Fracture during high-velocity impact of copper plates: a molecular dynamics study

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Abstract. High velocity impact of copper plates has been studied using the molecular dynamics code LAMMPS. The impact of copper plates at 1100 m/s impact velocity shows that spall of the material takes place at 160 kbar tensile pressure. Void nucleation is not observed at lower impact velocities where the peak tensile pressure stays below 160 kbar. No significant void nucleation occurs in the neighbouring regions where the peak tensile pressure stays below 160 kbar. For impact velocities close to the threshold, we observe stochastic behaviour of the spall process with respect to small changes in the initial atomic coordinates.

1. Introduction
Solid fracture under high strain-rate deformation is of interest for high velocity impact and penetration problems. The impact of a flyer onto the target produces compressive stress waves which travel toward the respective free surfaces of the flyer and target. When they reach the free surfaces, they are reflected back as release waves and interact at some location in the target. The interaction of release waves produces tension in the target material. If the tension created exceeds the tensile strength of the material, nucleation, growth and coalescence of the voids take place, leading to spall. This process is called spallation.

We have simulated high velocity impact of copper plates using the LAMMPS [1] code. In the present work, we validate the void nucleation threshold (160 kbar) obtained under triaxial strain conditions [2] by studying the impact of copper plates at 1100 m/s. We also show the stochastic behaviour of spall process for the impact velocities close to the spall threshold of the material. The summary of work done by other workers is presented in [3].

2. Computational Method
The classical molecular dynamics code LAMMPS [1] has been used for this study. We have used embedded-atom method potential parameters generated by Foiles et al [4]. As a first step, the simulations have been validated by reproducing the Hugoniot for crystal copper [5]. The simulation domain contains $1.08 \times 10^6$ atoms corresponding to $300 \times 30 \times 30$ unit cells. Free boundary conditions are applied along the impact direction ($x$-direction) and periodic boundary conditions are applied along the transverse directions ($y$- and $z$- directions). The thickness of the target plate is taken as twice that of the flyer. The target is divided into small bins and pressure is computed in each bin of the target using binning analysis. Impact is done with an
impact velocity of 1100 m/s. The typical strain-rate in this impact simulation is $\sim 10^9$/s, comparable with the triaxial strain simulation [2].

3. Results and Discussion

3.1. Free surface velocity

The free surface velocity of the target for an impact velocity of 1100 m/s is shown in figure 1 (a). The impact at 1100 m/s produces compressive stress waves at the point of impact. These waves propagate toward the respective free surfaces of the flyer and target. When they reach the free surfaces, they reflect as release waves. In this process, the free surface of the target is accelerated to approximately twice the particle velocity behind the shock [6]. The shock arrives at the free surface of the target at 14 ps as shown in figure 1(a). The interaction of release waves at some location in the target creates tension in the material. The centro-symmetry parameter analysis [3] shows that defects are created only during the tension. This means that plastic deformation of the material takes place only under the tension not under the compression state of the material. If the tension created exceeds the tensile strength of the material, nucleation, growth and coalescence of the voids take place leading to spall of the material. It is seen in the figure 1 (a) that there is a pullback in the free surface velocity which is the signature of spall [7]. Snapshots of the domain at different time points are shown in the side panel of figure 1(a).

3.2. Pressure-time history

The pressure-time history in the region where spall occurs is shown in figure 1 (b). Spall region here refers to the region where failure of the material takes place. It is different from other regions where only voids are created and material does not fail. It is seen in figure 1 (b) that spall of the material takes place at 160 kbar tensile pressure. No significant void nucleation is observed in the neighbouring regions where tensile pressure stays below 160 kbar. This validates the void nucleation threshold (160 kbar) obtained for crystal copper under triaxial strain conditions [2]. As soon as spall of the material takes place, pressure in the region rapidly drops to zero. The flat portion of the curve around zero beyond 40 pico-second (ps) is the signature of spall in the material.

Figure 1. (a) Free surface velocity of the target for an impact velocity of 1100 m/s (b) Pressure as a function of time in the spall region

4. Stochastic effect on the spallation process

To study the stochastic effect on the spallation process, we have performed following two exercises
• Impact at 1000 m/s without perturbing initial atomic coordinates
• Impact at 1000 m/s by perturbing initial atomic coordinates

4.1. Impact at 1000 m/s without perturbing initial atomic coordinates

4.1.1. Free surface velocity  The free surface velocity of the target as a function of time is shown in figure 2 (a). In figure 2 (a), it is seen that there is no pullback in the free surface velocity of the target corresponding to first traversal of the shock. Note that the pullback in the free surface velocity is the signature of the spall [7]. This means that there is no spall corresponding to first traversal of the shock. The pullback in the free surface velocity occurs corresponding to second traversal of the shock which is due to the creation of voids, not due to spall of the material. In this case, voids grow and coalesce leading to incipient spall like condition [7]. However, spallation does not occur as shown in the side panel of the figure 2 (a).

![Figure 2](image)

(a) Free surface velocity of the target for an impact velocity of 1000 m/s (b) Pressure as a function of time in the spall region

4.1.2. Pressure-time history  The pressure-time history in the region where voids nucleate is shown in figure 2 (b). It is seen that there is no void nucleation during the tension corresponding to first traversal of the shock. Void nucleation and growth occur during the tension created by second reverberation of the shock at lower value of tensile pressure. The tension created by first traversal of the shock creates many defects (dislocations, stacking faults, etc) in the material. These defects accumulate and become void nucleation sites for the tension created by second traversal of the shock leading to void nucleation at lower value of tensile pressure.

4.2. Impact at 1000 m/s by perturbing initial atomic coordinates

We perturb the initial x-coordinates of the atoms randomly between ± 0.001 Å. No perturbation is applied to the y and z coordinates.

4.2.1. Free surface velocity  The free surface velocity of the target for this case is shown in figure 3 (a). In figure 3 (a), there is no pullback in the free surface velocity of the target corresponding to first traversal of the shock. The pullback in the free surface velocity occurs after 80 ps due to nucleation and growth of the voids. In this case, growth and coalescence of the voids lead to the spall of the material. The compressive wave resulting from the stress...
relaxation due to spall of the material reverberates between the free surface and spall surface of the scab. The ringing in the free surface velocity after 90 ps (figure 3 (a)) corresponds to the reverberations of the trapped compressive wave. The snapshots at different time points in the free surface velocity are shown in the side panel of the figure 3 (a).

4.2.2. Pressure-time history The pressure as a function of time in the spall region is shown in figure 3 (b). No void nucleation occurs during the tension created by first traversal of the shock. However, various defects (partial dislocations, stacking faults, etc) are created. These defects become void nucleation sites for the tension corresponding to second traversal of the wave and hence lead to the nucleation and growth of voids at very low tensile pressure. This, in turn, results in spall. Therefore we see that, close to the spall threshold of the material, a small change in the atomic coordinates affects the spallation process of the material.

![Figure 3. (a) Free surface velocity of the target for an impact velocity of 1000 m/s (b) Pressure as a function of time in the spall region](image)

5. Conclusions
We have performed molecular dynamics simulations of high velocity impact of copper plates to validate the void nucleation threshold obtained under triaxial strain conditions and to study the stochastic effect on the spallation process. For the impact of copper plates at 1100 m/s impact velocity, the spall of the material takes place at 160 kbar pressure. This validates the void nucleation threshold (160 kbar) obtained under triaxial strain conditions [2].

The stochastic effect on spallation process has been studied by performing impact of copper plates at 1000 m/s impact velocity. We find that a small change in the initial atomic coordinates affects the spallation process. This means that for impact velocities close to the spall threshold, spallation process is stochastic.

References
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