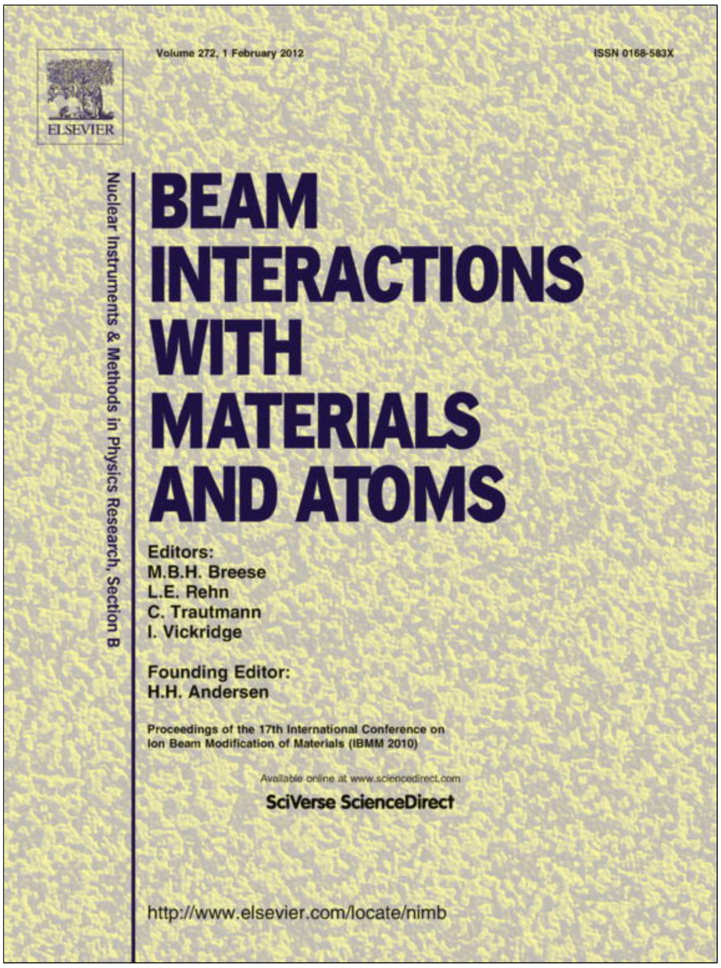
Volume 272, 1 February 2012
ISSN 0168-583X
ELSEVIER
Nuclear Instruments & Methods in Physics Research, Section B
BEAM INTERACTIONS WITH MATERIALS AND ATOMS
Editors:
M.B.H. Breese
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Founding Editor:
H.H. Andersen
Proceedings of the 17th International Conference on Ion Beam Modification of Materials (IBMM 2010)
Available online at www.sciencedirect.com
SciVerse ScienceDirect
http://www.elsevier.com/locate/nimb

Nuclear Instruments and Methods in Physics Research B 272 (2012) 374–376

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

Crater formation by single ions, cluster ions and ion "showers"

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ARTICLE INFO

Article history:
Available online 2 February 2011

Keywords:
Molecular dynamics simulation
Craters
Plasma–wall interaction

ABSTRACT

The various craters formed by giant objects, macroscopic collisions and nanoscale impacts exhibit an intriguing resemblance in shapes. At the same time, the arc plasma built up in the presence of sufficiently high electric fields at close look causes very similar damage on the surfaces. Although the plasma–wall interaction is far from a single heavy ion impact over dense metal surfaces or the one of a cluster ion, the craters seen on metal surfaces after a plasma discharge make it possible to link this event to the known mechanisms of the crater formations. During the plasma discharge in a high electric field the surface is subject to high fluxes ($\sim 10^{25}$ cm^{-2} s^{-1}) of ions with roughly equal energies typically of the order of a few keV. To simulate such a process it is possible to use a cloud of ions of the same energy. In the present work we follow the effect of such a flux of ions impinging the surface in the "shower" manner, to find the transition between the different mechanisms of crater formation. We also introduce the "shower"-like regime of ion bombardment (underdense cloud of ions) as a subsequent regime between the single ion impact (a rare "shower") and cluster ions (densely packed cloud).

1. Introduction

That huge craters modify faces of planets is part of common knowledge since the ancient times. Although they seem to be well investigated, the link between the shape of the damage and the impact energy as well as the nature of the projectiles (as single piece, extensive front of material or "staccato" mode of several pieces) still rises scientific interest. The similarity of crater shapes caused by giant asteroids and meteorites, bombs, explosives, gun bullets, and the microcraters seen on solid surfaces exposed to cluster ion irradiation is very well know. In addition, the similarity of scaling of crater volume in large metal clusters impacts and meteorite impacts has been clearly established [1]. The application of a very high electric field does also cause a damage in the shape of craters, seen on the surfaces of metal parts after a plasma discharge (Fig. 1). This evokes the idea of a possible combination of the crater formation mechanisms by the different kinds of impacts to derive a common law to enable the prediction of the crater shapes and the size of damage from a certain ion impact.

The shapes of the craters obtained from single ion and cluster ion impacts have been intensively studied over the last decades [1–7]. However, these studies have always excluded the third possibility of an impact, namely the "staccato" mode, or "shower" of ions, in which instead of being packed in a single cluster, scattered ions are carrying the energy towards the surface, each behaving as a single ion, but with minutely small delay between the impacts. MD simulations of such ion "showers" give results very close to the experimentally observed ones [8], which strongly suggests that the side craters are formed by the "ion shower". Although mostly this damage comprises a large area of a solidified metal liquid, the craters seen aside from the main spot resemble greatly the craters from ion and cluster ion impacts (Fig. 1).

Is it the same phenomenon that is observed during the plasma discharge and single ion/cluster ion impacts? Can common features be found between the three cases? In the present paper we consider the surface damage evolution during impacts in three different regimes: (i) from a single ion, (ii) ion "shower", and (iii) a cluster ion. All three regimes are considered until the formation of a crater on the surface. By the ion "shower" we understand a regime of ion impacts with the ultra high fluxes, observed when a plasma is formed in sufficiently high electric fields.

1.1. Ion "shower" impact during plasma development

If an electric field between two plane electrodes is gradually increased, the plasma starts building up inevitably, filling the gap between the electrodes and subsequently damaging their surfaces. If the plasma is formed in the relatively low fields, the surface exhibits no damage seen by a bare eye. This fact makes the practical application of plasma in industry possible. The situation changes

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doi:10.1016/j.nimb.2011.01.104

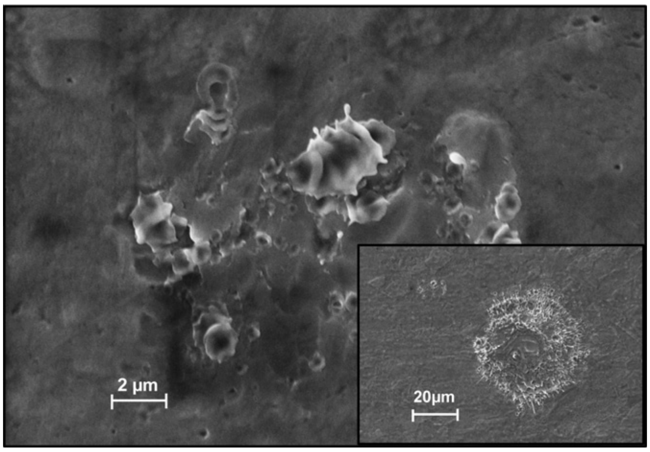

Fig. 1. Experimental craters on a Cu surface caused by the plasma formed in the high electric field ($E_0 \approx 400\ \frac{\text{MeV}}{\text{m}}$). The inset in the right bottom corner shows the overall view of the entire damaged area.

dramatically when the electrodes are operating in high and ultra high vacuum. Under such condition, the electric field can grow to the value close to the critical one, when the breakage of the metal surface is foreseen [9,10]. Modern technologies require an extensive insight into the ongoing processes during this particular kind of plasma–wall interaction, when the ions escape plasma with the high fluxes and energies of the order of a few keV. The damage caused by such a dense cloud of energetic ions cannot be neglected, since it may affect the performance of sensitive parts of high-precision machinery. This is a major problem at hand, for instance, in the accelerating structures of linear colliders of the next generation [11]. A high formation probability of tiny arcs, which deflect electron and positron bunches and result in bunch loss, reduces the efficiency of the costly machine.

The study of the mechanisms which lead to the damage clearly visible on the cathode surface will give a valuable information, which can enable the high level prediction of surface damage as well as a partial suppression of the probability of arcs in the structures.

Our previous studies of the formation of a 1D plasma, using the same condition as in experiments carried out at CERN [12], showed that the huge fluxes of plasma ions are accelerated towards the surface through the plasma sheath formed near the cathode. The energies of the ions are distributed between 0 and a few keV (depending on the voltage applied to the electrodes, and the distance between them) with a clear peak close to the maximum energy defined by the applied voltage. The simplified approach to the simulation of plasma formation provided us with values of the ion current close to those observed in the experiment [12]. In fact, these fluxes are of the order of $10^{25}\ \text{cm}^{-2}\ \text{s}^{-1}$ and the peak of the energy distribution appears at ~8 keV. Moreover, before the plasma is built up, the surface is exposed to impacts of single ions accelerated towards the surface with the maximum energy. Thus, during the process of plasma formation, the surface is subject to a gradual increase of the rate of ion impacts, from a single ion till the dense ion "shower" when the plasma can sustain the densities of a dynamic equilibrium.

Such a combination of ion impacts of many different kinds makes evident the complexity of a plasma–wall interaction, when the plasma is maintained in a sufficiently high electric field. A valuable insight can be obtained from a scaling law which can enable the prediction of a transition between the different regimes (mechanisms) of crater formation. Previously we have intensively studied the Au cluster ion impacts for such a scaling law [1]. Hence our aim in the present work is to broaden the scope of the studied impacts by including the case of dense ion cloud ("shower").

Some details of the simulation of Cu surface damage by the ions from self-plasma built-up in the presence of sufficiently high electric field can be found in [8]. For the current article, we carried out a new set of simulations of Au projectiles to be consistent with the single ions and Au cluster ion impacts investigations. The results are combined with the previous conclusions.

2. Method

To simulate the interaction within the Au sample we used the MD/MC CEM potential, which includes a high-energy repulsive part [13]. This potential was chosen since it has been previously found to describe the sputtering yields of Au quantitatively correct over three orders of magnitude in energy [14].

The principles of the Au cluster ion simulations were described in detail in [1]. To simulate the ion "shower" impact we used the following model. We created a set of simulations with variable flux where only one parameter of the projectile(s) was varied, as follows. We began with a normal 8 nm diameter Au nanocrystal. We then started scaling its z size up with factors of $f = 1$ (original nanocrystal), 3, 10, 100, 1000 and 10,000. After the elongation, the positions of atoms in the z-direction were fluctuated randomly between $-1/4$ and $+1/4$ of the enhanced lattice constant. Thus the higher-elongation cases corresponded to the arc plasma "ion shower". We did not consider explicitly "shower" ions ionically interacting between each other. In fact, the elongation of $f = 10{,}000$ corresponded to a typical arc plasma flux $\phi = 1.3 \times 10^{25}\ \text{cm}^{-2}\ \text{s}^{-1}$ [8,12]. We note that the intermediate fluxes (~10^{27}–10^{28}) are used only to find the transition between the "shower" and cluster impacts and do not correspond to any likely experimental condition. After creation, a kinetic energy of 500 eV was given to all atoms in the cluster or ion shower towards the surface.

To contain the energy of the projectile, we used simulations cells of 32 million atoms (a cube with 82 nm side length), and cooled down the system towards 0 K at 2–5 nm thick regions at the side and bottom boundaries. The atoms in the bottom unit cell layer of the box were held fixed. The simulations were ran until all atoms in the projectile had hit the simulation cell, and any overheated or densified regions of the cell had relaxed to normal temperatures and densities. The simulations were carried out using the classical MD code parcas on 128–1024 processors [15].

3. Results and discussion

The simulation technique allowed us to investigate the effect of the flux on the mechanism of the crater formation. The flux has been changed by increasing the average distance between atoms, thus we could cover all the possible fluxes from the compact cluster to the cloud representing a realistic plasma flux using the same amount of ions, and hence, fixed fluence.

Fig. 2 depicts a typical shape evolution of a crater formed by a 100 times underdensified cluster ($\phi = 1.3 \times 10^{28}\ \text{cm}^{-2}\ \text{s}^{-1}$). The

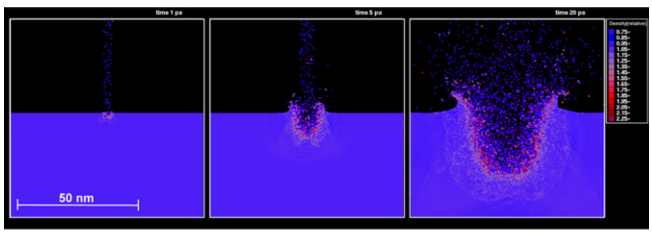

Fig. 2. Snapshots of the evolution of the crater formed by the cloud obtained as an Au cluster underdensified by a factor of 100. The last image to the right shows a clear overdensified front, which is observed despite the fact that the impact is not by a condensed cluster of ions (simultaneous impact of all ions).

decrease of the flux leads to the transition in the mechanism of crater formation. In fact, we observed the explosion on the Au surface which was subject to a cluster impact with an energy of 500 eV. Here we follow our definition of explosive cratering on the atomic level introduced in [1], namely, that the impact causes on the surface the well defined continuous overdensified front. Fig. 3 shows the results for the different cloud impacts (different fluxes) as distribution of the local densities around all atoms below the 8 nm radius diameter projectile impact area. This was analyzed by finding all neighbours within 3.1 Å from atoms in this region (including the atoms from the projectile), then calculating the inverse of the average bond lengths to these atoms and scaling this to a relative density, such that the equilibrium bond length leads to a relative density of 1.0. The data is taken at the time in each different simulation when the number of atoms with a density higher than 1.8 times the normal one was the maximum.

Fig. 3 clearly shows the that explosive mechanism can be expected at fairly high fluxes ($\phi = 1.3 \times 10^{28}$ cm^{-2} s^{-1}), at least at the explored impact energy. Although a single Au ion can form a crater on Au surface, this can happen only at the impact energy of about 5 keV and higher [16]. The 500 eV Au single ions form a linear atomic cascade, which due to the high flux overlap and form a crater according to the thermal spike mechanism. Only if the density of the cloud grows to a sufficient value, the overlap of the cascades becomes more intense and the mechanism of crater formation undergoes a transition to the regime of an explosion.

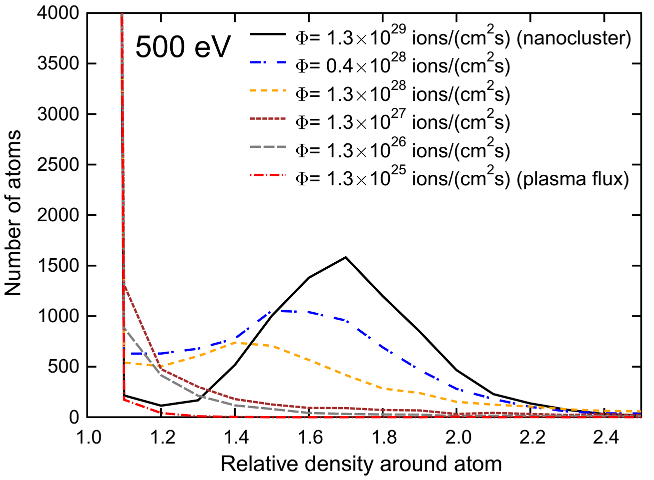

Fig. 3. (Color online) Density distribution in the crater region overdensified by the ion clouds with different fluxes. The second peak which corresponds to the continuous overdensified front is seen at the fluxes $\geqslant 1.3 \times 10^{28}$ cm^{-2} s^{-1}. The times used are 0.5 ps, 1 ps, 0.75 ps, 5 ps, 40 ps and 20 ps, in order of decreasing flux.

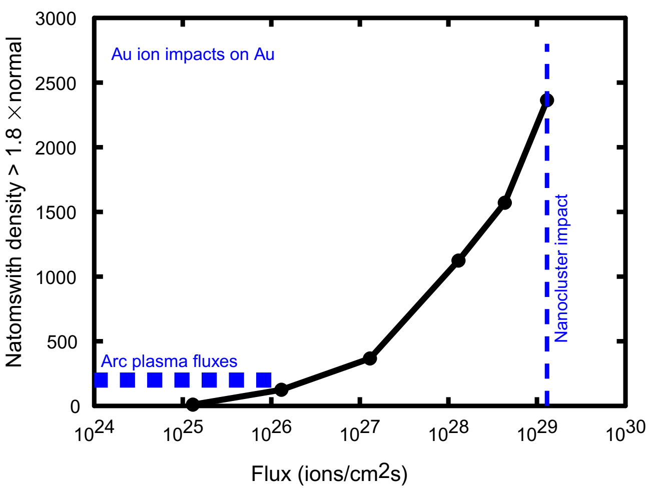

Fig. 4. (Color online) Transition from a thermal spike mechanism seen at the arc plasma fluxes to an explosive mechanism at the cluster ion impact. The energy of the impacting atoms is in all the cases 500 eV/atom.

In Fig. 4 we show the number of atoms which have overdensified neighbourhood versus ion flux, in the range between the arc plasma fluxes and the case of a cloud condensed back into a cluster. This figure thus provides a clear evidence of the presence of a transition between a thermal spike and an explosion mechanism of crater formation. The effect of the energy of bombarding ions requires further investigation to derive a common scaling law for the damage prediction.

4. Conclusions

In the present paper we show that the irradiation of a surface with the high fluxes can lead to the similar damage as that which is observed at the cluster ion bombardment. In spite of the fact that the ion "showers" are a combination of single ion impacts, which do not damage the surface significantly, the combined effect leads to the overlapping of the single atomic cascade, resulting in intensive thermal spikes, which form a crater on the surface. The increase of the ion flux leads to the transition of the mechanism of crater formation as the density of the overlapped cascades grows significantly leading to the explosion effect. Further investigations of the effect of the energy of the ions are required to derive a general law for the prediction of surface damage due to the ion impacts in the different regimes.

Acknowledgements

This work was performed within the Finnish Centre of Excellence in Computational Molecular Science (CMS), financed by The Academy of Finland and the University of Helsinki, and also financed by Academy projects OPNA and CONADEP. Grants of computer time from the Center for Scientific Computing in Espoo, Finland, are gratefully acknowledged. We also thank the Australian Synchrotron Research Program, funded by the Commonwealth of Australia, and the Australian Research Council for support.

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