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On shock response of nano-void closed/open cell copper material: Non-equilibrium molecular dynamic simulations

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Non-equilibrium molecular dynamic simulations were carried out on model three-dimensional nano-void copper material with different idealised pore structure and porosity to highlight differences in response behaviour between them when subjected to various piston velocities simulating planar shock loading of different intensities. This article demonstrates and explains from a mechanistic perspective the differences in response observed with respect to Hugoniot elastic limits, dislocation line and jet formation, void collapse mechanism and hot spot generation, specific volume, partial recrystallisation and temperature evolution in void collapsed regions, shock and particle velocity curves. © 2014 AIP Publishing LLC. [http://dx.doi.org/10.1063/1.4861029]

I. INTRODUCTION

The presence of porosity in the form of nano-voids induces unique and tunable properties in materials. Sometimes porosities are a result of defects (cracks or voids of several hundred nanometres) in a material structure which in turn affects the global response of the material.1 Porosity can be present in a material either as a closed- or open-cell pore structure. The effect of these different pore structures on shock response of materials is the main highlight of this paper. The material chosen for this study is nano-void Cu foam. It should be mentioned in here that even though there exists a lot of literature on molecular dynamic (MD) simulation of shock response of single crystal solids, there is limited literature on shock response of metallic nano-void materials.1–9 To the best of the authors knowledge, even within these limited literature on shock response of MD simulations of metallic nano-void foams, there does not exist any previous literature which addresses the influence of pore structure on shock response through non-equilibrium molecular dynamic (NEMD) simulation.

II. SIMULATION METHODOLOGY

A large scale explicit NEMD simulation of Cu samples with different porosities and different pore structures have been carried out in this study using Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) developed by Sandia Labs.10 A small bulk sample (4 × 4 × 4 unitcell) with periodic boundary condition applied in all orthogonal directions was prepared by equilibrating it at NPT ensemble for 75 ps followed by NVT ensemble for 100 ps with time step size of 0.5 fs. This small bulk sample was replicated in all the respective directions to generate a 1000 × 100 × 100 large bulk supercell of Cu with (100), (010), and (001) Miller planes oriented in X, Y, and Z directions, respectively. Equilibration of the large bulk sample was also carried out at 50 K temperature and ambient pressure by NPT followed by NVT ensemble for 40 ps each. A total of 4 × 107 Cu atoms, thus generated, have been utilized for simulation using embedded-atom method (EAM) potential.11

Spherical nano-sized voids, centred at predefined atomic coordinates in the large bulk domain, were then inserted in the bulk domain. It should be noted that even with introduction of voids in closed/open cell pore structure the uniformity of the entire structure was maintained. The acceptability of the voids was checked by performing energy minimization. After void insertion, equilibration of sample was again carried out at 50 K temperature and ambient pressure by NPT followed by NVT ensemble for 55 ps each. To obtain a model of close and open-cell pore structure and to reach desired percentage of porosity, the radius, scaled position coordinate of voids, and also total number of voids were varied to obtain Cu nano-void foams with porosity approximately 18%, 38%, and 54%. It should be noted that for open-cell pore structure the radii and number of the voids in three directions were not identical; the voids were created to maintain almost same porosity ratios as that of its corresponding closed-cell pore structure. Table I highlights all sample details. Figure 1 shows initial XZ planes for samples used in simulation in this article. Voronoi tessellation was done to obtain atomic volume and density data of the samples.

To simulate a planar shock wave loading in (100) direction, the piston is kept at rest with unshocked target materials given an initial velocity of −Vp, the shock wave then moves out from the stationary piston face.12–14 The direction of shock wave propagation was chosen along the X axis whereas periodic boundary conditions were applied in Y and Z directions. Fixed boundary condition was applied along the direction of shock propagation. NVE ensemble with a timestep of 0.5 fs was utilised during the simulation of shock wave propagation. Some empty region was intentionally

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invoked at the right edge of the foam sample to see the free surface jetting at considerable shock strengths.

III. RESULTS AND DISCUSSIONS

Shock response of nano-void Cu materials with different pore structures and porosities has been investigated in this study. Shock loading has been applied at different piston velocities ranging from $u_p = 0.05 - 3.5$ km/s generating elastic-plastic and fully plastic waves in the nanofoams. Detailed investigations were performed regarding plastic deformations, Hugoniot elastic limit (HEL) positions, specific volume change, shock velocity, temperature profile, void collapse, recrystallisation, nano-jetting within the pores, hotspot formation, as well as underlying atomistic mechanisms involved during the process of shock wave propagation through the nano-void material. Center of mass velocity has been removed during calculation of pressure and temperature in the following subsections. Ovito software\textsuperscript{15} has been utilized for visualization and color rendering purpose.

For different piston velocities, two different regimes of behaviour can be observed:

\begin{itemize}
  \item regime in which elastic wave front precedes the plastic wave front. This regime is typically below the HEL position. No change in the pore structure is observed while the elastic wave front crosses them whereas the pore structures are deformed and/or gets collapsed while the plastic wave front passes over them. This regime is typically achieved with low piston velocities.
  \item regime above the HEL position where the plastic wave front has overtaken the elastic wave front. At high piston velocities, fully plastic wave fronts could be observed. Mechanisms such as void-collapse, jetting, and shock induced melting are observed in this regime.
\end{itemize}

A. Hugoniot elastic limit position

HEL is typically defined as maximum stress sustainable by a solid in one-dimensional shock compression without significant irreversible deformation taking place at the shock front.\textsuperscript{3} Thereby, this corresponds to the stress at which plastic wave front just precedes the elastic wave front in a solid subjected to shock loading. Figure 2 shows variation of HEL position (expressed in terms of stress (GPa)) with different porosities for closed- and open-cell pore structure. It can be

\begin{table}[h]
\centering
\caption{Cu nano-void foams of different pore structure and porosity used in this manuscript for simulation.}
\begin{tabular}{ccc}
\hline
        & Close-cell & Open-cell \\
\hline
4.11 & 54.08 & 0.24 & 4.05 & 54.78 & 0.25 \\
5.56 & 37.92 & 0.18 & 5.55 & 38.06 & 0.18 \\
7.30 & 18.52 & 0.14 & 7.28 & 18.74 & 0.14 \\
\hline
\end{tabular}
\end{table}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{Cross section (XZ plane) of different pore structures and porosities used in simulation: (a) high porosity close-cell, (b) medium porosity close-cell, (c) low porosity close-cell, (d) high porosity open-cell, (e) medium porosity open-cell, and (f) low porosity open-cell.}
\end{figure}
observed from the figure that with increase in porosity (for both closed and open-cell pore structure) the HEL position decreases thereby demonstrating that plastic shock front overtakes the elastic wave front at lower values of stress with decrease in density of the entire sample. Typically, increase in porosity results in lower density as well as lower yield strength. The lower yield strength is easily exceeded by the stress induced to the material due to shock resulting in plastic waves overtaking the elastic waves earlier which in-turn results in lower values of stress at HEL position. It can also be observed from the figure that for almost same porosity, the HEL position is lower for open-cell in comparison to closed-cell pore structure for lower porosities (or higher densities). However, as the porosity is increased the difference in HEL position between the two types of pore-structures diminishes.

B. Void collapse mechanism

Dislocation lines, identified by using a centrosymmetry parameter filter, could be observed for both closed and open-cell pore structure at low piston velocities for different porosities in $(111)$ direction. Enhancement of dislocation density around the voids can be observed in the simulations supporting the theory of formation of shear loops and sessile junctions when a shock wave passes through a nano-void region within a bulk fcc medium. For close-cell pore structure, the observed dislocation lines are more prominent and are stable for a longer time for low porosities in comparison to high porosities (Figure 3). The primary reason for this can be attributed to larger intervoid bulk material region in low porosity samples. Small inter-void bulk material region typically accounts for development of disordered particle structure instead of stable formation of dislocation lines.

For open-cell pore structure (Figure 4), the behaviour regarding observation of dislocation lines is different from that of the close-cell pore structure; however, not much difference could be observed in between different porosity levels within an open-cell pore structure. Enhancement of dislocation density around a void can be observed leading to formation of ligaments in initially void-interconnected regions. These ligaments eventually evolve leading to void collapse. As observed in Figure 4, along with time more particles accumulate in these ligament region, which eventually helps in the process of collapse of the pore region. Ligaments which are already formed and/or being formed have been highlighted in the Figure 4 by white rectangular regions whereas initial interconnected void regions are shown by red rounded rectangular regions. Comparing Figures 3 and 4, it can be stated that voids completely collapse along the direction of shock propagation at a faster rate in close-cell pores in comparison to open-cell pores. It can also be observed that void collapse occurs at a much faster rate at low porosities for both closed and open-cell structure in comparison to high porosities.

The phenomenon of void collapse is significantly different for higher piston velocities in comparison to low piston velocities. At high piston velocities, no dislocation lines are formed but phenomenon of jetting could be observed. Similar observations on jetting (constituting of spalled particle from upstream side of the void) have been reported previously by other researchers. Figure 5 shows formation of jetting in close-cell pore structure. For higher porosities,
apart from jetting, spraying phenomenon can also be observed. The phenomenon of spraying is different from that of jetting in which the jets formed are not focussed at one point but are dispersed. These phenomena of jetting and/or spraying eventually result in complete void collapse before the shock front moves to the next array of voids along the shock wave propagation direction. The jets and/or sprays containing particles of higher kinetic energy generated from the concave upstream void surface walls hit the downstream convex walls of the pore resulting in hot-spot formation.

It can be observed from Figure 6 that jets formed in open-cell pore structure travel freely through the interconnected pores as ejecta materials and thereby the complete void collapse in open pore structure (of an array of voids) takes more time in comparison to close-cell pore structure. Ligaments which are already formed and/or being formed have been highlighted in the figure by white rectangular regions whereas initial interconnected void regions are shown by red rounded rectangular regions. The freely travelling jets and ejecta materials through interconnected pore regions result in increase in the height of the jet but do not result in formation of hot spot regions due to collision of particles with a wall of bulk materials. The height of the jet and ejecta materials along shock wave propagation direction was observed to increase with increase in piston velocity. Comparison of Figures 5 and 6 demonstrates that because of unrestrained open region of propagation for the jets and ejecta particles in open-cell pore structure, the kinetic energy

![Figure 4](https://example.com/fig4)

**Figure 4.** Void collapse mechanism and dislocation band formations (along XZ plane) at a specific time instance of 12 ps in open-cell pore structure at 0.5 km/s piston velocity at different porosities: (a) low, (b) medium, (c) high porosity. Red arrow indicates shock front location. Color bar indicates centrosymmetry parameter. Red rounded rectangular region indicates initial inter-void regions; white rectangular regions indicate formed ligaments and/or ligaments being formed.

![Figure 5](https://example.com/fig5)

**Figure 5.** Void collapse mechanism and jetting (along XZ plane) in close-cell pore structure at 3.5 km/s piston velocity: (a) low, (b) high porosity. Color bar indicates temperature in Kelvins. $k$ in the color bar represents multiplication by 1000.

![Figure 6](https://example.com/fig6)

**Figure 6.** Void collapse mechanism and jetting (along XZ plane) in open-cell pore structure at 3.5 km/s piston velocity: (a) low, (b) high porosity. Color bar indicates temperature in Kelvins. $k$ in the color bar represents multiplication by 1000.
TABLE II. Specific volume and stress for Cu bulk as well as foam materials with different pore structure and different porosities (Prop.: property; Por.: porosity; SpV.: specific volume).

<table>
<thead>
<tr>
<th>Prop.</th>
<th>Bulk</th>
<th>Close-cell</th>
<th>Open-cell</th>
</tr>
</thead>
<tbody>
<tr>
<td>Por. (%)</td>
<td>0</td>
<td>18.52</td>
<td>37.92</td>
</tr>
<tr>
<td>Str. (Gpa)</td>
<td>275</td>
<td>117</td>
<td>98.14</td>
</tr>
<tr>
<td>SpV. (cc/gm)</td>
<td>0.112</td>
<td>0.087</td>
<td>0.0978</td>
</tr>
</tbody>
</table>

is higher (resulting in higher temperature) in comparison to close-cell pore structure of similar porosity.

C. Specific volume

Specific volume (or inverse of average mass density) has been obtained in the simulation from a particular region within the entire domain. Boundary atoms corresponding to 3 layers of unitcells (approximately 11 Å) were excluded from both sides of the entire domain in X direction. The remaining region was then divided into 10 regions of equal dimensions with the region where shock starts propagating (from left side of the entire domain) being referred to as the tenth region. The region to the extreme right along the X direction was labelled as the first region where the shock reaches last. The calculations corresponding to specific volume were done as the shock front enters the ninth region. The specific volume vs. stress curves are shown in Figure 7 for the ninth region till the point stability in stress values has been achieved as the shock front traverses through the entire domain at a specific piston velocity. It can be observed from Figure 7 that stress increases whereas ultimate specific volume decreases for decreasing porosity for both closed and open-cell pore structure. For the case of closed-cell pore structure, the simulation results are found to match experimental observation as well as previous MD simulation results carried out at similar porosity. No such validations could be made for open-cell pore structure due to unavailability of any previous data. Table II shows the values of specific volume and stress for bulk Cu material along with values obtained from simulation (at a piston velocity of 3.5 km/s) for closed and open-cell pore structure with different porosities. It can be concluded from Table II that as porosity is increased for both open and close-cell pore structure, the compressed density is lowered (specific volume is increased). Based on values obtained from Table II, it can also be concluded that at a piston velocity of 3.5 km/s the compressed portion of open-cell pore structure has higher density (lower specific volume) in comparison to close-cell pore structure of comparable porosity. It can be mentioned from the table that at a specific piston velocity open-cell pore structure achieves a density (or specific volume) closer to that of the compressed bulk material in comparison to that of close-cell pore structure with similar porosity. This indicates a potential for more compaction in samples with close-cell pores unless melting occurs prior to that. It should be noted that based on phase diagram, melting may be considered as a complex procedure involving a combination of pressure applied as well as temperature attained in the sample.

A comparative evaluation of specific volume vs. stress for two different cell pore structures with high and low porosity is shown in Figure 8. The figures reveal that there is a gradual change in values of stress as the specific volume gets decreased for open-cell pore structure with higher piston velocities; whereas there is a more drastic change in stress as specific volume is decreased for close-cell pore structure with higher piston velocities. The reason from this can be observed from the atomistic response plots (shown in Figures 5 and 6) which typically indicates a sudden collapse of the pore for close-cell pore structure (due to jetting) in comparison to a more gradual collapse of the pore for open-cell pore structure (due to jetting propagation through interconnected pores) at higher piston velocities. An intersection is observed between the two curves for both porosities, which demonstrates a behavioural change for higher piston velocities in comparison to low piston velocities. The ultimate stress calculated at a piston velocity of 3.5 km/s is observed to be lower for close-cell in comparison to open-cell pore structure. Ultimate density (inverse of specific volume) at 3.5 km/s is also observed to be higher for open-cell in comparison to close-cell pore structure and this difference was observed to be more for lower porosity in comparison to higher porosity of the samples.

D. Partial recrystallisation after void collapse

After void collapse at low piston velocities in close-cell pore structure, no proper crystal structure is observed and a
fully disordered system exists in initial void regions due to high thermal energy. Based on common neighbour analysis, Figure 9 shows that as the shock moves further into the material, partial recrystallisation is observed in the initially fully disordered void collapse regions for low piston velocities (0.5 km/s) in low porosity close-cell pore structures which indicates gradual decrease of kinetic energy of the collapsed region as the shock front moves forward. No such phenomena are observed at low piston velocities for high porosity close-cell pore structures. For open-cell pore structure, even though development of inter-void ligaments regions are observed in Figure 4, no definitive crystal structure could be observed in the ligament regions where the atoms remain in a disordered state. It should be pointed out that this recrystallisation was also not observed for both the cell pore structures at higher piston velocities. Figure 9 shows formation and evolution of recrystallisation region for a specific pore region at different temporal instances as the shock front propagates through the material. At 5 ps, the atoms in the collapsed void region are in state of complete disorder. Gradually along with time as the shock front moves away this disordered region partially recrystallises into bcc, or hcp or fcc crystals. However, no specific pattern could be obtained regarding the crystal structure temporally. Moreover, as the piston velocity is increased to 1 km/s for low porosity close-cell pore structure, partial recrystallisation could be observed for only a limited time after which the collapsed void region again moves back to the disordered state.

E. Temperature profile in a region

The average temperature of the void region (obtained from the kinetic energy of the particles by using equipartition theorem) has also been recorded during the process of void collapse in the ninth region (refer to region division of bulk domain in Subsection III C). Figure 10 shows temperature vs. simulation time for closed and open-cell pore structure with different porosities at a piston velocity of 2.5 km/s. The equilibrated temperature of the sample was 50 K prior to...
shock wave initiation; but as the shock front enters in the tenth region, the kinetic energy behind the front rises which causes drastic increase in the temperature and subsequent void collapse. In order to observe the maximum temperature and plateau of the void collapsed region during the propagation of the shock front, the temperature variation beyond 2.5 ps after entering into the ninth region has only been plotted to accommodate the plateau more clearly. The plot has been continued till the shock front leaves the eighth region and an equilibrated temperature is achieved in the collapsed pore area of the ninth region. High local temperatures in the range of 5000–9000 K were observed in the samples (similar observation has been made in previous literature\textsuperscript{7}). For both closed and open-cell pore structures, the temperature recorded in the pore collapse region is observed to be higher for higher porosities in comparison to lower porosities (refer Figure 10 and Table III). It is also observed from Figure 10 and Table III that the length of the plateau of high temperature before attainment of temperature surrounding the pore is higher for higher porosities both for closed and open-cell pore structures. The reason for this can be explained by the size of the voids influencing the kinetic energy of the particle which in turn affects the temperature (Table III). Higher temperatures are observed in open-cell in comparison to close-cell pore structure, primarily because of higher velocities attained by particles in the open-cell pore structure.

F. Shock velocity vs. piston velocity

Utilizing measurements from binning analysis in the ninth region (refer Subsection III C), shock velocity was obtained using the Rankine Hugoniot mass conservation equations (where the initial density was taken as the density of the unshocked region, whereas the current density was taken as the mean density of the same region after being shocked). Figure 11 shows shock-piston velocity curve \((U_s-U_p)\) for different porosities for two different pore structures. Good correlation could be observed between experimental and simulation results\textsuperscript{17} carried out for closed-cell pore structure with approximate porosities of 16\% and 34\%. Similarly, good correlation of simulation results could also be observed with previous MD simulations of close-cell Cu foams\textsuperscript{8} with around 50\% porosity. Since no such data were available for open-cell pore structure, comparison and/or validations with current MD simulations could not be made. An interesting observation could be made on comparing these curves for closed- and open-cell pore structures. A

\begin{table}[h]
\centering
\begin{tabular}{|c|ccc|ccc|}
\hline
Properties & Close-cell & Open-cell & & & & \\
\hline
Porosity (\%) & 18.52 & 37.92 & 54.08 & 18.74 & 38.06 & 54.78 \\
Max. Temp. (K) & 6250 & 7100 & 8000 & 7500 & 8000 & 9000 \\
Plateau (ps) & 20 & 12.5 & 7 & 24 & 10 & 3 \\
\hline
\end{tabular}
\caption{Maximum temperature and Maximum temperature plateau for both cell pore structure at different porosities.}
\end{table}

FIG. 10. Temperature profile of a region for 2.5 km/s piston velocity: (a) close-cell, (b) open-cell pore structure.

FIG. 11. Shock velocity vs. piston velocity: (a) close-cell, (b) open-cell pore structure.
difference in slope could be observed in between the linear fit of \( U_s - u_p \) lines for closed and open-cell pore structure with different porosities. Table IV shows the statistic for the intercept with the shock velocity axis, slope of the linear fit and also \( R^2 \) goodness of fit to the linear regression line for \( U_s - u_p \) curve. The difference in slope between the two cell-pore structures can be explained by taking a deeper look into the void collapse mechanism of the two cell pore structures at low and high piston velocities. At lower piston velocities in open-cell pore structure, ligaments are formed and as a result energy utilized for shock wave propagation (which can be related to a function of shock velocity) is reduced. This leads to lower shock velocities (for low and medium porosities) for open-cell pore structure at lower piston velocities in comparison to its close-cell counterpart. Since voids occupy a significant region of the entire bulk region and inter-void connection regions are small for high porosity open-cell pore structure samples, energy required for ligament formation is less and thereby shock velocity is almost same as that of samples with high porosity close-cell pore structure. On the other hand, for higher velocities, atoms are seen to move through the inter-void regions and thereby complete pore collapse of an array of voids is delayed for the open-cell pore structure in comparison to the close-cell pore structure. These phenomena eventually result in higher shock velocities in open-cell pore structures in comparison to close-cell pore structures at a specific porosity level. This interesting response behavior has been highlighted in Figure 12 which compares linear \( U_s - u_p \) curve fits for a specific porosity between the two types of cell pore structures. For samples with low to medium range of porosities, lower shock velocities were observed for lower piston velocities for an open-cell pore structure in comparison to a close-cell pore structure. This behavioural pattern changed at piston velocities of around 2 km/s and after that the pattern was reversed with open-cells showing higher shock velocities in comparison to close-cell pore structure. However, for higher porosities, it was observed that shock velocity for open-cell was always more at all piston velocities than for closed-cell pore structure. Support to the above proposed hypothesis explaining difference in slopes between two cell pore structures can also be obtained from Figure 8 demonstrating changes in mean density (inverse of specific volume) which in turn would obviously result in changes in shock velocity.

**IV. CONCLUSIONS**

The article elucidate atomistic mechanisms which results in differences in shock response between closed and open-cell pore structures of different porosities. Major differences are highlighted as follows:

- HEL point lowers with increase in porosity. Typically, HEL is lower in open-cell compared to close-cell pore structures.
- Dislocation lines observed at low piston velocities are prominent for lower porosities. Rate of complete void collapse is faster for close-cell compared to open-cell pore structures.
- At higher piston velocity, jetting and spraying behaviour is observed. Jets and/or sprays of ejecta particles are observed to travel through inter-void regions for open-cell pore structure.
- Ultimate specific volume of a region decreases with decreasing porosity. The ultimate specific volume,
calculated at 3.5 km/s piston velocity, was observed to be lower for open cells in comparison to close-cell pore structure.

- Partial recrystallisation after void collapse is observed for closed cells with low porosity at low piston velocities but not for open-cell pore structures.
- Local temperature in a region after shock wave propagation is higher with higher porosity and also observed to be higher for open cells in comparison to close-cell pore structure.
- Differences are observed in shock velocity–piston velocity curves for two pore structures regarding slope of the linear fit line.

This study can help in answering questions such as why open-cell metallic nano-foams are being used in double shell inertial confinement fusion target. The reason for this is primarily significant increase in shock velocity with open-cell pore structure in comparison to closed-cell pore structure at higher piston velocities.

This study also raises questions over whether pure close-cell nano-foams at any porosity level should only be utilized for mitigation of shock response of all intensities. It has found from this study that open-cell pore structure of low-medium porosity can demonstrate better energy absorption characteristics for low-medium shock intensities since the shock velocity is significantly reduced in comparison to close-cell pore structure. On the other hand, a definitive prescription of use of pure open-cell pore structure for shock wave absorption at low-medium shock intensities cannot also be made since HEL position is lower and local temperature in a region after shock wave propagation is higher for open cells in comparison to close-cell pore structures. Therefore, the engineers/physicists may need to manufacture tailored nano-void fcc crystal materials containing combinations of closed and open-cell pore structure for different applications involving energy absorption for low-medium intensity shock loading situations. For high intensity shock loading situations, closed-cell pore structure of comparable porosities demonstrate better energy absorbing characteristics in comparison to open-cell pore structure.

Nano-voids of open/close-cell pore structure may result during initial fabrication of the material or due to in-service defects; this study will also help in fundamental understanding of different phenomena associated with shock loading of these structures/materials at different intensities.

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