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Atomistic mechanism of shock-induced void collapse in nano-porous metals

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We have investigated the microstructural changes in ductile porous metals during high pressure-high strain rate loading employing atomistic simulations and explored their relation to recent experiments on polycrystalline copper samples. Molecular-dynamics simulations of shocks in porous, single crystal samples show the formation of nano-grains due to localized massive plastic deformation induced by the presence of voids. In the process of grain formation the individual voids serve as dislocation sources. The efficiency of these sources is further enhanced by their collective interaction which eventually leads to very high dislocation densities. In agreement with experimental studies, the simulations display a temporal delay of the particle velocity in comparison to perfectly crystalline samples. This delay increases with porosity. Our results point towards the importance of void-void interactions and collective effects during dynamic loading of porous materials.

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The presence of porosity significantly alters the response of materials under conditions of high pressure-high strain rate loading, creating the opportunity to systematically tune materials properties. In fact, porous materials and in particular metallic foams have attracted considerable attention with regard to potential applications in the absorption of high energy impacts[1–4]. Metallic foams with nano-scale porosity are also being considered as possible target capsule materials for inertial confinement fusion at the National Ignition Facility (NIF)[5]. Furthermore, the influence of voids on materials properties is of fundamental interest in connection with radiation damage[6]. While the behavior of solids under conditions of high pressures and high strain rates has been intensively studied for many decades[7,8], a thorough understanding of many processes at the atomic scale is still pending. In order to resolve these open questions, considerable efforts are being undertaken to push the spatial and temporal resolution of experimental techniques towards the ps-nm regime[9]. Despite continuous progress, *in situ* diagnostic techniques are still far from resolving this regime and simulations play an important role in the interpretation of experimental results and the dynamical processes involved. Traditionally, continuum modeling is widely applied to complement experiments[6] but such calculations do not provide microscopic detail and possible effects of porosity at the nano-scale are *per se* not included. On the other hand, thanks to the continuous increase in computer power, molecular-dynamics (MD) simulations have become a powerful tool in the study of the high-strain rate response of materials[10]. Due to their importance in the mechanical failure of ductile materials under tensile loading as well as under spall conditions, nucleation and growth of voids under external *tension* have been studied quite extensively using MD simulations[11–13]. In contrast, so far only relatively few MD studies have dealt with the behavior of voids under *compression*[14–17], most of which have focused on hot-spot initiation above the melting pressure. To our knowledge, the only atomistic simulation of a void distribution up to date has been conducted by Phillips and co-workers who simulated a strong shock traversing a two-dimensional Lennard-Jones sample leading to amorphization and the emergence of a hexagonal crystallite in a square matrix[15]. In view of this situation, it is desirable to gain a more detailed picture of the mechanism of void compaction based on more realistic models and taking into account the three-dimensionality of the problem. We have performed large-scale MD simulations of high-strain rate compression of porous Al and Cu samples with different degrees of porosity, focusing on the collective effects of voids during shock compaction. Simulations have been carried out with the massively parallel MD code *MDCASK*[18] using embedded-atom method (EAM) potentials to describe the atomic interactions[27]. The voids were randomly distributed over the sample and their size distribution was chosen in qualitative agreement with a power-law distribution[11]. We simulated the response of an aluminum sample containing 5% voids shocked at pressures between 25 and 100 GPa ($1.15\,\mathrm{km/s} \leq u_p \leq 3.55\,\mathrm{km/s}$, where u_p is the piston velocity). For copper, we tested void volume fractions of 3, 6 and 12% and shock pressures between 10 and 48 GPa ($0.25\,\mathrm{km/s} \leq u_p \leq 1.0\,\mathrm{km/s}$).

In Fig. 1 we show snapshots of parts of the aluminum sample which illustrate the passage of a shock wave through a porous material. The atoms have been colored according to their centro-symmetry parameter (CSP)[19]. The first four slides show the closure of a single void. As the shock front arrives at the rear end of the void the surface atoms are pushed into the void diminishing its free volume. As the shock front moves forward the void is crushed up completely and a highly disordered region is created which is confined approximately to the original void volume. During the collapse leading partial dislocations are emitted on {111} planes as previously observed

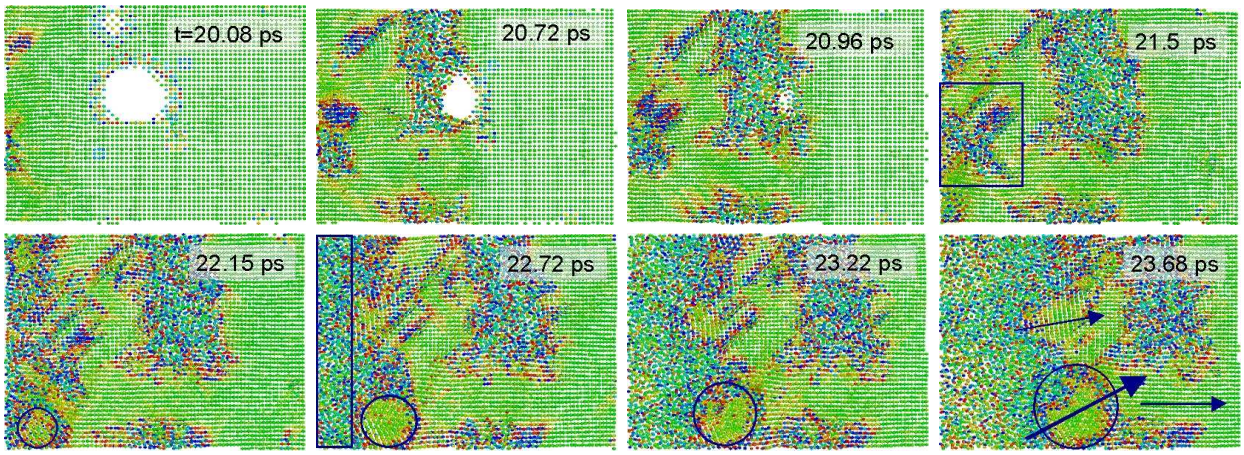

FIG. 1: (Color online) Series of snapshots of a part of the aluminum sample loaded with 25 GPa. Only a few layers perpendicular to the shock front are shown. The shock proceeds from the left to the right. Warm colors indicate large CSP values. The emission of dislocations from the surface of a void on the fcc glide system $\{111\}\langle 110\rangle$ is marked in the frame at 21.5 ps. The circles in the last four frames indicate the evolution of a small crystalline region in front of the piston, which appears in the frame at 22.72 ps entering from the left. The arrows in the very last frame show the shock induced orientation change of two nano-crystallites projected onto the paper plane.

for single voids in copper[20]. In agreement with previous studies, the voids exhibit a focusing effect which initiates the creation of hot-spots in the sample. The last four slides show the sample after the elastic as well as the plastic shock front have passed. Due to the high volume fraction of voids extended disordered regions have been created. On the left side of the observation frame, directly in front of the piston, a crystalline region can be identified whose orientation is rotated with respect to the original lattice. The sequence of slides suggests this being due to localized massive plastic deformation involving large dislocation densities (rectangular box in the slide at 21.50 ps). We observed similar events also in other parts of the sample. In a foregoing study[21] the EA potential was found to predict an entirely elastic response up to melting which occurs between 100 and 120 GPa. Here, we observe strong plastic deformation and strong local disorder at a pressure of only 25 GPa. This finding illustrates the importance of lattice imperfections as nucleation sites for plasticity.

Fig. 2 shows a typical snapshot of our copper simulations at a pressure below the threshold for homogeneous nucleation of dislocations in a perfect crystal, i.e. the same shock propagating in a sample without voids would not induce any plastic deformation. We observe large dislocation densities in the immediate vicinity of the voids and the formation of detached partial dislocation loops due to the presence of a highly non-uniform strain field. As the shock strength is raised the dislocation density increases further and extended dislocation networks are formed.

In recent experiments on the recompression of polycrystalline pre-shocked copper samples[22] (average grain size 50 μm), which contained a void distribution due to spall, grain refinement down to the nanometer scale has been observed. The electron backscatter diffraction (EBSD) orientation map shown in Fig. 3, which was obtained from a cross-section of the sample, reveals the spall plane. The first shock release creates a spall region in the interior of the specimen while the trailing (second) shock causes closure of voids in the spall region. The associated plasticity in the region of the voids is revealed by the rotations of the crystal lattice. Grains which did not undergo this severe plastic deformation are shown to have somewhat uniform coloring indicating that the rotations are generally within a degree or two of the average grain orientation. In contrast, in the regions where the spall voids are closed, crystal rotations on the order of 5 de-

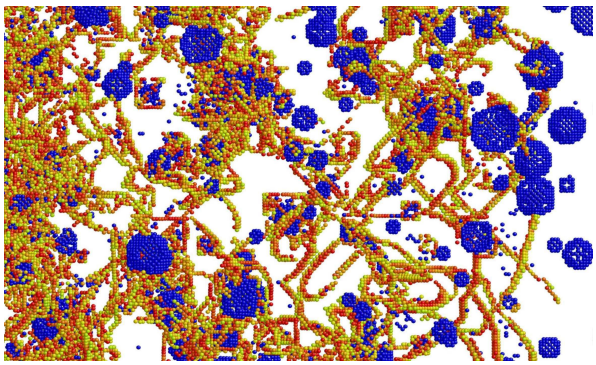

FIG. 2: (Color online) Slice of the copper sample with 3% porosity subjected to a shock at 10 GPa (0.25 km/s). Color coding as in Fig. 1. Only defective atoms are shown (void surfaces and dislocations). While the pressure is too low to induce crush up of voids, a significant number of (partial) dislocations is being emitted from the void surfaces leading to several dislocation loops. The plastic front moves from the left to the right side of the figure.

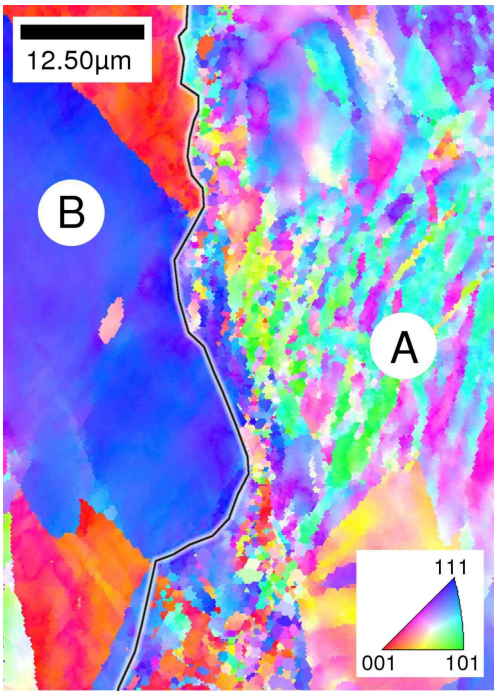

FIG. 3: (Color online) Electron backscatter diffraction (EBSD) orientation map of a cross-section of a double-shocked polycrystalline copper sample. The EBSD color map indicates the orientation of the grains in the standard stereographic triangle. Region A is part of the spall plane in which grain refinement down to nanometer scale is observed. Region B is representative for the grain structure outside the spall plane.

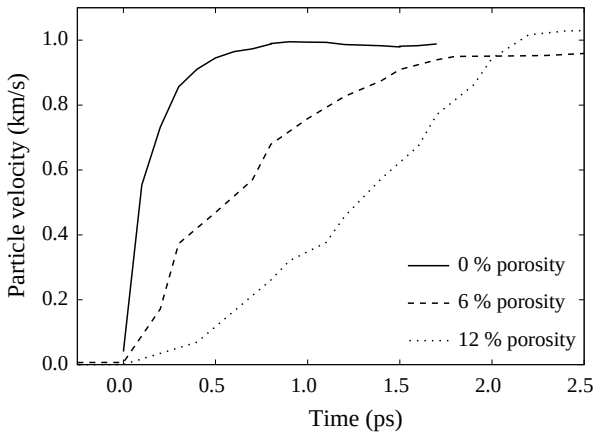

FIG. 4: Particle velocity vs. time after shock launch for a fixed slice near the back of our simulated copper sample for different porosities at a piston velocity of 1.0 km/s ($P = 48$ GPa).

grees or more are observed and these nano-scale regions are separated in some instances by high-angle boundaries. Since the experiment is integrated over time and the observations are made *post mortem*, it is not easy to determine the exact time at which the grain sub-division process is initiated. The high quality of the EBSD patterns obtained from these regions does suggest that some form of annealing of the deformed regions has occurred.

Due to the time and length scale restrictions of MD simulations, it is impossible to replicate exactly the experimental conditions which have led to the configuration shown in Fig. 3, i.e. void sizes on the order of up to several microns in conjunction with time scales in the ps to μs range. In previous studies, it has been established that for small voids ($\lesssim 10$ nm) there exists a strong dependence of the critical pressure for dislocation nucleation on the void size, which is the pre-condition for void collapse[20]. Therefore, using the experimental shock pressure in the simulations will not be sufficient to induce the degree of void collapse observed in the experiments. However, our simulations suggest that extensive void collapse is crucial for the massive local plastic deformation which according to our simulations is in turn the pre-requisite for the evolution of a nano-sized grain structure. In this spirit, in the present context aluminum serves as a suitable model material to study the problem on more easily accessible scales for two major reasons: (1) the shear modulus of aluminum is about half as large as for copper leading to a significant lowering of the critical pressure for void collapse[20]; (2) compared to copper the melting temperature and pressure of aluminum are considerably lower which should facilitate the creation of local disorder required for the formation of nano-crystalline regions[28].

One of the most important experimental techniques to monitor the dynamic response of shocked samples is the measurement of the particle velocity via VISAR. Experiments[2,6,22] on porous samples have revealed a delay in the particle velocity vs. time plot. The delay is due to void compaction which leads to a change in the density and accordingly the bulk modulus[6]. In order to establish a link to existing experimental studies, we have evaluated the time dependence of the particle velocity from our large scale simulations of Cu for a thin slab of material near the back of the sample. The results are shown in Fig. 4 and display a temporal delay of the particle velocity in the porous samples with respect to the perfect case. The delay becomes more pronounced with increasing porosity in qualitative agreement with experimental measurements[2,6,22]. The delay observed in the velocity-time plot extracted from the simulations is similar to the one observed experimentally, albeit the time scales are quite different. However, it does reflect the role of extensive plastic deformation in the closure of the voids, and the hysteresis in effective strength associated with the opening and closing of voids.

We note that the initial mechanism observed in our simulations is consistent with the qualitative model suggested by Reisman and co-workers[6]. However, we find void collapse to be due to emission of shear loops rather than prismatic loops[20]. These loops form, grow, and intersect other voids, without gliding far away from the void from which they nucleated, changing the overall en-

ergy balance presented in Ref. 6. Similar observations were made at other pressures. A simple model giving elastic properties as a function of porosity can be used to calculate a delay due to bulk modulus and density changes in the material[23]. However, as expected, the thus obtained delays do not compare well with our simulations, since most of the porosity disappears after the shock, and because the model cannot capture the complexity of the plastic deformation process which takes place in the material.

Summarizing our results, EBSD mapping of double-shocked polycrystalline copper samples reveals the presence of nano-crystallites in the post-shock sample. Molecular dynamics simulations of shocks in porous metals motivated by this experiment show formation of nano-crystallites as well. Although the time and length scales are different, it seems plausible that in both cases the formation of nano-grains occurs by massive local plastic deformation. In the simulations, this is triggered by the collapse of multiple interacting voids. We have also calculated the time dependence of the particle velocity for our shock simulations in copper. In qualitative agreement with experiments we find a temporal delay which increases with porosity. Our results point out the importance of void-void interactions and collective processes during the compression (and expansion) of porous samples. Complex dislocation structures and possible solid-state re-crystallization that result from these interactions can change the strength of the material and should not be neglected. On-going experiments[24] show increased hardness during void collapse, which is consistent with our simulation results of extended plastic zones around the collapsing voids.

Reliable continuum models of porous materials would be an important tool for tailoring material properties at the nano-scale for specific applications. They require, however, accurate dynamical information that cannot be captured by present day *in situ* diagnostics or observed in *post mortem* microscopy investigations. The present study complements the existing studies on void nucleation and growth and opens the way for the development of improved continuum models. Choosing the present work as a starting point, future studies could aim to derive a quantitative relationship betwen porosity, density and temporal delay based on atomistic simulations. In order to extend the length and time scales towards experiment coupling of MD simulations with hydro-dynamic and dislocation-dynamics modeling must be pursued.

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[27] Aluminum was modeled with the embedded-atom method (EAM) potential due to Ercolessi and Adams (EA)[25] while the EAM potential due to Mishin *et al.* (MMP)[26] was em-

ployed to represent copper. Both potentials have been previously used in simulations of shock loading[18,20,21]. While the MMP potential has proven to yield a very good description of copper under pressure, the EA potential exhibits some deficiencies in the description of these properties[21]. However, in the present context we consider it as a model system which correctly reproduces the Hugoniot relation as well as the melting temperature and pressure. The simulation cell comprised $25\times25\times100$ fcc unit cells for aluminum ($10.8\times10.8\times43.2\,\mathrm{nm}^3$) and $100\times100\times150$ unit cells for copper ($36.2\times36.2\times54.2\,\mathrm{nm}^3$). In both cases the samples were oriented along [001].

[28] In polycrystalline samples such as those usually employed in experiments grain boundaries can act as dislocation sources. Furthermore, voids are often located at grain boundary triple points. In contrast, in our simulations we consider single crystalline samples. For grain sizes on the order of micrometers the surface-volume ratio is however very small whence grain boundaries should play a comparably small role. Equivalently, we can consider our simulations as a model for the material behavior in the interior of a grain sufficiently remote from its boundaries.