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Microstructure effects on shock response of Cu nanofoams

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Microstructure effects on shock response of Cu nanofoams are investigated with molecular dynamics simulations, including elastic-plastic deformation, Hugoniot states, void collapse, nanojetting, and vaporization. The microstructure features examined include pore shape, arrangement and size, as well as grain boundaries. The elastic-plastic transition, void collapse, and jetting including vaporization, are dependent on the microstructure, although to different extents. The void arrangement and aspect ratio play an important role. The effects of grain boundaries and void size are less pronounced. Considering the measurement scatter inherent for porous materials, the high pressure Hugoniot states are not sensitive to microstructure. Jetting during void collapse is due to tensorial velocity gradients (direction and amplitude), and a combined result of forward, divergent, and convergent flows with varying contributions; this mechanism and related processes are common for different microstructures. Free surface jetting involves necking and cavitation. Elliptical voids with large aspect ratios, and with their centers aligned linearly with the shock direction, are particularly efficient in inducing high speed jetting and vaporization.

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I. INTRODUCTION

Metallic and polymeric foams can find applications in diverse areas, including materials and structure engineering, and shock physics (e.g., as laser ablaters).1–4 Metallic nanofoams5,6 are of particular interest since their routine synthesis offers relevance to molecular dynamics (MD) simulations, and to real applications (e.g., light-weight structural members and energy absorbers).

A foam’s low density and pronounced structural inhomogeneities often make temporally or spatially resolved measurements extremely difficult, to which MD can serve as a useful complement. Direct MD simulations of high porosity nanofoams under shock loading are still underexplored. Very recently, polymer and Cu nanofoams were investigated with MD simulations.2,7 Here, we extend our earlier study on an idealized Cu nanofoam7 to microstructure effects, including pore shape, arrangement and size, as well as grain boundaries. We explore circular, elliptical, square, and hexagonal voids, and different arrangements of void centers which form either a square or hexagon/honeycomb pattern. Besides deformation (elastic-plastic, void collapse, jetting) and Hugoniot states, we also look into the phenomenon of shock-induced vaporization that accompanies surface jetting. The internal and free surface jetting are analyzed in detail via vector plots, which reveal some general mechanisms of jetting for different microstructures. It is found that deformation and vaporization depend on the pore characteristics, but to a less extent, on grain boundaries. The bulk Hugoniot states for different microstructures agree within measurement scatter. We present methodology in Sec. II, results and discussion in Sec. III, followed by summary in Sec. IV.

II. METHODOLOGY

We use the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS),8 and an accurate embedded-atom-method potential of Cu,9 in our MD simulations. For a nanofoam with an initial specific volume (V0), we characterize its porosity with the ratio of its specific volume at a state of interest (V) to that of the full-density solid at ambient conditions (V0), χ ≡ V/V0, and χ0 = V00/V0.

Closed-cell nanofoams with idealized columnar voids are considered here. To examine the effects of void shape, void center arrangement, void size, and grain boundaries, we create various voids from (100) single crystal Cu or (100) columnar nanocrystalline Cu, while keeping χ0 fixed at ≈2 (Fig. 1). The x-, y- and z-axes are along [100], [010], and [001], respectively. Six unit foam configurations (types 1–6) are constructed from (100) single crystal Cu, with circular (types 1 and 2), square (type 3), elliptical (types 4 and 5), and hexagonal (type 6) voids; the yz-cross-section is 20 nm × 5 nm. For type 1, the void diameter is 15.8 nm; type 2 is similar to type 1 except that the void diameter is reduced to 7.7 nm, but the number of voids is doubled in x- and y-directions. For type 3, the edge length of the void is 14 nm. For types 4 and 5, the major and minor axes of the ellipse are 18.7 nm and 13.4 nm, respectively. The aspect ratio is about 1.4 for type 4 and 0.7 for type 5. For types 1–5, the void centers form two-dimensional (2D) square patterns. For type 6, hexagonal voids are created, and their centers form a honeycomb pattern. The wall thickness is 3.35 nm, and the outer...
piston-driven shock loading. In shock simulations, periodic boundary conditions are applied only along the $y$- and $z$-axes. The time step for integration of the equation of motion is 1 fs, and the run durations are up to 250 ps. If needed, a Lennard-Jones absorbing wall is applied to the plastic wave region with the wall velocity equaling to the average particle velocity in the plastic wave region, in order to achieve long equilibration durations. The Lennard-Jones absorbing wall is applied in this way. We take the plastic region from the last configuration before the reflected wave encounters the plastic wave front, and apply an virtual Lennard-Jones absorbing wall. The interactions between the Cu atoms and the wall are described with a 9-3 Lennard-Jones potential. Since the added wall has the same particle velocity as that in the plastic region, no waves will be reflected from the absorbing wall, and equilibration of the plastic region can be simulated for an extended duration without the complexity of wave interactions. No additional constraints are applied to the classical trajectories beyond the shock loading and the absorbing wall.

We perform 1D and 2D binning analyses\(^\text{10,11}\) to resolve spatially such physical properties as density ($\rho = 1/V$), stress tensor ($\sigma_{ij}$), von Mises stress ($\sigma_{VM}$), particle velocity ($\mathbf{u}$), and temperature ($T$) profiles at different stages of compression and release. The binning width is 5 Å or 10 Å. Averaging along the $z$-axis is applied for 2D analysis. To calculate $T$ and $\sigma_{ij}$ within each bin, we need to remove its center-of-mass velocity, $\mathbf{v}_i$ ($i = x, y$ and $z$), or apply corrections: $\Delta T = -(m/3k_B)(\overline{v_x^2} + \overline{v_y^2} + \overline{v_z^2})$ and $\Delta \sigma_{ij} = -(Nm/V)\mathbf{v}_i\mathbf{v}_j$, where $m$ is the atomic mass, $V$ is the bin volume, and $N$ is the number of Cu atoms in the volume under consideration. We also characterize the local deformation and local structure around an atom with the local von Mises shear strain invariant ($\eta_{VM}$)\(^\text{12,13}\) and centrosymmetry parameter.\(^\text{14}\)

For a full density solid, the Hugoniot is centered at $V_0$. Different states with the same $V$, e.g., Hugoniots centered at $V_0$ and $V_{00}$, can be related with the Mie-Grüneisen equation in the finite difference form via the Grüneisen parameter.\(^\text{15,16}\) Its volume dependence is normally assumed to be $\gamma_0/V_0 = \gamma/V$ and $\gamma_0 = 2$ for Cu.\(^\text{16}\) For a porous solid ($V_{00}$), if we suppose that the specific volume collapses from $V_{00}$ to $V_0$ instantaneously upon compression, then the theoretical compacted Hugoniot is\(^\text{15,16}\)

$$P_H = \frac{[2V - \gamma(V_0 - V)]C_0^2(V_0 - V)}{[2V - \gamma(V_{00} - V)][V_0 - s(V_0 - V)]^2}. \tag{1}$$

For full density Cu, the shock velocity ($U_s$) and particle velocity ($u_p$) relation $U_s = C_0 + s u_p$ are obtained from experiments and MD simulations,\(^\text{17,18}\) and $C_0 = 3.94$ km s$^{-1}$ and $s = 1.5$ are used here.

There are different models for compaction of porous or powder materials, including the $P - \alpha$ model and its variations,\(^\text{19,20}\) $P - \lambda$ model,\(^\text{21}\) and Wu-Jung model.\(^\text{22}\) The $P - \alpha$ model involves two critical pressures for the onset of plasticity ($P_s$) and full compaction ($P_c$), and a modified power-law $P - \alpha$ model\(^\text{7}\) with finite $P_s$ is
\[ P_H - P_e = (P_s - P_e) \left( \frac{V_0}{V} \right)^n \]  

(2)

III. RESULTS AND DISCUSSION

Shock loading is applied at two representative piston velocities, \( u_p = 0.625 \text{ km s}^{-1} \) and \( 2 \text{ km s}^{-1} \). Shock front and the region behind show 2D features owing to the microstructure. Based on 1D/2D binning and atomic-level structure/deformation analyses, we examine elastic and plastic deformation, Hugoniot states, void collapse, and internal and free surface jetting, and address both phenomenology and mechanisms (Figs. 2–11).

Figure 2 shows the 1D particle velocity profiles for type-2 nanofoams shocked at \( u_p = 0.625 \text{ km s}^{-1} \) and \( 2 \text{ km s}^{-1} \), showing an elastic–plastic or two–wave structure, and a single shock, respectively. The single shock formation is due to the overtake of the elastic precursor by the faster plastic shock at sufficiently high shock strengths. The pronounced fluctuations for \( u_p = 2 \text{ km s}^{-1} \) are caused by the particle velocity gradients between the collapsed void regimes and walls. For example, high speed jets may form inside voids (see discussion below).

For the two-wave structures, we can deduce the Hugoniot elastic limit (HEL), and the corresponding particle velocity and shock velocity of the elastic precursors. Figure 3 shows dependences, although to different degrees, of \( \sigma_{\text{HEL}} \), von Mises shear stress \( \sigma_{\text{VM,HEL}} \), \( u_p, \) and \( U_s, \) on microstructure, i.e., the nanofoam types. For a given microstructure, \( U_s,\) is determined by the effective, “shortest,” path length a wave traverses, as well as the void aspect ratio (horizontal/vertical dimensions), void size, and crystal orientation (e.g., \([100]\) vs. other orientations as in the cases of types 7 and 8), and void center geometry. Larger aspect ratios (type 4 vs. type 5), smaller void sizes (type 1 vs. type 2), crystal orientations other than \([100]\) (types 7 and 8 vs. type 6), and shorter paths (type 2 vs. type 6) should result in higher \( U_s,\) Type 5 is the slowest (\( U_s,\)), \( \sigma_{\text{VM,HEL}} \) is an indicator of the resistance to shear or plastic flow. Types 1–3 are similar, and slightly stronger than the honeycomb structures (types 6–8), so the grain boundaries and void sizes only play a secondary role in deformation of nanofoams. The drastic difference between types 4 and 5 (the strongest and the weakest, respectively) may be attributed to the horizontal wall thickness.

We examine next the dependence of the \( P-V \) Hugoniot states on the microstructure or nanofoam types. These states for \( u_p = 0.625 \text{ km s}^{-1} \) and \( 2 \text{ km s}^{-1} \) are obtained from 1D binning analysis and plotted in Fig. 4. For comparison,
experiment results on porous Cu\textsuperscript{17,23} full density Hugoniot [Eq. (1) with $V_{00} = V_0$], compacted Hugoniot [Eq. (1)], and a $P - z$ model fit\textsuperscript{7} [Eq. (2)] are also included. Despite the relative large scatter in high pressure data, the overall agreement among different nanofoam types, and between the simulations and experiments or predictions, is reasonable. The scatter for $u_p = 2 \text{km s}^{-1}$ is due to the large fluctuations that are inherent in the 1D profiles, for example, Fig. 2. Therefore, the Hugoniot states at high pressures appear to have weak dependence on the microstructure of foams. Note that the errors of measurements on foams or porous materials both in experiments and simulations are large because of their large structural inhomogeneities.

The above 1D analyses only describe the average shock responses of nanofoams, and may not be sufficient, or even appropriate, for other purposes since they are highly structured. To reveal the mechanisms of void collapse, we compare local atomic shear strain distributions ($\gamma_{vM}$) for different nanofoams shocked at $u_p = 0.625 \text{km s}^{-1}$ (Fig. 5). The results of centrosymmetry parameter analysis are consistent. The passage of the “elastic precursor” (Fig. 1) leaves traces of weak plasticity in the walls (types 1–6) or the grain boundaries (types 7 and 8). So the “elastic wave” is not purely elastic. For monocrystalline void configurations, plastic deformation is largely nucleated from void edges with activated \{111\} slip systems, while for nanocrystalline void configurations...
configurations, it initiates from grain boundaries. For the plastic wave, the nucleation and growth of plasticity are rapid. The strain concentrations are localized initially on the top and bottom of a void, or the tips along the long axis for type 4.

For void collapse, the transverse flow prevails in the cases of circular voids (types 1 and 2). For square voids (type 3), plastic flow begins with the left two corners towards the void center. The horizontally (type 4) and vertically (type 5) oriented elliptical voids collapse differently. The left wall in type 4 is so thin that it easily yields and caves forward, accompanied by slow moving, broad transverse flow. In contrast, type-5 voids yield from top and bottom walls, i.e., predominantly via transverse flows. The plastic flow in types 6–8 is more uniform, owing to their more “random” distributions of void centers. For type 6, strain concentration occurs at the top and bottom tips, and flow follows the void shape. For type 7, the regions near the small “triangular” voids undergo more plastic deformation. The void collapse leads to nanodomains of different extents of plastic deformations, which can be correlated with void (size, shape, and arrangement). In particular, the uniformity of deformation is dictated by the randomness of void center arrangement. For example, the deformation bands apparent in types 1–5

FIG. 7. Internal jetting: vector plots of the distribution of velocity projected onto the $xy$-plane for different types of foams shocked at $u_p = 2 \text{ km s}^{-1}$. The snapshots are for $t = 90 \text{ ps}$. Numbers denote foam types. Shock direction: left → right.
nanofoams are replaced by homogeneous deformation in types 6–8.

With piston velocity increased to 2.0 km s\(^{-1}\), forward plastic flow may dominate transverse plastic flow, leading to internal jets (Fig. 6). An internal jet is stopped by a front wall and this impact gives rise to the next internal jet. Foam microstructure has pronounced effects on the head shape of an internal jet. For circular voids (types 1 and 2), the jet heads assume a “circular” shape. For the square voids (type 3), the jets are not smooth and show two protuberances at the corners, due to wave convergence. Horizontally oriented elliptical void (type 4) is so long in the shock direction that its internal jet is similar to free surface jet (see below). A jet head can grow as long as possible until it reaches a wall. Small curvature on the left side of an elliptical void (type 5) leads to a flat jet head, as well as small gradients in \(u_x\) along the transverse direction (\(y\)). Similar to type-3 foams with square voids, two protuberances form on the corners due to shock convergence. Hexagonally arranged voids in monocristalline (type 6) and nanocrystalline (types 7–8) induce more homogeneous deformation. The jet head shape for type 6 assumes the void shape (hexagon), and those for types 7 and 8 are similar to types 1 and 2. Thus, the shape of an internal jet head (or the curvature) is approximately the mirror image of the portion of a void the shock traverses, except the “secondary jets” at the sharp corners. Grain boundaries appear to have very limited effects on internal jet at high impact velocities.

To better reveal the mechanisms of internal jetting, we compare vector plots of particle velocities (\(u\)) for different nanofoams shocked at \(u_p = 2.0 \text{ km s}^{-1}\) (Fig. 7), obtained from 2D binning analysis. Different foam microstructures manifest apparent differences in flow patterns within and behind internal jets, in terms of tensorial velocity gradients, which describe the deviation of flow direction from the forward direction, and the gradients in amplitude. A major difference is due to the geometric arrangements of void centers. For the foams with linearly aligned void centers (types 1–5), the forward flow along the void center line prevails, although the gradients for type 5 are much smaller. In contrast, the flow pattern also shows an “X” feature, for foams with hexagonally arranged void centers (types 6–8); this pattern is a direct consequence of wave propagation along the tortuous paths formed by ligaments while circumventing voids. These
“random” voids serve as homogenizing “scattering” centers and lead to more homogeneous velocity distribution.

Despite the apparent differences in flow patterns for different void shapes and arrangements, there are some common mechanisms in the development of internal jetting, as illustrated in Fig. 8 for foam type 3. Upon initialization of internal jetting [Fig. 8(a)], there are four zones labelled as A–D. When the vertical wall (zone A) is impacted by a jet, the shock wave traveling along the horizontal wall has just arrived at zone D and lags behind the jet. The vertical wall moves forward (A) as well as sideways due to the stress gradient along the y-direction (B). Zone C is vacuum, so atoms in zone D move towards zone C, again due to the stress gradient. As a result, divergent flows are initiated from A to D, and their convergence at the corners leads to the formation of two high speed protrusions [E, Fig. 8(b)]. Since the \( u_y \) component in A is still highest, the jet center arrives at the vertical wall first, and two vacuum spaces form at the corners in the currently collapsed void [F, Fig. 8(c)]. F and C are equivalent. This process [Figs. 8(a)–8(c)] repeats itself until the jet reaches the free surface, and an unconstrained, divergent flow leads to free surface jetting [Figs. 8(d) and 9]. For different foam types, voids all collapse via forward, divergent, and convergent flows, and the jet formation processes are largely similar. However, the exact contributions of such flows and flow patterns depend on pore shape and arrangement.

Free surface jet evolution is of particular interest, and we thus examine the processes (including vaporization) and mechanisms involved (Figs. 9–11). Necking, cavitation, and atomization accompany jet growth, breaking, fragmentation, and vaporization, and are driven by tensorial velocity gradients originated from the inherent heterogeneities or microstructure in a foam.

Various morphologies of free surface jets are observed for the eight types of foams (Fig. 9). Initially, a free surface jet necks to form a head. The head then grows with or without cavities formed inside. The velocity distribution is relatively homogeneous for types 5–8 (Figs. 9 and 10), and the free surface jets become steady and then merge. The type-5 foam is a special case with thin horizontal wall and small curvature along the shock direction, and no cavitation is observed. For other foam types (1–4), cavitation and jet breaking are evident. In particular, pronounced fragmentation and vaporization occur for the type 4 foam (Figs. 9–11). For types 1 and 2 foams, the divergent flow in the jet head and uniform flow in the region behind result in necking. Roughly speaking, divergent flows with finite transverse gradient, \( \partial u / \partial y \), lead to cavities in the jet head [e.g., zone A, Fig. 10(a)]. For type 3, cavitation in region C [Fig. 10(b)] is due to the longitudinal gradient \( \partial u / \partial x \) between A and B (similar for cavitation in D). Cavitation in type 4 foams shows the effects of both longitudinal (A) and transverse (B) gradients [Figs. 10(c) and 10(d)]. In contrast, small values of \( u_y \) and velocity gradients along the x- and y-directions, result in no cavitation for types 5–8 [Figs. 10(e) and 10(f)].
High speed, narrow, straight flow “channels” form inside type-4 foams via internal jetting. At a free surface, the confinement as supplied by the foam ligaments does not exist anymore. So the free surface jet is initially under inertia confinement after it exits the free surface. The strong tensorial stress and velocity gradients then give rise to “exploding” cavitation, which in turn create more gradients, and fragmentation and atomization follow (Fig. 11). The leading front is essentially a fast moving vapor, as seen from the velocity and density plots. The vaporization also erodes the compressed foam from the free surface into the interior (in a sense similar to multiple spallation in solids). It is also worth pointing that jets at the exit surfaces may bend sideways and become twisted (Fig. 11), likely caused by velocity perturbations.

Our MD simulation results bear important implications to larger scale processes in shocked foams, including phenomenology and mechanisms for deformation, void collapse, jetting, and vaporization, and their microstructure dependence. However, simulations at larger time and spatial scales, and with different ligament thicknesses and boundary conditions, are highly desirable for future study.

IV. SUMMARY

We have investigated the effects of microstructure (including void shape, arrangement, and size) and grain boundaries on dynamic response of high porosity nanofoams under shock loading at two representative piston velocities. The elastic-plastic transition, void collapse, and jetting including vaporization, display dependences on the microstructure. The void arrangement and aspect ratio play an important role, while the effects of grain boundaries and void size are secondary. The high pressure Hugoniot states are not sensitive to microstructure. Jetting during void collapse is caused by local tensorial velocity gradients, and a combined result of forward, divergent, and convergent flows with varying contributions; this mechanism and related processes are common for different microstructures. Necking, cavitation, and atomization accompany jet growth, breaking, fragmentation, and vaporization, and are originated from the inherent heterogeneities or microstructure in a foam. In particular, elliptical voids with large aspect ratios, and with their centers aligned linearly with the shock direction, yield high speed jetting and vaporization.

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