

Nanocrater formation via Coulomb explosion initiated by impingement of highly charged xenon ions with silicon surface

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ABSTRACT

The aim of this work is to study the dynamics of nanocrater formation induced by Coulomb explosion. The Molecular Dynamics (MD) method is used with realistic interaction potentials. The time and space distribution of density, pressure and temperature of the simulated Si sample and, finally, the time-velocity dependence of the charges and neutrals yield are investigated.

1. INTRODUCTION

The interaction between a highly charged ion (HCI) impinging on a solid surface with a low translational energy has extensively been investigated recently. It is well known that a HCI is neutralized very fast (<10 fs) even if the HCI does not still reach the surface [1-5]. Therefore the electronic potential energy of HCI is released very near the surface and the more charged the ion, the more effect it produces on the surface before the impact itself takes place [6]. The dependence of the potential HCI energy (the energy needed to strip the atomic electrons to the q charge state) on q is presented in Fig.1.

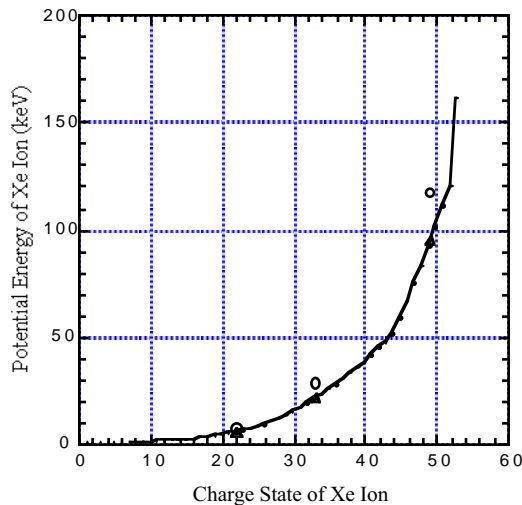


Fig.1. Potential energy of HCI versus its charge state. Circles are estimate by (2). Triangles are MD computation.

strong Coulomb field of HCI can pull the electrons from the solid surface. These electrons are then captured into Rydberg (high levels) states of the ion. Thus, a superexcited 'atom' with empty inner shells (so called hollow atom) is created. The "hollow" atom then relaxes to its ground state via Auger processes, with ejecting electrons and/or photons. Therefore the total number of electrons pulled out of the solid can be greater than the initial charge of the ion q .

If the process of HCI relaxation is fast enough, the charged zone is formed close 'below' the falling ion, with the charge $N > q$. Strong repulsion interaction between the newly formed ions, that belonged to the solid, produce so called "Coulomb explosion" effect which, in turn, leads to formation of a nanocrater on the surface.

Coulomb explosion of Si(111) surface was investigated by Molecular Dynamics (MD) method in [8]. About 35,000 Si atoms were considered in the simulated block of solid and from 265 to 360 Si ions were placed in a hemisphere region in the center of solid surface. The choice of ions number N was rather arbitrary. It was based on the experimental observations [9,10] and was not dependent directly on the potential energy of HCI (E_p). However, one can connect the number of ions to the potential energy from a simplified estimate of the system energy balance. Neglecting the potential energy of interaction between Si atoms which are to be ionized with each other and with the rest of the solid (before HCI neutralization) and interaction energy between Si ions and the rest of the solid (after neutralization), the energy balance can be written as follows:

$$E_C = E_p - NI - E_a \quad (1)$$

where E_C is the total energy of the Coulomb interaction of the surface ions, I is the ionization potential of Si atom, E_a is the energy brought away in the process of the hollow atom relaxation. Dropping two last terms in (1) and taking into account the fact that $E_C = ae^2N^2/R$ (a is a dimensionless coefficient of the order of unity, $R = (3N/(2Pin_{Si}))^{1/3}$ is the radius of ion hemisphere, n_{Si} is the number density of FCC silicon crystal) one can obtain the estimate from above

$$6N^{5/3} < E_p \quad (2)$$

where E_p is in eV.

The aim of this work is to study the dynamics of crater

finally, the time-velocity dependence of the charges and neutrals yield of the Coulomb explosion.

2. SIMULATION MODEL AND NUMERICAL COMPUTATIONS

The simulated block of Si FCC crystal consists of 157,216 Si particles distributed in approximately 88x88x44 layers cell and placed in the nodes of the FCC lattice. We consider that HCI (Xe) ion impacts onto a Si(100) surface in normal direction and the number 88 corresponds to a lateral direction. To stabilize the system, movable particles (132,000) are placed in a 'box' made of fixed atoms (4 layers from each side of the block except the upper one). No periodical boundary conditions were used.

The particles in a central hemisphere with its equator lying on the upper plane of the sample are considered to be ions bearing the charge $+e$ each. Of course, these initial conditions are physically meaningful only if Xe^{q+} ion is neutralized before the surface ions begin to displace noticeably.

The Si^+ ions interact via pure pair Coulomb repulsive potential. Stillinger-Weber 3-body potential was chosen for the interaction of Si atoms with each other [11]. For the interaction $Si-Si^+$ a model was taken including polarization attraction ($1/r^4$) and ZBL repulsion

$$U(r_{ij}) = U_{ZBL}(r_{ij}) - (\sigma / r_{ij})^4 \quad (3)$$

Here σ is a characteristic length of the interaction depending on a polarizability of silicon,

The parameters of the potential were fitted so that to give the potential curve minimum of 9.17 eV at a distance 1.85 Å [8]. This potential is not, of course, a first-principle one, but it can allow one to obtain a basic insight to the process dynamics investigated.

A simple numerical algorithm of 'leap-frog' type was used with the numerical integration time-step of 0.1 fs. It was sufficient to provide the necessary accuracy and the total energy conservation during the computations.

3. RESULTS AND DISCUSSION

The initial energies of charged subsystem ($N=68, 159, 375$. Only Coulomb interaction is taken into account) are shown in Fig.1 along with the Eq. (2) results. It is seen that the latter gives quite reasonable estimate. The numbers of particles chosen correspond to $q = 21, 33, 49$ respectively.

The snapshots of a system with $N= 375$ in several moments after the beginning of the Coulomb explosion is presented in Fig.2. The process is fairly developed up to the moment $t=385fs$. Many charges and neutrals have quitted the crater. The increased Si atom density (shock wave) and fairly destroyed structure are observed in the area near the crater surface. The accelerated propagation of the shock wave is clearly seen in Fig.3 (3d plot). Moreover, a weak rarefaction wave behind the shock wave can be seen in Fig.4.

The dynamics of ion potential, kinetic and total energies, as well as Si atoms potential energies are

energy of atoms grows which leads to an additional acceleration of ions.

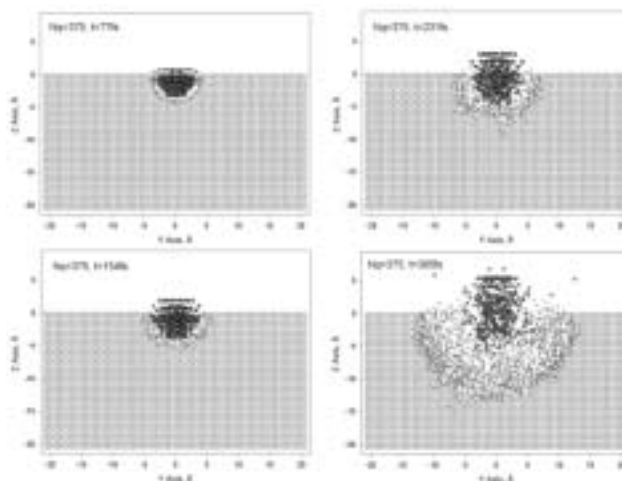


Fig.2. Snapshots of crater formation

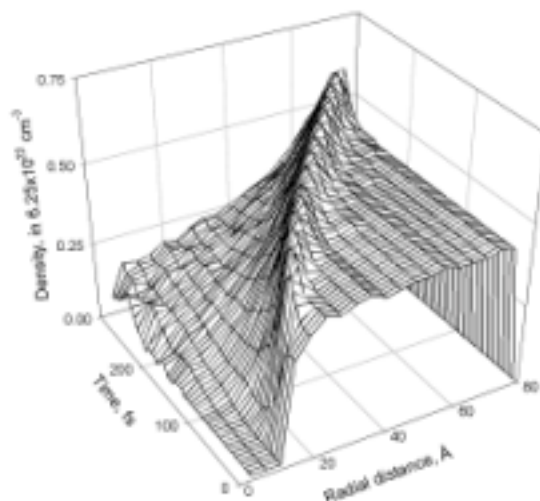


Fig.3. Time and space dependence of crater density (3d plot)

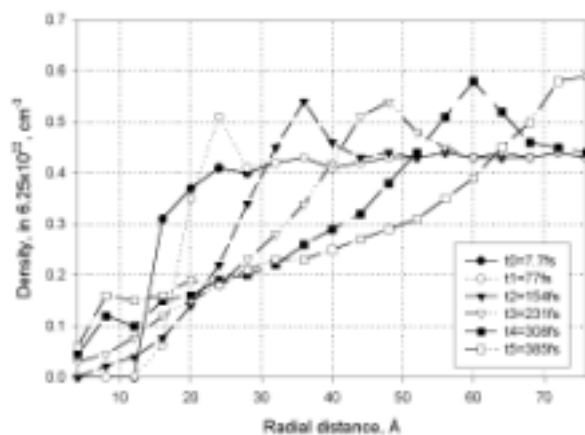


Fig.4. Radial distance dependence of crater density

The time-dependend velocity distribution of the total yield of the particle from the crater (Fig.6) reveals that there are two sets of peaks. The first (low velocities) is due to Coulomb repulsion and the second one is induced by the rarefaction wave. This means that the whole layer by whole layer evaporates from the bottom of the crater.

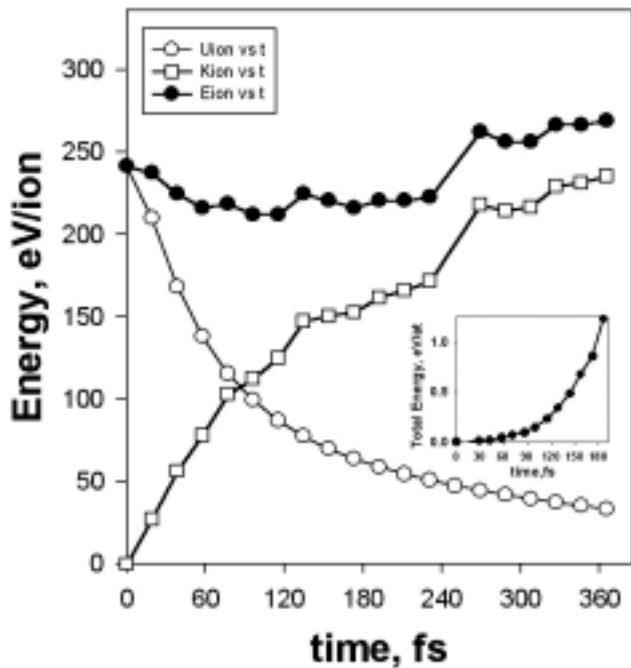


Fig.5. Time-dependence of kinetic and potential energies of neutral atoms and ions.

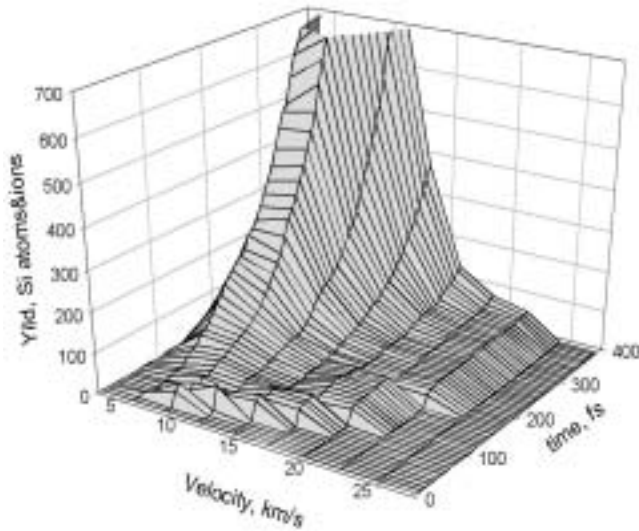


Fig.6. Sputtering yield versus time and velocity

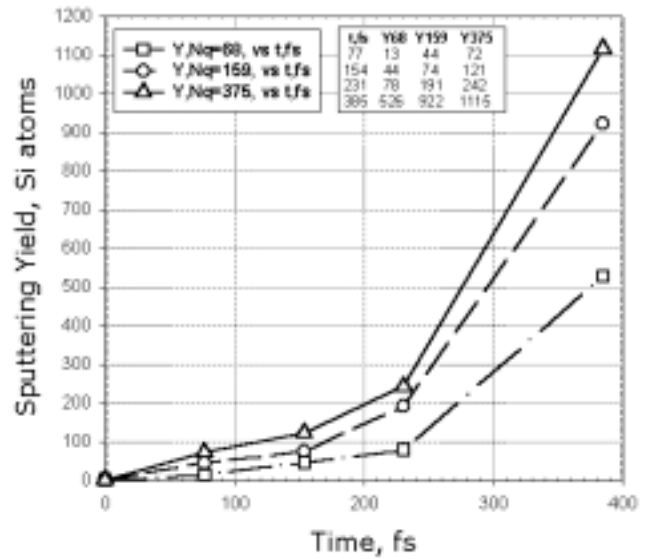


Fig.7. Sputtering yield versus time for different ion numbers

4. SUMMARY

The computations of the dynamics of nanocrater formation at Coulomb explosion were performed for realistic values of surface ion number, their potential energy being corresponding to the potential energy of falling HCl. The results obtained predict some new features in the behavior the material structure such as shock and rarefaction waves formation, two peaks energy distribution of the particles thrown out of the crater and so on.

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