

Recoils, flows and explosions: surface damage mechanisms in metals and semiconductors during 50 eV – 50 keV ion bombardment

K. Nordlund * ^{† ‡}, J. Keinonen [‡], M. Ghaly[†] and R. S. Averback[†]

[†] *Materials Research Laboratory, University of Illinois, Urbana, IL 61801, USA*

[‡] *Accelerator Laboratory, P.O. Box 43, FIN-00014 University of Helsinki, Finland*

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We review some recent simulation results on mechanisms of damage production close to a surface during ion irradiation. The simulation work encompasses studies of several metals and semiconductors at irradiation energies ranging from a few tens of eV:s to 50 keV. The results show that in dense metals the presence of a surface can dramatically enhance the damage production up to energies of at least 50 keV. The added damage is mostly in the form of vacancy clusters, which can extend quite deep, ~ 10 nm, in the sample. In semiconductors, by contrast, the surface in general has little effect on the damage production in bulk.

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I. INTRODUCTION

Since the effects of ion irradiation of materials occur to a large extent within the bulk region of a sample, it is very difficult to directly observe these effects. Most techniques used for observing irradiation damage, like transmission electron microscopy, field ion microscopy and scanning probe techniques, in fact examine defect structures close to the surface. Hence much of the understanding of bulk radiation effects comes from analytical and computer simulation analysis of experiments [1,2]. Most of the computer simulation analysis of ion irradiation effects was until recently carried out using binary collision approximation (BCA) methods [3]. While these methods have been successful in predicting effects like ballistic sputtering, depth distributions of implanted ions and the overall spatial extension of collision cascades, they can not account for the thermodynamic aspects of heat spike development [4]. This can be a problem especially in the vicinity of surfaces, where it has recently become clear that thermodynamic effects can be an important part of the cascade development [5].

Molecular dynamics (MD) simulation methods can treat the thermodynamic aspects of surface cascades realistically, but since computer capacity has only quite recently reached the point where MD methods can be used to simulate high-energy cascades, a comprehensive picture of when surface effects are important has not yet emerged. While in the present paper we can not yet provide such a complete description, by summarizing a num-

ber of recent simulation results obtained by our groups we can already deduce some general trends.

We divide surface effects in collision cascades induced by a single ion into four categories, which are illustrated schematically in Fig. 1. The first effect (Fig. 1 a), sputtering of single recoil atoms by ballistic collisions, is well-understood from classical theory [6,7] and simulations (see e.g. [8–13]). For light materials and ions penetrating deep into the sample sputtering can be the only surface effect of a cascade. In dense materials the collisions produced by a heavy ion (typically with an energy of at least a few keV) can be so well-localized that they can produce a liquid-like zone inside the material or close to the surface [4]. The other three surface effects all require that such a zone is formed somewhere in the cascade.

The second effect, plastic flow of hot liquid onto the surface, can result when a cascade is centered inside the sample, but is bounded by the surface so that liquid atoms can flow onto the surface (Fig. 1 b) [5].

The third effect, 'microexplosions', occurs when the liquid zone is so close to a surface that the pressure wave from the cascade essentially ruptures the surface (Fig. 1 c). In this case, pockets of hot liquid can explode out from the surface as a direct result of the collision cascade [12,14].

We also have now observed a new, fourth kind of surface damage effect, coherent displacement (Fig. 1 d). [15]. It will be discussed in detail in Section II D below.

The microexplosion effect corresponds to the nonlinear sputtering regime, and has thus been indirectly observed in numerous experimental sputtering studies. Furthermore, it is expected to produce craters on the sample surface, and such craters have indeed been observed in several experimental studies [16,17]. A recent compari-

*Corresponding author. Email kai.nordlund@helsinki.fi, phone +358-9-19140007, fax +358-9-19140042

son of simulation and experiment has shown that the observed crater formation can indeed be explained by the microexplosion mechanism seen in simulations [14,18]. Since the liquid flow effect was first predicted by Ghaly and Averback using MD simulations [14], experimental evidence supporting the presence of such a mechanism has emerged [19,20].

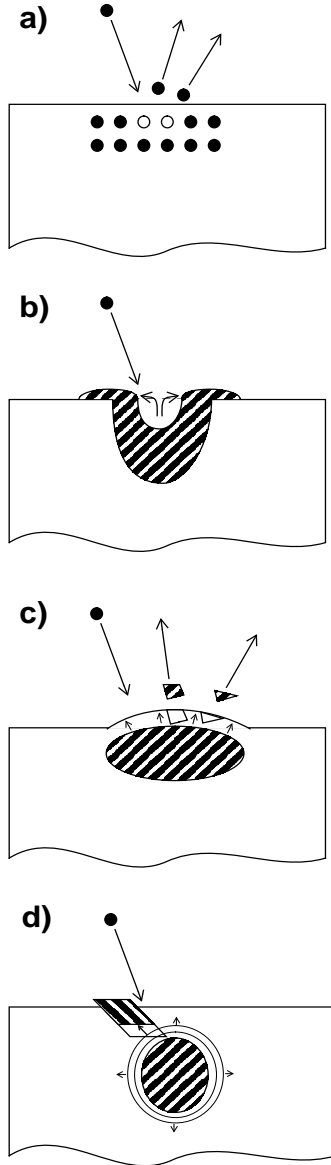


FIG. 1. Schematic illustration of different kinds of surface effects in cascades; a) recoils, b) liquid flow, c) microexplosions, d) coherent displacement. The shaded area illustrates liquid zones in a cascade. Note that for reasons of clarity the effects have been exaggerated in the figures. See text for a description of the effects.

The simulation methods used in the studies discussed here have been described in detail elsewhere [14,21,22], so we only recall some basic principles here. In simulating

“surface cascades” we place an incident ion on a random position a few Å above the surface, and give it a high velocity towards the sample. The incident angle is usually chosen in an off-channeling direction close to the surface normal, corresponding to the most usual experimental conditions. In the “bulk cascades” a recoil is started from a lattice site inside the sample. The development of the system of atoms is followed using MD simulations until the cascade has cooled down close to the ambient temperature (usually 0 K). In both cases, varying the initial velocity direction and position of the recoil atom can cause the resulting cascades to behave quite differently (even for the same ion-energy-sample combination) depending on where the strongest collisions occur.

In the next section, we present some results of surface effects in metals in detail, and describe the coherent displacement mechanism. In section III we explore whether surface effects can be significant in semiconductors as well. Finally, in the last section we discuss what general trends can be deduced from the results presented.

II. METALS

A. 4.5 – 20 keV ion bombardment of Ni, Cu, Pt and Au

We recently studied ion irradiation of nickel, copper, platinum and gold with ions in a wide mass range with energies from 4.5 to 20 keV [14]. 10 keV Pt ion impacts on Pt surfaces were found to exhibit quite different behaviour depending on how deep in the sample the cascade was centered. One event behaved essentially like a bulk-like cascade, another as a liquid flow-like event and a third exploded into the vacuum. This illustrates the important point that the same kind irradiation can produce quite different results in individual events, depending mostly on at what depths the incident ion happens to collide most strongly and thus transfer kinetic energy to the lattice. Hence a complete description of given irradiation conditions, or a quantitative comparison of experiments and simulations, requires simulations of enough events to obtain a representative picture of the possible kinds of behaviour for the given case.

10 and 20 keV gold surface cascades were most frequently found to exhibit liquid-flow or microexplosion-like behaviour. One of the micro-explosion-like events produced by a 20 keV event in gold is illustrated in Fig. 2. In this event about 300 atoms were sputtered, most of them in six large clusters with sizes ranging from 18 to 113 atoms. 10-15 keV surface events in Ni and Cu induced by self-ions were found to behave similarly to the Pt and Au cascades, some events being bulk-like, others producing large surface effects.

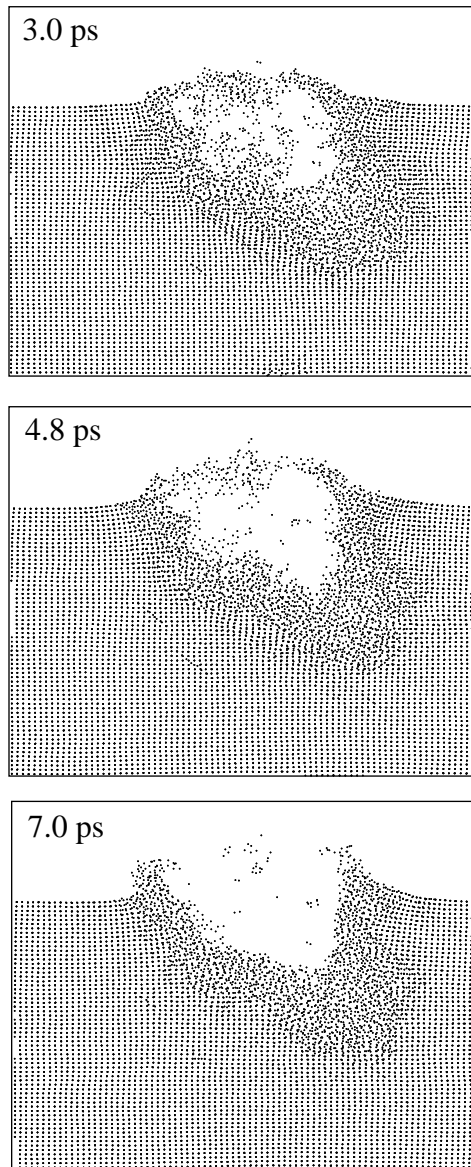


FIG. 2. Illustration of the development of a 20 keV cascade induced by a self-ion hitting a (100) Au surface. Each dot shows the position of one atom in a slice with a thickness of one unit cell. From Ref. [14].

Finally, several 4.5 keV Ne and Xe impact events on Pt (111) surfaces were simulated to provide a quantitative comparison of experiments produced by the same ions. The Ne bombardments behaved mostly like linear cascades, similar to the description given by BCA models, with adatoms produced by isolated primary and secondary recoils. The Xe events, on the other hand, produced craters through the microexplosion and liquid flow mechanisms, with adatom islands surrounding the crater center. Direct comparison of these events with experiment showed agreement to within about $\sim 20\%$ for both the Ne and Xe ions [18], providing strong support for the validity of these simulations.

Most experimental and simulation results indicate that the Kinchin-Pease (K-P) equation overestimates the damage production in metals by keV-energy heavy ions by a factor of ~ 3 or more [2]. Field-ion microscopy (FIM) experiments, however, indicated that during ion irradiation of tungsten the Kinchin-Pease equation is valid to a reasonable accuracy [23]. Since the FIM experiments directly observed the vacancies produced inside the samples, they are considered to be the best observation of cascade damage, and hence the discrepancy between the FIM and all other experiments has certainly been unsettling.

The comparison with the K-P equation, however, assumes that the damage is produced in bulk-like events. To test whether surface effects can be responsible for the discrepancy, we simulated 20 - 30 keV cascades produced by self-ions in the bulk and close to the (100) W surface [22]. Although it is clear that surface effects are quite significant in gold in this energy range, the presence of such effects in W, which has a different crystal structure, high cohesive energy and very high melting point, is not self-evident. Our simulations showed that the liquid flow mechanism is indeed present in W, and enhances the damage production compared to the bulk by a factor of 3 - 6 depending on the incident angle. The results are summarized in Table I.

TABLE I. Average defect production results by 30 keV W ions in W obtained by simulation and experiment. θ denotes the incident angle in degrees off the normal of the surface. N_{vac} is the total number of vacancies, and N_{int} is the number of interstitials. The statistical uncertainty of the simulations is about 25 % and of the 30 keV experiments 10 %. From Ref. [22].

Event type	θ	N_{vac}	N_{int}
Bulk sim.		23	23
Surf. sim.	70-80°	63	0.8
Surf. sim.	22°	136	6.7
Surf. exp. ^a	70-85°	125	-

^a Ref. [23]

The comparison with experiment is not completely direct, since the curvature of the tip and various vicinal planes of impact were not included in the simulations. Still, the results show that the experimental result is in the range expected for the surface simulation events, and thus shows that the FIM results can be understood in terms of the surfaces enhancing damage production. The low number of interstitials observed in the surface simulations (primarily due to in-cascade recombination effects) also explains why very few interstitials were observed in the FIM experiments [24].

C. 50 keV self-irradiation of Cu and Ni

Most simulations of cascade effects to date have been performed at energies below 30 keV, whereas most experiments on damage production have used ions with energies of 50 keV or more. Since extrapolation of the low-energy simulation results is not straightforward, a direct comparison with experiments has usually not been possible until now. Using massively parallel supercomputers we can now simulate the development of several full 50 keV collision cascades and have quantitatively studied the production of defect clusters in this energy range in Cu and Ni, where most experiments have been performed.

The experimental results on loop yields in metals during irradiation show great variation probably due to experimental difficulties and differences in the measuring equipment [23,25,26]. To compare results between different materials we therefore use data obtained by the same group using similar equipment. Studies on ion damage production in Ni and Cu performed at low temperatures show that about 3 – 5 times more loops is produced in Cu than in Ni for ion energies less than about 200 keV [27,25,28]. During neutron irradiation, on the other hand, the same difference appears to be between 1 and 2, with the most recent studies giving values of roughly 1.5 [29–34].

The large difference between Cu and Ni during ion irradiation has been attributed to either electron-phonon coupling [35] or to heat spike mechanisms [25]. Our recent comparison of experimental and simulated ion beam mixing, however, indicates that electron-phonon coupling affects the mixing at most by about a factor of ~ 1.3 in Ni, Pd and Pt, much less than previously thought [36]. This makes it unlikely that the electron-phonon coupling could explain the large ion irradiation difference. The smaller Cu-Ni-difference during neutron irradiation along with recent results which show that the size of loops produced in Cu is larger close to the surface than deeper in, and that they are closer to the surface than expected from range calculations [26], suggest the presence of a surface effect in Cu.

To examine this question we simulated 7 surface and 5 bulk events induced by self-ions in both Cu and Ni [15]. In the surface events, an MDRANGE simulation [37] was used to find an optimal off-channeling direction close to the surface normal. Primarily due to the liquid flow mechanism, but also in part due to the coherent displacement mechanism described below, the damage production by 50 keV ions in the Cu surface events is roughly a factor of 4 larger than in Cu bulk events, and a factor of 3 larger than in Ni (see Table II). The bulk vacancies resulting from these surface effects can be produced deep inside the sample, typically some 5 – 10 nm in, and can be well-separated from the adatoms produced on the

surface.

TABLE II. Average number of defects produced by 50 keV self-cascades in Cu and Ni. n is the number of events simulated, N_{vac} is the number of vacancies, N_{int} the number of interstitials, N_{ad} the number of adatoms and N_{sput} the number of sputtered atoms. V_{max} is the average number of vacancies in the largest vacancy cluster produced in each event.

Event	n	N_{vac}	N_{int}	N_{ad}	N_{sput}	V_{max}
Cu bulk	5	110 ± 10	110 ± 10	–	–	32 ± 7
Cu surf.	7	410 ± 120	103 ± 13	300 ± 110	12 ± 3	238 ± 44
Ni bulk	5	98 ± 14	98 ± 14	–	–	26 ± 12
Ni surf.	7	140 ± 20	84 ± 10	46 ± 20	11 ± 4	38 ± 6

The ratio between the damage production in Cu and Ni is in good agreement with the experimental results. The difference in the size of the largest loops is even more dramatic, about a factor of 6 in terms of the vacancy numbers shown in the table. This also agrees well with the experimental observation that loops in Ni are smaller than those in Cu [25]. The similar loop production at 50 and 100 keV [25] is also consistent with our surface model – since 100 keV ions have a longer range the surface enhancement effect is not expected to increase with increasing energy. One of the surface events in Cu produced 810 vacancies, which is more than 7 times the bulk average. In Ni, by contrast, the surface enhancement in vacancy production was no more than two in any of the events.

Since we did not incorporate a model for electron-phonon coupling in our simulations, and since the damage production results in the bulk are the same in Ni and Cu, the simulation results show that at least most of the experimental difference between damage production in these materials during ion irradiation can be explained as a surface heat spike effect. The lower melting point of Cu compared to Ni causes the liquid flow mechanism to produce on average more damage in Cu, and the lower shear modulus of Cu makes damage production by the shear mechanism more probable in Cu.

The smaller difference of ~ 1.5 between Cu and Ni during neutron irradiation can not be explained by this argument, though. This difference could be related to larger subcascades in Cu due to the higher melting point, or an electron-phonon coupling effect not affecting the mixing strongly. Further study is clearly needed to illuminate this question.

D. Coherent displacement

In the 14 surface events simulated in Cu and Ni, coherent displacement of atoms towards the surface was observed three times. In this kind of an event, the strong pressure wave emanating from the cascade caused entire

planes of atoms to slide coherently along the $\{111\}$ slip planes of FCC metals towards the surface, forming an adatom island. We recognized this “shear mechanism” by tracking the motion of all atoms displaced from their initial lattice site during the course of the cascade. In the shear events all adatoms, and the same number of atoms in several atom layers below them, were all displaced exactly one nearest-neighbour distance in the same $[110]$ direction. In the liquid flow events, by contrast, the motion of the adatoms and the atoms below them was largely random, as expected for a liquid.

In one Cu event, one large adatom island with about 180 adatoms formed mainly by shear, although a few atoms in the same island also formed by liquid flow. To obtain a better understanding of the mechanism, we analyzed this one event in detail. The event is illustrated in Figs. 3 – 4.

Figure 3 shows the final shape of the adatom island seen from above. It is remarkable to note that two sides of the island form straight edges encompassing about 15 atom rows. Figure 4 shows a side view of the initial and final positions of all atoms in the top 45 Å displaced from their initial site during the cascade. It is clearly evident that most of the adatoms are results of a uniform shear in the $[110]$ direction, although some flow of liquid has also taken place in the center. A detailed analysis showed that 117 out of the 177 adatoms were displaced exactly one nearest-neighbour distance in the $[110]$ direction. The slip has occurred over up to 20 atom layers. The side planes of the slipped region were found to be two different $\{111\}$ planes, confirming that the motion occurs along the ordinary slip system of FCC metals.

Since about 200 adatoms are formed in the event, a corresponding number of vacancies must be present in the bulk. Analysis of the final positions of all adatoms, interstitials and vacancies formed in the event showed that most vacancies are clustered in one large cluster well below the surface, extending roughly from 5 to 10 nm. The crystal just below the surface has regenerated almost perfectly, a consequence of the large number of atom planes involved in the slip. Thus the damage produced due to a surface mechanism extends surprisingly deep, tens of atomic planes, in the bulk. The total number of vacancies produced is 250, about 2.5 times the average in bulk events. In the liquid flow events, the vacancy cluster formed inside the sample was similar to the one observed here, but the adatoms were less regularly distributed. This coherent displacement mechanism can also be considered (prismatic) loop punching on the $(111)\parallel(110)$ FCC slip system, with the interstitial platelet resulting in an adatom island on the surface [38].

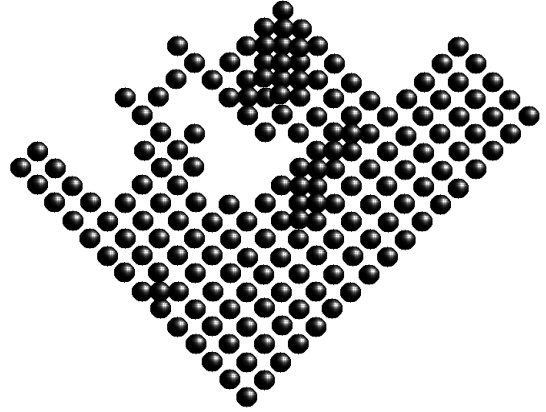


FIG. 3. Shape of the adatom island produced by the shear mechanism in the 50 keV Cu cascade described in the text. Note that the regular shape of the islands results directly from the shear during the cascade - on diffusion timescales the shape can be expected to become even more regular due to adatom migration. From Ref. [15].

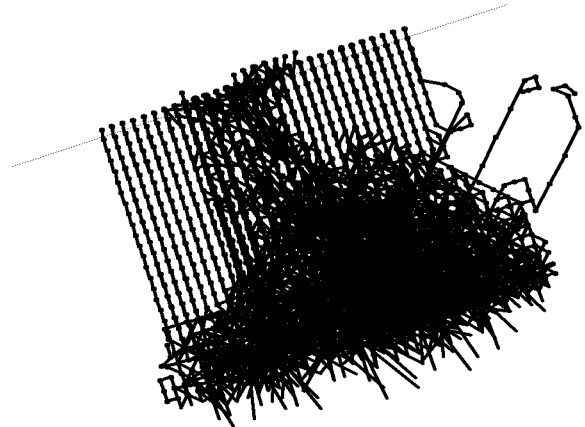


FIG. 4. Side view of atoms displaced by more than half a nearest-neighbour distance in the top 45 Å from the surface in a 50 keV cascade event. Each line connects the initial and final position of one atom; the sphere at the end of the lines denotes the final position. The weak straight line shows the position of the surface. Inside the sample, where the cascade forms a liquid region, the motion is essentially random, but near the surface most atoms have moved coherently towards the surface. From Ref. [15].

III. SEMICONDUCTORS

We have seen above that surfaces can cause a dramatic increase on the bulk damage production in dense metals. Since the most common semiconductors have a lower atomic density and more open structure than metals, making cascades less dense, it can be expected that surface effects are less significant in them. On the other

hand, we have just seen that a wide range of metal irradiations can produce surface effects, so some effects might be expected in heavier semiconductors (with low melting points) like Ge. To examine this question, we have simulated low-energy cascades in silicon induced by self-ions [39], and (for the present paper) high-energy cascades in Si and Ge induced by heavy ions like Kr and Xe.

A few results for the cascades in Si are summarized in Table III, comparing the vacancy production of bulk and surface cascades. We see that even at the lowest energies close to the displacement threshold the difference between the surface and bulk results are similar, even though the mechanism by which a displacement occurs is quite different in the two cases [39]. At higher energies the relative difference decreases; at energies above 400 eV the difference is less than 10 %.

TABLE III. Average vacancy production results by 50 - 200 eV Si ions in Si for surface and bulk cascades. The numbers are averages over at least 50 events in each case. From Ref. [39]

Energy (eV)	$N_{\text{vac}}(\text{surface})$	$N_{\text{vac}}(\text{bulk})$
50	0.8	1.1
100	2.1	2.0
200	4.8	4.3
400	9.5	9.0
800	17.0	16.3

Results for high-energy heavy-ion-induced cascades in Si and Ge are shown in Table IV. Although the statistical uncertainties are large, it is clear from the number of adatoms and sputtered atoms that the surface effects are quite small in all events in unstrained samples. The reason is partly the low atomic density and crystal structure of silicon and germanium [40], but more importantly the higher density of liquid silicon and germanium compared to the density of the crystalline state. Because of this, the liquid formed in the cascade does not need to expand outwards towards the surface, contrary to metals [14]. On the other hand, this still does not rule out the possibility of microexplosions. We have not observed any major explosions in the present events. Experimentally craters have been observed during 20 keV Ga irradiation of Ge, but with a probability of only $\sim 1/1000$ [41], so it is not surprising we do not observe them in the few events simulated now.

If the main reason for why liquid flow does not occur in semiconductors indeed is the high density of the liquid phase, some liquid flow should be expected in samples under sufficient compressive strain. To test the idea, we simulated five 5 keV Xe cascades in Ge under 1.7 % compressive strain in the surface plane. The cell was allowed to relax in the direction of the surface normal before the initiation of the cascade. The results in Table IV show that in this case the number of adatoms is indeed some-

what increased from the unstrained sample, indicating that some of the liquid has flowed to the surface.

TABLE IV. Average defect production results by Kr and Xe ions in Si and Ge for surface cascades. Note that the number of ions simulated in these events is only 3 - 5. The statistical uncertainty of the interstitial and vacancy results and the number of adatoms for strained Ge is roughly 20 % and for the other numbers roughly 50 %.

Event type	N_{int}	N_{vac}	N_{ad}	N_{sput}
5 keV Xe \rightarrow Si	100	105	6	1
20 keV Kr \rightarrow Si	240	240	3	2
40 keV Xe \rightarrow Si	830	830	3	1
5 keV Xe \rightarrow Ge	270	270	6	4
5 keV Xe \rightarrow Ge (strained)	200	220	20	3
40 keV Xe \rightarrow Ge	1400	1400	5	3

IV. DISCUSSION AND CONCLUSIONS

Some general trends in the damage production mechanisms can be deduced from the results presented here. Low-mass ions (like Ne in Pt) tend to mostly produce linear cascades with no large heat spikes and thus no surface effects except for recoils. Likewise, cascades in materials with a low mass or open crystal structure like silicon also do not exhibit a large surface enhancement of damage production. The behaviour in Si can in fact be not too badly represented by binary collision approximation simulations [42], except of course for the nature of the amorphous zones produced [43].

For heavy ions in dense, close-packed materials like Ni, Cu, W, Pt and Au, on the other hand, large heat spikes are produced, and the thermodynamic and mechanical aspects of materials become important. The presence of a surface can strongly affect the behaviour of cascades by the microexplosion, liquid flow and coherent displacement methods. Comparison of cascades in pairs of materials expected to behave similarly in a ballistic manner, namely Pt and Au, and Ni and Cu, showed that the melting point and elastic hardness of a material are important parameters in determining the behaviour of cascades. Because in all these materials the liquid has a lower density than the solid, the microexplosion and liquid flow mechanisms can be present. But since Pt and Ni have relatively high melting points, the effects in these materials tend to be smaller than in Au and Cu for similar irradiations.

In semiconductors one factor making surface effects less important is the open crystal structure, which leads to medium-energy recoils traveling further than in FCC lattices [40] and thus diminishing the energy density in the heat spike. The study of cascades in compressed and regular germanium showed that another important factor is the high density of the liquid phase in these materials.

Since the liquid has a similar or smaller volume than the same number of atoms in the solid phase, the heat spike tends to relax inwards rather than outwards, making all the three “thermodynamic” surface mechanisms unlikely to occur. In fact, it can be argued that an inverse “sucking” effect may be present in these materials [14].

In conclusion, the simulation results discussed in the present article allowed us to deduce some rough trends about during what kinds of ion irradiation thermodynamic surface effects are large, and affect the bulk damage production. In dense metals we found that a large range of irradiation conditions results in effects like microexplosions and liquid flow, and can enhance the vacancy production in bulk by almost an order of magnitude. In semiconductors, by contrast, the amount of surface damage is quite small compared to the bulk damage production in most cases. We also observed a coherent displacement mechanism of damage production during irradiation (“loop punching at surfaces”).

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