yield is nearly 20% of the yield for  $Y(\tau = \infty)$ , indicating that CE could be important in ejection processes if the neutralization (quenching) time  $\tau \gtrsim 0.2\tau_D$ .

Fig. 3 shows a series of snapshots of a CE simulation and illustrates ejection due to ‘direct’ Coulomb repulsion: two large red circles (hot charged particles) being ejected by 0.26 ps. Later ejection involves neutrals (small circles) which are

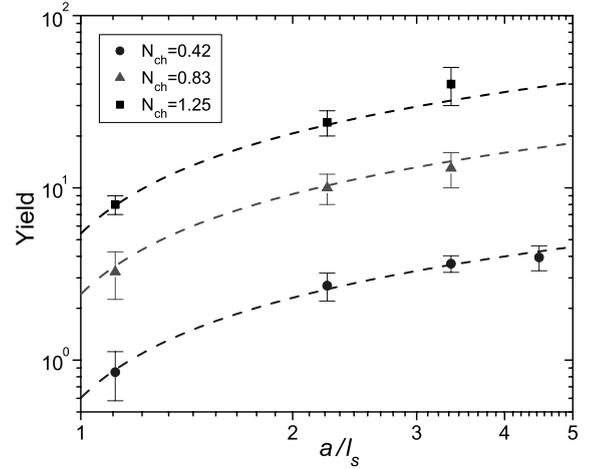


Fig. 1. The sputtering yield from a repulsive track versus the screening constant  $a$ . The dashed lines are from Eq. (1).

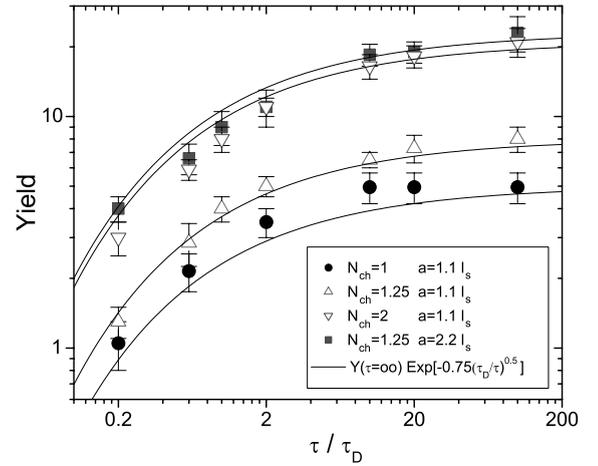


Fig. 2. Yield versus  $\tau$ , the neutralization/recombination time. The solid lines are from Eq. (1),  $Y(\tau = \infty) \exp[-\alpha(\tau_D/\tau)^p]$  with  $\alpha = 0.75$  and  $p = 0.5$ . A better fit can be obtained varying  $\alpha$  and  $p$  slowly with  $(l_s dJ/dx)$ .

both hot and ‘cold’. In the last snapshot the crystal structure near the surface shows some damage, but it is well reconstructed away from the surface.

Figs. 4(a) and (b) show depth and radial distributions of ejecta, normalized to unit area, for two different neutralization times. The longer the neutralization time, the deeper and farther from

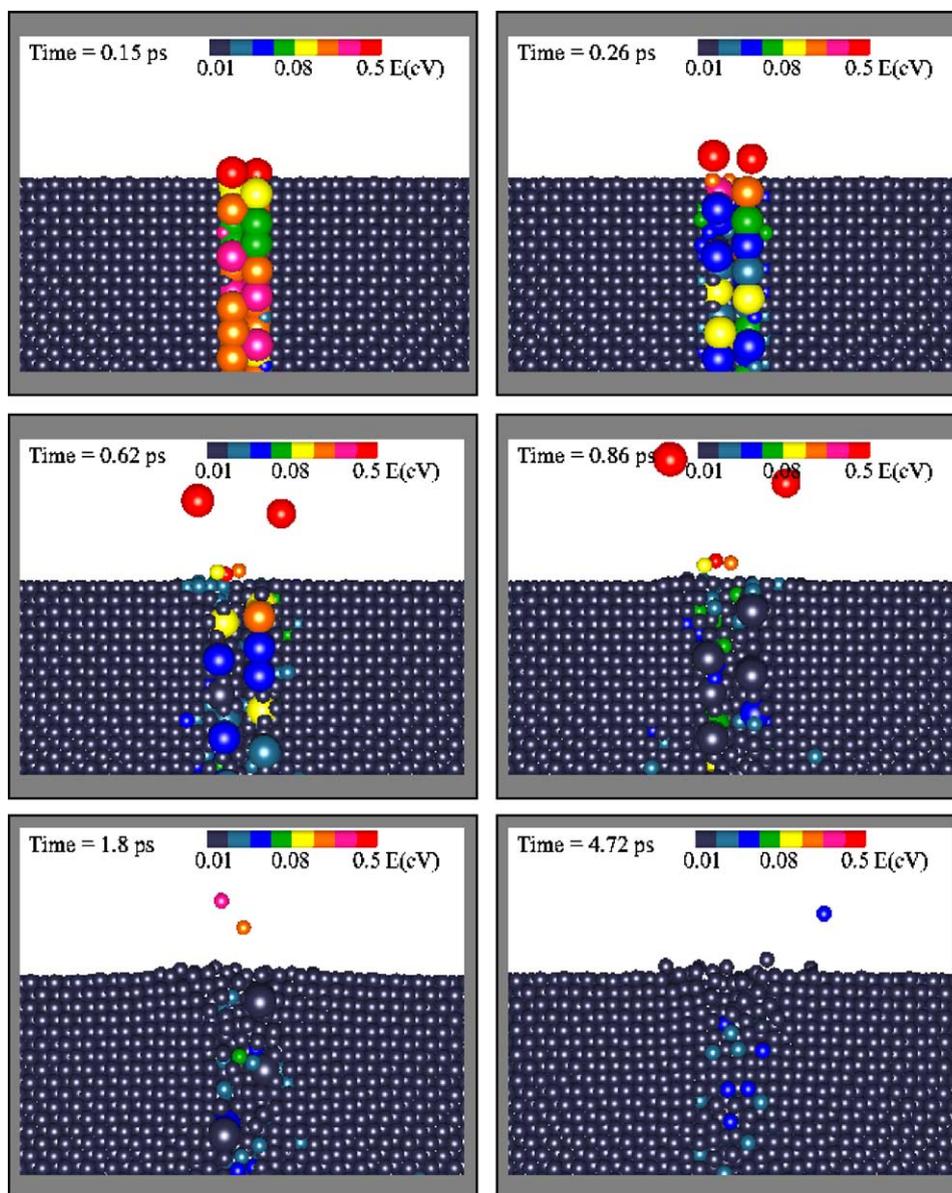


Fig. 3. Snapshots from a MD simulation of CE. Screening constant  $a \approx l_s$ , neutralization time  $\tau = 2\tau_D$ , and  $N_{ch} = 2$  in the fully excited track of  $r_{tr} \approx l_s$ .  $U = 0.08$  eV and  $\tau_D = 0.5$  ps. Charged particles have twice the size of neutrals. Color code correspond to KE of the particles (red hotter, blue colder).

the track the ejecta can originate. Figs. 5(a) and (b) show the KE distribution of ejecta for the same neutralization times as in Fig. 4. At large KE,  $E \geq 10U$ , the spectra exhibits peaks due to prompt ejection from the surface layers in the initial track (second frame in Fig. 3). This includes initially

‘ionized’ species and accounts for  $\sim 20\%$  of the ejecta at large  $dJ/dx$ , but dominates at very small  $dJ/dx$ . On the other hand, the principal component of the ejecta in Fig. 5 has an energy distribution like that found in our studies of ejection from a cylindrical spike (dashed line) [10]. That is,

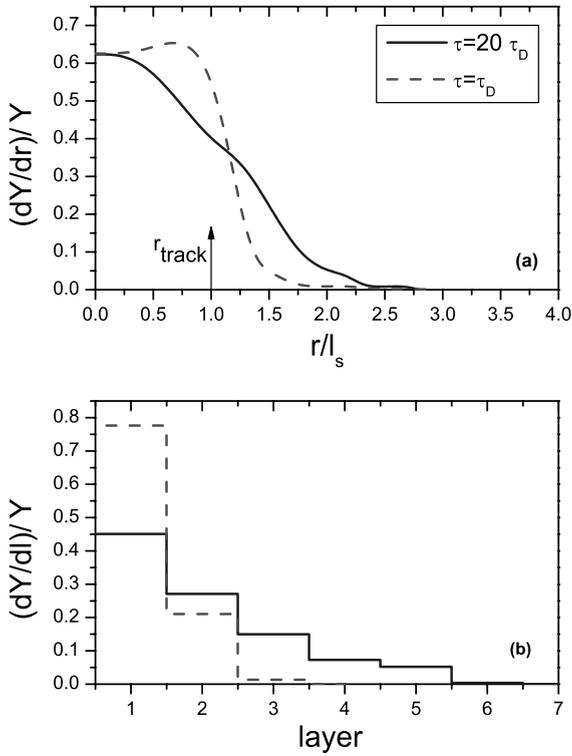


Fig. 4. Depth and radial distribution of ejecta for  $N_{\text{ch}} = l(dJ/dx)_{\text{eff}} = 2$ ,  $a \approx l_s$  and  $r_{\text{tr}} \approx l_s$ . Both  $\tau = \tau_D$  and  $\tau = 20\tau_D$  are shown.

there is a broad, quasi-thermal distribution at low ejecta energies,  $E < U$ , which gives way to a  $\sim E^{-2}$  dependence at  $E > U$  differing from TS model predictions [10]. This is the ejection seen in frames 4–6 in Fig. 3. If CE contributes to sputtering, the experimental energy spectra would have a peak due to ejection of surface ions (which may be neutralized on their way to the detector). In an experiment, the size of this peak will be small and may be hidden by the background noise. The position of the peak is related to  $(dJ/dx)_{\text{eff}}$ :  $\text{KE} \approx C_1 U [l(dJ/dx)]^2 - U - E_{\text{pol}}$ , where  $C_1$  depends strongly on the track radius,  $r_{\text{tr}}$ , and screening length,  $a$ , and slightly on the neutralization time,  $\tau$ .  $E_{\text{pol}}$  is the energy required to extract an ion from the surface due to polarization forces. For our MD simulation,  $E_{\text{pol}} = 0$ ,  $r_{\text{tr}} \approx l_s$ , and  $C_1 \sim 35$  for  $a \approx l_s$ . Therefore, the CE should exhibit a peak at  $\text{KE} \sim 34U$  for  $[l(dJ/dx)] = N_{\text{ch}} = 2$ . The peak in the

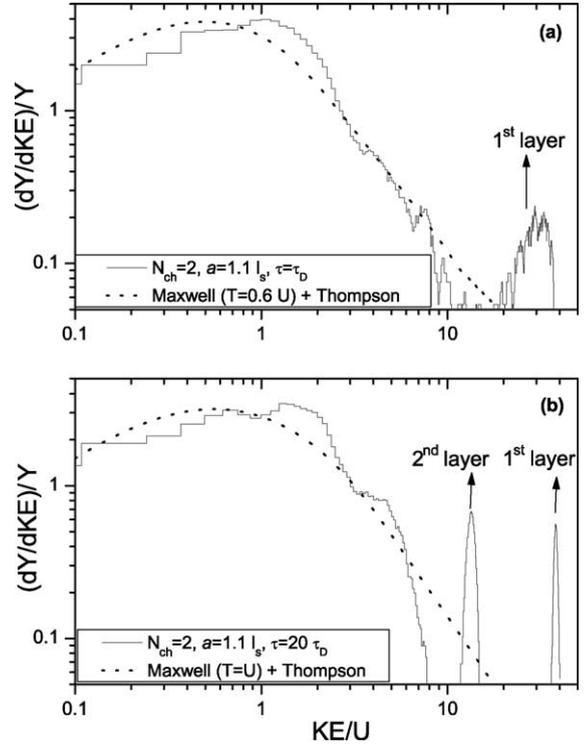


Fig. 5. Energy distribution of the ejecta for  $(l_s dJ/dx) = 2$ ,  $a \approx l_s$  and  $r_{\text{tr}} \approx l_s$ , for  $\tau = \tau_D$  (a) and  $\tau = 20\tau_D$  (b). Dotted line: energy spectrum obtained adding a Maxwellian distribution to a Sigmund–Thompson distribution. High energy peaks are prompt ejecta determined by the potential energy between neighbors and  $U$ .

MD simulations, in fact, appears at  $\text{KE} \sim 38U$  for  $\tau = 0$  in agreement with this estimate. For  $\tau = \tau_D$  a broad peak with a height  $\sim 15$  times smaller than the height of the maximum is located at  $\text{KE} \sim 32U$ .

In order to verify if the repulsive energy transferred to the lattice indeed forms a TS, energy transport at the atomic level should be extracted from these simulations [8]. When we compare the nature of the energy transport beyond  $\sim 0.2\tau_D$ , the sputtering yield, and the ejecta energy spectra with the results from our earlier TS MD simulations, the quantitative agreement is good. In both cases, the transport is not simply by thermal diffusion. At large  $dJ/dx$  most of the ejecta are generated by the “thermal” hot spike produced. That is, the ionization track rapidly

produces a heat spike which determines the subsequent energy transport, sputtering and bulk damage. This means that ‘CE’ and spikes are the *early and late* aspects of an ionization track and differences in predictions occur due to the use of *incorrect* spike models.

### 2.1. Electronic sputtering of molecular condensed gas solids

One of the principal outstanding problems in electronic sputtering is the fact that yields for molecular condensed gas solids appear to vary roughly quadratically with the electronic stopping  $(dE/dx)_e$ , at high  $(dE/dx)_e$ , as initially shown by Brown and co-workers (see e.g. [5]). Since both CE and analytic TS models directly give such a dependence, they have been used to analyze the laboratory data [34]. The standard analytic TS model, which has now been shown to be incorrect [10], can be modified [35]. Here we note that our CE MD simulations confirm that a CE model can also be applied. That is, a CE can produce a TS at high  $dJ/dx$ . If the neutralization times and electron densities are such that  $\tau \gtrsim 0.2\tau_D$  and  $a \sim l$  for  $0.02\tau_D < t < 0.2\tau_D$ , a quadratic dependence of the yield  $dJ/dx$  occurs and the ejecta energy spectra are similar to those observed for molecular condensed gas solids [36,37]. Since  $(dJ/dx) \propto (dE/dx)_e$ , the resulting yield is also quadratic in  $(dE/dx)_e$ . Because electron density and neutralization times are difficult to measure or evaluate theoretically, it is not clear if the above conditions are fulfilled for the tracks in molecular condensed gas solids. If the screening length varies with  $(dE/dx)_e$  the yield might not be quadratic and the neutralization times are not well known but may be short. The sizes of the yield in the model MD simulations are consistent with the experimental yield for solid  $O_2$  at high  $(dE/dx)_e$ . However, if only Coulomb repulsion were driving sputtering, the sputtering yields of solid  $O_2$  and  $N_2$  should be close in size, since they have the same binding energy,  $U$ , and, one would assume, similar neutralization times and hole diffusion. However, the yield for  $O_2$  is almost one order of magnitude larger suggesting that differences in the relaxation processes are critical: differences in ionization lev-

els, luminescence [34] and chemistry of the dissociation products [38].

### 3. Summary

We carried out MD simulations of a simplified CE model, which roughly described that when the electrons are excited by a fast ion the average track potential experienced by the ions is repulsive. Using a screened Coulomb potential with constant screening length, the simulations verified predictions that the sputtering yield is quadratic in the ionization per unit path length,  $dJ/dx$ , created in the track of a fast ion over a broad range of  $dJ/dx$ .

The yield consists of two components: prompt ejecta from the track core, which dominates at small  $dJ/dx$ , and ejection from the heat spike formed, which dominates at high  $dJ/dx$ . That is, the potential energy was seen to evolve into kinetic energy of the ions in the track and of the surrounding neutrals. This can form a cylindrical spike with a radius larger than the initial track radius producing sputtering.

The mechanism for converting electronic energy into lattice motion can be either the transfer of energy to the lattice directly by the secondary electrons or by a repulsive force. The repulsion may result when electronic recombination occurs ( $O_2^+ + e \rightarrow$  repulsive state  $\rightarrow O + O + \Delta E$ ), due to the repulsive track of holes partially screened by free electrons, or by the interaction between ‘excited atoms’ in the track. At high excitation densities, once the energy is in the lattice motion, the evolution of this energy can be described by that spike model shown to be correct by MD [10] and hydrodynamic simulations [11], rather than the convenient but incorrect analytic diffusive spike model. In order to determine the evolution of the ion track it is crucial to accurately describe the electron screening and neutralization [8]. When neutralization is introduced, the yield can decrease. Neutralization times longer than one tenth of the Debye period are needed in order for CE to be effective in heating the lattice and producing sputtering. Information on electron temperature in the track, for instance from Auger electron spectra [32,39], can be used to test models. Measurements

of luminescence in condensed gas solids [40], response of semiconductor detectors to radiation [41] and the survival probabilities of ions in liquids [28,29] can also provide information on neutralization.

Although sputtering is a very old field of physics, the discovery of electronically-induced sputtering and the possibility of creating extremely high energy densities in very narrow regions will continue to test our ability to describe solid state processes under extreme conditions.

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