Atomistic modeling of shock-induced void collapse in copper

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Nonequilibrium molecular-dynamics (MD) simulations show that shock-induced void collapse in copper occurs by emission of shear loops. These loops carry away the vacancies which comprise the void. The growth of the loops continues even after they collide and form sessile junctions, creating a hardened region around the collapsing void. The scenario seen in our simulations differs from current models that assume that prismatic loop emission is responsible for void collapse. We propose a dislocation-based model that gives excellent agreement with the stress threshold found in the MD simulations for void collapse as a function of void radius. © *2005 American Institute of Physics*. [DOI: 10.1063/1.1906307]

Shock waves in solids have been studied for decades, but only recently a detailed microscopic picture of the evolution of defects under shock compression is emerging.[1,2] Most "real" materials contain large concentrations of defects that change their response to shocks: vacancies, dislocations, boundaries, secondary phases, voids, etc. For the sake of simplicity the role of these defects is often either neglected or absorbed into some fitting parameters. However, it is important to understand in detail the shock response of porous materials,[3] materials that experienced radiation damage,[4,5] materials that have been previously shocked,[2] and materials that undergo pressure-induced phase transitions.[6] Recent work on radiation-damaged Fe showed that changes in void fraction modified the back velocity of the shocked sample.[5] Voids are instrumental in the initiation and propagation of energetic reactions in explosives,[7–11] and void nucleation due to release/tension waves controls the spall behavior of the material. There has been a large number of both experimental[12,13] and atomistic modeling studies[14–16] on spall and void growth, but models that include dislocation-level information are scarce.[17,18] The mathematical description of collapsing voids has been an important component in the development of constitutive equations for distended materials under shock compression.[19,20] These models have been successfully applied to the propagation of shock waves through porous materials and powders but do not address the physical processes responsible for void collapse. On the other hand, there have been comparatively few studies on shock-induced void collapse,[7–11,21] and there is only one current dislocation-based model describing this, in which void collapse occurs by formation of prismatic dislocation loops which rapidly glide away after emission.[5]

The equilibrium states accessed by a shock wave can be described by the Hugoniot equations, and these states can be predicted from high-fidelity atomistic simulations at thermodynamic equilibrium. However, these simulations do not give any information on how the material can reach the final state or if there will be any plasticity or phase transition involved. Nonequilibrium atomistic simulations instead do provide this kind of information.[22,23] There have been a few molecular-dynamics (MD) studies of shocks interacting with

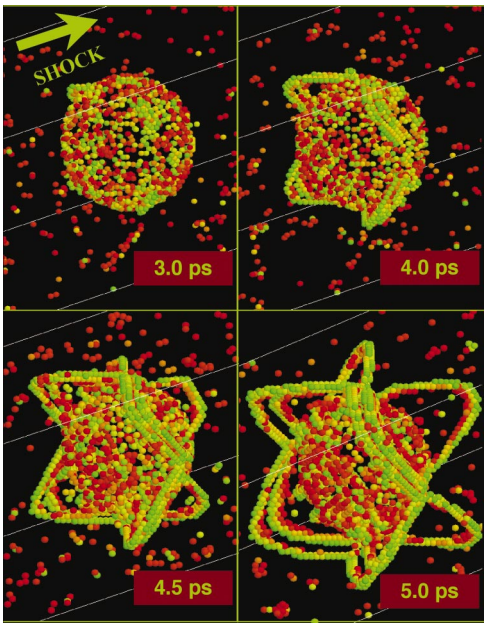

FIG. 1. (Color) Snapshots from an MD simulation, showing evolution of void collapse for a shock of 8 GPa and a void radius $R=1.5$ nm (~1200 vacancies). Only defective atoms are shown. Numbers in boxes indicate time in ps after shock was applied; emission of loops starts at 3 ps.

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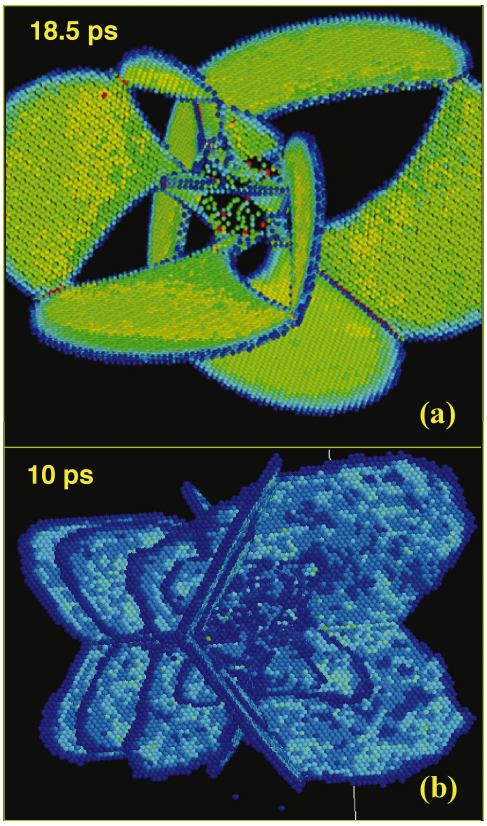

FIG. 2. (Color) Snapshots from an MD simulation for a void with $R=2$ nm ($\sim$2850 vacancies). (a) 8-GPa shock. Shear loops grow with a velocity $v/c_0 \sim 0.15$, where c_0 is the sound speed at normal conditions. Snapshot from a similar MD simulation for (b) a 21-GPa shock. Loops grow at nearly the sound speed c_0. In both (a) and (b) only defective atoms are shown.

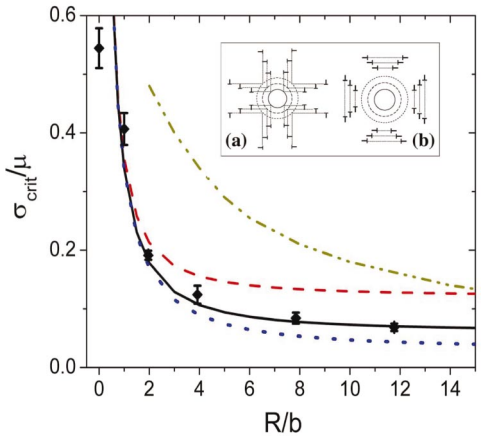

FIG. 3. (Color) Calculated stress thresholds for emission of dislocations, normalized by shear modulus μ, as a function of void radius, R normalized to the Burgers vector b. MD simulations (diamond), model from Reisman *et al.* (Ref. 5) (dash-dot-dot), analytical model [Eq. (1)] for different dislocation core (r_{core}) sizes: b (dashed), $2b$ (solid), and $4b$ (dotted). Inset: Proposed loop mechanism for void collapse: (a) shear loops and (b) prismatic loops. Successive loops are formed as the void diameter is decreased. The relative positions of the loops correspond to their sequence of generation.

voids in two dimensions,[7,8] for infinite cylindrical voids,[9] and on prismatic voids inducing detonation.[10] There are few studies on the interaction of a shock wave below melting/reactivity with a three-dimensional (3D) void.[24,25] Recent electron backscattered diffraction images of a shocked Cu sample with pre-existing voids that were recompressed reveal dark band regions between voids that are associated with several collapsed voids and the plastic deformation surrounding them.[26] Identifying void collapse of nm-sized voids using high-resolution transmission electron microscopy has also proven difficult, and therefore the role of simulations is crucial in understanding this process.

The goal of this investigation is to focus on the interaction of a shock wave with a pre-existing void. We have carried out large-scale MD simulations of shocks interacting with 3D voids in copper.[27,28] Partial dislocation cores were identified using a centrosymmetry parameter filter.[29] The atoms inside the desired void volume were removed from the simulations, and then the sample was relaxed for several ps at 5 K before applying the shock. The use of lateral periodic boundary conditions entails that there is a periodic array of voids. However, due to the r^{-3} dependence of the stress field produced by one void (r is the distance from the center of the void), the change in the stress at the boundaries induced by the void was negligible for the sample sizes used.

Figure 1 (8-GPa shock) shows how a void with radius $R=1.5$ nm begins to collapse due to the emission of partial vacancy loops. For shocks along $\langle 100 \rangle$ there are four different, equally active slip planes. One loop is nucleated in each slip plane on the leading side of the shock (side of the void being hit first). After the shock passes, the stress state is roughly hydrostatic, and therefore four additional loops are nucleated in the back of the void (trailing side). Additional loops are also nucleated on the leading side, on planes parallel to the ones where dislocations nucleated initially. Figure 2(a) displays a larger and longer simulation, also for an 8-GPa shock, but for $R=2$ nm. The loops meet and form sessile junctions, which change the shape of the evolving loops. The shear loops stay attached to the void for at least 10 ps after the void collapse, when the shock hits the back surface. There is a possibility that they may form prismatic loops which would glide away,[30] but this would happen at much longer times. The shear loops and sessile junctions lead to a large enhancement of the dislocation density around the void with associated hardening of the material. In a real single crystal the presence of pre-existing dislocation sources with low activation threshold would provide the "background" dislocation density which is missing in our simulations for a crystal which is perfect except for the void. Figure 2(b) shows the effect of larger pressure (21 GPa) on the void collapse process, for $R=2$ nm. Due to the higher available stress, there are numerous loops nucleated at the surface of the void. It is important to point out that the threshold for homogeneous nucleation of dislocations for this particular potential is 32 GPa (Ref. 23), and therefore any shock pressure below that value in a perfect crystal would lead only to elastic compression of the material.

Both prismatic and shear loops have been postulated as mechanisms to transfer matter *away* from voids. Here we present an analytical dislocation-based model for a collapsing void, based on an analogous model recently proposed[18] for expanding voids. The dislocation signs are changed in order to transport matter *into* the void. At the present stage, the model is two-dimensional. Figure 3 (inset, left) shows the two alternative loop emission mechanisms. As the void is collapsed, successive shear loops are formed. They have decreasing diameters, since dislocations are generated at the surface of the void where the resolved shear stresses are at a maximum. The other alternative mechanism, prismatic loop

emission, is shown in Fig. 3 (inset, right). By comparing Fig. 3 (inset) to the MD simulations (Figs. 1 and 2), shear loop emission appears to be the mechanism for void collapse. The equation that predicts the stress required for dislocation emission from a growing void can also be used for void collapse.[18] The critical stress normalized by the shear modulus, σ_{cr}/μ, is given by

$$\frac{\sigma_{cr}}{\mu} = \frac{b/R}{\sqrt{2}\pi(1-\nu)} \frac{(1+\sqrt{2}r_{\text{core}}/R)^4+1}{(1+\sqrt{2}r_{\text{core}}/R)^4-1}, \tag{1}$$

where b is the Burgers vector, R is the void radius, ν is Poisson's ratio, and r_{core} is the dislocation core radius. Figure 3 shows the threshold stress to induce dislocation emission from the surface as a function of void radius; both the continuum model and the MD simulations are presented. Results from a model assuming emission of prismatic loops[5] are also shown. Our new dislocation-based model gives an excellent fit to the simulation results using $r_{\text{core}}=2b$. Calculations were carried out at zero pressure and temperature ($b=0.255$ nm and $\mu=48.7$ GPa). Using pressure-dependent values for μ and b gives a correction of only few percent at pressures below 10 GPa. Note that continuum models are not reliable for small R, $R<3r_{\text{core}}$, but can easily handle large initial void sizes, while MD can be used for any void size, provided that enough computer power is available. In practice this limitation means $R<15b$ for MD. Our MD results on void collapse in Cu are similar to those by Hatano[25] for a Lennard-Jones solid, and the "nonlinear" behavior that he finds for the threshold stress is easily explained here with our dislocation-based model.

In summary, we have presented atomistic simulations and a dislocation-based model showing the evolution of shock-induced plasticity in void collapse. The agreement between the two approaches suggests that the results can be extrapolated to larger void sizes, paving the way for more reliable constitutive models. Our calculations for copper do not support a model using prismatic loops to transport the vacancies away from the collapsing void.[5] The model presented here, based on shear loop nucleation, agrees better with the observed MD mechanism and gives excellent agreement with the critical stress needed for void collapse from our MD simulations. Although the simulations were performed for Cu, preliminary calculations show similar features in other fcc metals, including Al (Ref. 31) and Ni. The energy difference between production of shear and prismatic loops would lead to different constitutive models and different void fractions as a function of pressure.[5] In addition, prismatic loops that easily glide away[30] would not contribute significantly to hardening of the material near the void, while shear loops would form a tight network of junctions that would harden the material near the void. The formation of sessile junctions has also been recently observed in quasicontinuum simulations of void growth.[32] Simulations of shock-induced void collapse in bcc metals are in progress.

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