Molecular dynamics simulations of jet breakup and ejecta production from a grooved Cu surface under shock loading*

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Large-scale non-equilibrium molecular dynamics simulations are performed to explore the jet breakup and ejecta production of single crystal Cu with a triangular grooved surface defect under shock loading. The morphology of the jet breakup and ejecta formation is obtained where the ejecta clusters remain spherical after a long simulation time. The effects of shock strength as well as groove size on the steady size distribution of ejecta clusters are investigated. It is shown that the size distribution of ejecta exhibits a scaling power law independent of the simulated shock strengths and groove sizes. This distribution, which has been observed in many fragmentation processes, can be well described by percolation theory.

Keywords: molecular dynamics, ejection

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1. Introduction

Ejection is a kind of complex dynamic phenomenon that occurs when a shock wave interacts at a material/vacuum or material/gas interface accompanied by the emitting of a great amount of matter (ejecta). Extensive studies have been conducted on the phenomenon since the pioneering studies of Asay and co-workers in the 1970s,[1–3] and significant achievements have been gained. Previous research on the ejection of roughened surface has shown that the mass, size, and velocity of the ejecta vary depending closely on the surface status, the initial shock conditions, and the material properties of the sample.[4–9]

Based on a great number of experiments on metals with well characterized surface perturbations, several models have been proposed to quantify the total amount and maximum velocity of ejecta. Asay and Bertholf[3] found that the amount of ejecta can be approximated by an effective defect mass. However, this model does not capture such important factors that affect the ejection process as the vertax angle and the shock breakout pressure. Adopting the concepts of the nonlinear Richtmyer–Meshkov instability, Dimonte *et al.*[10] developed a simple algebraic model for melted materials that describes the amount and velocity of ejecta as a function of shock conditions, material properties, and surface perturbations. This model is able to describe the common features of the preceding experiments and models with a physical basis. Besides these macroscopic characterization of ejection, atomistic approaches based on molecular dynamics (MD) simulations also provide efficient tools to reveal the microscopic mechanism of ejection and serve as an important complement to the classical approaches.[11–18] Prior works on the atomic scale ejecta from Cu or Al crystals under shock loading with or without free surface defects confirm that the surface roughness is one of the determining factors in ejecta production. By employing a hybrid MD method, Durand and Soulard[19] investigated the jet breakup and ejecta formation of copper with a sinusoidal surface defect under shock loading upon a purely liquid phase on nanosecond timescale. They found that the size distribution of ejected particles exhibits a power law scaling that reflects a self-similar behavior. However, the influence of the shape of the surface perturbation and the shock intensity on the ejecta distribution still remains unexplored.

In this paper, we perform large-scale non-equilibrium MD simulations to explore the jet breakup and ejecta production of single crystal Cu with a triangular grooved surface defect under shock loading. The morphology of the jet breakup and the size distribution of the ejected particles are obtained. The variation of the ejecta distribution with shock strength as well as the size of the surface groove are discussed in detail.

2. Computational details

The simulation sample is a face-centered cubic single crystal Cu with a groove of depth h and vertex angle θ on the upside surface along the x direction, as shown in Fig. 1. The Cartesian x, y, and z axes correspond to the [100], [010], and [001] crystallographic directions, respectively. The dimensions of the model are fixed as 145 nm × 72 nm along the x, y directions, while it can be varied to be a little greater than the width of the groove $2h\tan(\theta/2)$ along the z direction. The tabulated embedded-atom-method (EAM) potential developed by Mishin *et al.*[20] is adopted to describe the atomic interaction between Cu atoms. This potential has been successfully

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used to study the dynamic responses of Cu for a very wide pressure range.[21–23]

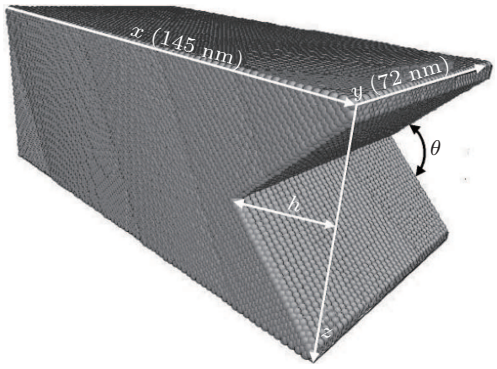


Fig. 1. Initial configuration of the single crystal Cu sample with a triangular surface groove.

Prior to shock wave loading, the system is equilibrated at 10 K and zero pressure with the constant-pressure-temperature (NPT) ensemble and three-dimensional (3D) periodic boundary conditions. Then, the microcanonical NVE ensemble is adopted in shock loading simulations, and periodic boundary conditions are applied only along the y and z axes. The shock wave is generated along the x axis using momentum mirror method where the target is thrown into a wall of infinite mass with a velocity $u_{\rm p}$ along the shock direction. Since ejection process only involves atoms near the surface region, the upside sample with a certain thickness in the fully release state can be separated from the system and the other part can be eliminated from the subsequent calculation. Consequently, we can get rid of the influence on the ejection from the wave reflected from the momentum mirror boundary and also reduce the computation cost.

In order to discern and quantify the size of the ejecta, a 3D grid of cubic cells is superimposed over the sample and clusters are identified as aggregates of atom-filled cells with distance smaller than a critical value. Moreover, the size distribution of the ejecta is studied by using a binning technique.[19,24] This technique groups the observed ejecta numbers into volume bins of a width that is equal to increasing powers of 2, so that large numbers of a few populated volume classes are clustered together.

3. Results and discussion

The typical pictures of jet breakup and ejecta formation are shown in Fig. 2 where the sample with surface groove of $h = 10$ nm and $\theta = 60^\circ$ is shocked with an impact velocity of $u_{\rm p} = 2.75$ km·s^{-1}. The interaction of the planar shock wave with the valley of the groove causes the generation of a sheet of jet that develops continuously in the (x,y) plane. As time increases, the jet begins to breakup, both in the x and y directions, while the tip of the jet maintains its shape for much longer times [Fig. 2(a)]. Subsequently, the degree of jet fragmentation increases and the tip of the jet starts to breakup [Figs. 2(b) and 2(c)]. Finally, the whole jet fragments into a series of spherical clusters due to the effects of surface tension [Fig. 2(d)]. Figure 2(e) shows the magnified atomic image of an isolated ejecta indicating a nearly perfect spherical liquid cluster structure.

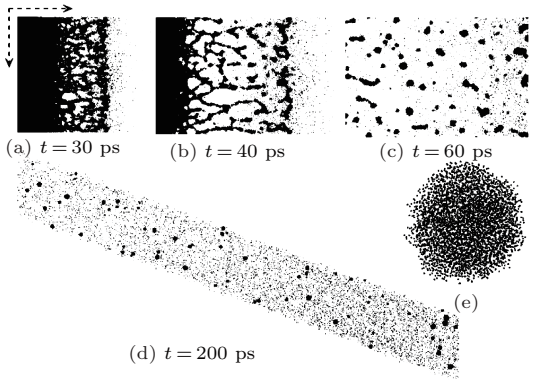


Fig. 2. Snapshots of the jet breakup and ejecta production for a shocked Cu with surface groove of $h = 10$ nm and $\theta = 60^\circ$, with $u_{\rm p} = 2.75$ km·s^{-1}. Panels (a)–(c) top view, and (d) oblique view.

Then cluster analysis method is used to discern and quantify the size of the ejecta. Figure 3 gives the analyzed result of the partial configuration of the ejecta that are shown in Fig. 2(d). We can see that this method identifies the ejecta clusters successfully, which enables us to obtain the detailed size information of the clusters.

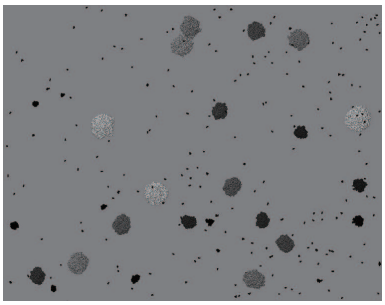


Fig. 3. Top view of the partial configuration of ejecta showing in Fig. 2(d) and the ejecta clusters are colored according to their volume.

The time evolutions of the ejecta size distributions as a function of their volume from the sample with surface groove of $h = 10$ nm and $\theta = 60^\circ$, shocked with $u_{\rm p} = 2.75$ km·s^{-1} are drawn in Fig. 4. We can seen from this figure that the ejecta distributions change gradually with the progression of fragmentation and reach nearly stable polydisperse distributions for times above 60 ps. For the steady distribution states, there are three distinct parts with two power law decays in the small and intermediate ejecta ranges and a rapid decrease in the large size limit. Since the volume of most of the ejecta in the first part is less than 100 Å^3, namely 10 atoms, this is attributed to the atomization of the surface (see the gray cloud in Fig. 2)

and is considered to be insignificant in the ejection process.[13] The rapid decrease part is interpreted as a finite size cutoff reflecting the finite dimension of the system. The intermediate power law range reflects the inherent distribution of the ejecta clusters[19] and will be focused on in the following discussion.

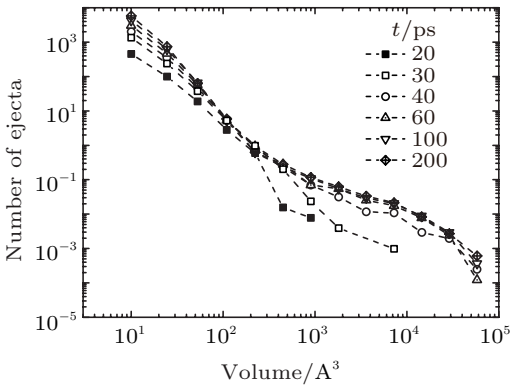


Fig. 4. Log–log volume distribution of the ejecta clusters at different times for Cu with $h = 10$ nm and $\theta = 60°$, shocked with $u_p = 2.75$ km·s^{-1}.

The above description of of jet breakup and ejecta formation of Cu with surface groove is basically similar to that of Cu with a sinusoidal surface studied by Durand *et al.*[19] and is universal for altered shock strengths and groove sizes explored below. It has been pointed out in a previous work that the mass of ejecta increases with the shock strength and could be significantly enhanced upon surface melting, but the effect of melting on the size distribution of ejecta remains unknown. Figure 5 shows the steady volume distribution of ejecta from the groove with fixed size of 5-nm depth and 60° vertex angle shocked with three representative strengths, $u_p = 2.0$, 2.75, and 3.5 km·s^{-1}, corresponding to solid, release melting, and shock-induced melting states of the sample, respectively.[25] It can be seen that the number N of ejecta clusters as a function of volume V can be described by a power law decay

$$N(V) \propto V^{-\kappa},$$

where $\kappa = 1.1 \pm 0.08$ for all the three shock strengths, independent of surface melting. The number of ejecta clusters increases correspondingly to the shock strengths demonstrating the enhancement of the total jet mass upon melting. Moreover, the scaling power law is in good agreement with the ejecta distribution from the sinusoidal surface defect where $\kappa = 1.15 \pm 0.03$ is given[19] and the experimental size distribution of debris generated by laser-induced shock waves in Cu target.[26]

Then, the variation of the size distribution of ejecta with the groove shape is investigated. The steady volume distributions of ejecta from the grooves with various depths and vertex angles shocked with $u_p = 2.75$ km·s^{-1} (release melting state) are illustrated in Fig. 6. Although the number of ejecta clusters differs, the scaling power law with the same exponent is observed once again for different grooves. Furthermore, for the two grooves with different depths and fixed vertex, the number of ejecta is nearly identical to each other in the small and intermediate ranges, but more ejecta clusters appear in the very large size limit range for the deeper groove, suggesting an increase of the total mass of ejecta. For the grooves with different vertex angles, an increase of ejecta number in the small and intermediate ranges for the smaller vertex is clearly exhibited, which reflects an enhanced fragmentation process due to the fact that the shock deposits more of its energy in the jet for the smaller vertex angle grooves, resulting in an enhanced driving force for the jet to breakup.[27]

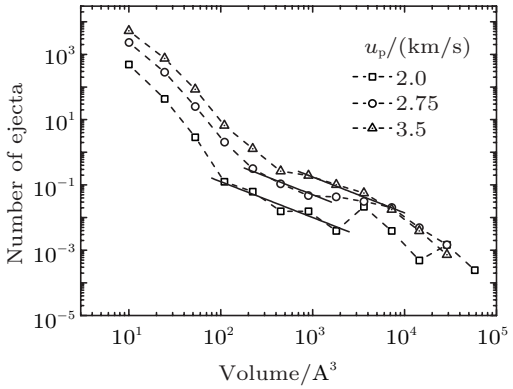


Fig. 5. The variation of size distribution of ejecta with shock intensities for Cu with $h = 5$ nm and $\theta = 90°$ at 200 ps after shock loading. The solid lines represent the power law functions fit with exponent of −1.1.

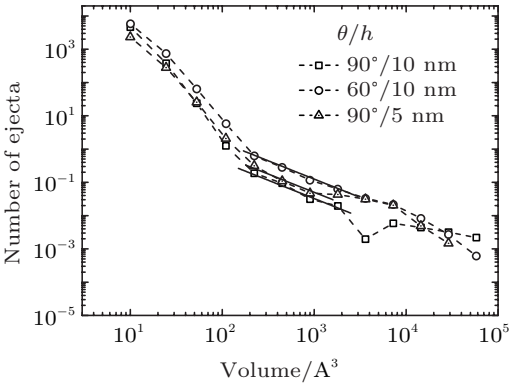


Fig. 6. The variation of size distribution of ejecta with groove depth h and vertex angle θ at 200 ps after shock loading with $u_p = 2.75$ km·s^{-1}. The solid lines represent the power law functions fit with exponent of −1.1.

Thus, we have obtained the size distributions of ejecta clusters from surface grooves with different sizes under various shock strengths. The scaling power law agrees well with the 2D percolation theory as pointed out by other authors.[5,13,14,19] The negligible influence of surface melting and groove size on the power law distribution demonstrates that the jet breakup is essentially a random 2D fragmentation process. In fact, for the simulated models in this paper, the

thickness of the jet along the z direction is too small compared with the other two directions, so the percolation develops following only two degrees of freedom in the (x,y) plane. However, the dimension of the breakup process would be changed if the thickness of the jet is non-negligible. Therefore, further simulations on much larger grooves need to be performed. Since material property is another crucial factor to the jet breakup and ejecta production, studies on other metals need also to be conducted.

4. Conclusion

In conclusion, the dynamic process of jet breakup and ejecta production of single crystal Cu with a triangular grooved surface defect under various shock strengths are investigated using MD simulations. For different shock strengths before and after surface melting, it is found that the steady size distributions of the ejecta clusters agree well with a scaling power law decay, which can be reproduced within the framework of 2D percolation theory, and the number of ejecta clusters increases with shock strengths. For different sizes of groove, the ejecta distributions also exhibit the scaling power law with the same exponent and the number of ejecta clusters increases for a groove with a smaller vertex angle, suggesting an enhanced breakup process prompted by the increased energy deposit in the jet from the shock waves. Although the groove size seems to have negligible influence on the ejecta distribution, models with much larger grooves need to be further studied to explore the scale effect on the jet breakup and ejecta production process.

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