Parallel Molecular Dynamics Simulations of Ejection from the Metal Cu and Al Under Shock Loading *

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Large-scale non-equilibrium molecular dynamics simulations are used to investigate the ejection of the metal under a shock loading. The present work focus on the dynamic process of ejection from the metal Cu and Al surface groove under shock loading, using parallel MD implementation and the Morse potential. The ejected mass coefficient and the size distribution of ejected particles (cluster for atoms) are investigated with changes of the half-angle or the depth of groove and shock strength.

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When a shock wave interacts with a metal sample at the surface, ejecta can be emitted from the surface. The mass, size, shape, and velocity of ejecta depend on the initial shock conditions and the material properties of the metal sample. The ejection of materials from shock surfaces has been experimentally and theoretically studied for many years, beginning in the modern era with the pioneering work of Asay and colleagues in the 1970s.[1] Prior works on roughened surfaces,[2−5] has demonstrated that the total ejected mass is approximately equal to the "detect" mass in the solid state and can be significantly enhanced upon surface melting. Measurements of particle size distributions exhibit a power-law scaling with exponents in agreement with two- or three-dimensional percolation theory for spall-dominated and jet-dominated breakup,[6,7] respectively. Large-scale non-equilibrium molecular dynamics (NEMD) simulations of metals subjected to high-strain rate loading (compression and/or shear) provide a unique insight into the fundamental mechanisms behind shock induced plasticity, phase transformations, tensile failure, and sliding friction.

We previously studied the fundamental mechanism of the dynamic process of ejection from the metal surface groove under a shock loading by using molecular dynamics (MD) simulations.[8] In this Letter, we present systematic microscopic investigations of the ejection mass dependence on shock strength and groove sizes by non-equilibrium parallel molecular dynamics simulations on the model of surface groove, which describes machined surfaces and surfaces scratches.

MD simulations would be large in two cases. Firstly, MD simulations usually require a large number of time steps and therefore should be as fast as possible. If we want to increase the speed of a simulation of given size, we should use processors as many as reasonable. Secondly, one often needs a large number of particles to compare with experimental data. Thus a new scalable parallel method has been implemented for large-scale MD simulations with seriously non-uniform particle distributions. In particular, based on cell-block date structures, this algorithm uses Hilbert space filling curve to convert high-dimensional domain decomposition for load distribution across processors into one-dimensional load balancing problems for which the measurement-based multilevel averaging weights (MAW) method can be applied successfully.[9] Numerical experimental results have shown that this new MD method based on the cell-block data structure is superior to the traditional link-cell method in rendering balanced load for large-scale multi-medium MD simulation in high temperature and high pressure physics. Excellent scalability has been demonstrated with a up-speed larger than 200 by 240 processors of one MPP, in simulating a metal micro-ejection system including about 10^8 particles distributed with non-uniform densities.[10]

Molecular dynamics simulation is a well-established technique in solids, especially for studying the proceeding of the dynamical evolution of metals under shock loading. Large-scale molecular dynamics simulations, integrating the classical equation of motion for millions of atoms over picosecond to nanosecond timescale, have been used to investigate funda-

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mental mechanisms of shock-induced plasticity[11,12] and polymorphic phase transformations,[13] among other phenomena. Germann and Holian's preliminary studies of ejecta indicate that the ejecta mass depends on shock strength and that for perfect *fcc* crystals shock loaded (below melting) in the ⟨100⟩ direction, atoms and small clusters of atoms are primarily ejected at trijunction.[14] Moreover, the amount of the ejected material can be significantly increased at surface heterogeneities, such as machining grooves.[15] To simulate the roughness of the metal surface and shock strength influence on the ejection, we assign the model structures as the same as Ref. [8]. A wave is generated by colliding a flying slice of atomic copper with a target of atomic copper on the surface ⟨100⟩. Mirror reflection boundary conditions are imposed perpendicular to the impact velocity. The initial velocity u_f of the flying slice was varied from 1 to 6 km/s. The systems of simulation are summed up to 422455 and 382113 atoms for Cu and Al, respectively. The system is then allowed to evolve in time by solving the classical equations of motion using a specified time step τ. We took a time step $\tau = 1$ fs. The peak pressure was calculated by using the particle velocity u_p behind the wave surface and the velocity u_s of the shock wave propagating in the material.

The interaction $V(r_{ij})$ of two atoms i and j separated by a distance r_{ij} uses the Morse potential

$$V(r_{ij}) = D[e^{-2\alpha(r_{ij}-r_0)} - 2e^{-\alpha(r_{ij}-r_0)}], \qquad (1)$$

where α and D are the constants with dimensions of reciprocal distance and energy, respectively, and r_0 is the equilibrium distance between two nearest-neighbouring atoms. Morse potential constants for the cubic metal Cu and Al are listed in Table 1. The Morse potential of the cubic metal can be applied to problems involving any kind of a lattice deformation, that is, either homogeneous expansion or contraction, or shear deformation.

Table 1. Morse potential parameters of the cubic metal Cu and Al used in the present work.[16]

Metal	α (Å^{-1})	r_0 (Å)	D (eV)
Cu	1.3588	2.866	0.3429
Al	1.1646	3.253	0.2703

To study the regularity of the ejected mass dependence on shock strength and groove sizes (including the half-angle and depth of groove), the ejected mass coefficient α is defined as

$$\alpha = \frac{m}{\rho V_0} = \frac{m}{M} = \frac{N_E}{N_g}, \qquad (2)$$

where N_E and N_g are the ejected particle number from the groove and the total particle number of groove.

The evolution of the ratio N_E/N_g with a half-angle of groove 30° and depth 320Å depending on the simulated time in different impact velocity u_f is given in Figs. 1 and 2 for metal Cu and Al, respectively. We note that the ejected mass coefficient α $(= N_E/N_g)$ is approached the saturation value (~ 1) in different impact velocities above the critical shock strength at which ejection occurs.[4] The time of the arrived saturation value is become shorter with increasing impact velocity (or shock strength), and the particles of ejection is significantly enhanced upon surface melting (shock melting, e.g., in Al and Cu impact velocity is above 6.0 km/s). It is indicated that the total ejected mass is approximately equal to the groove mass in the metal Cu and Al, above the melting region the ejected mass can be largely enhanced, but is not increased up to several orders of magnitude.

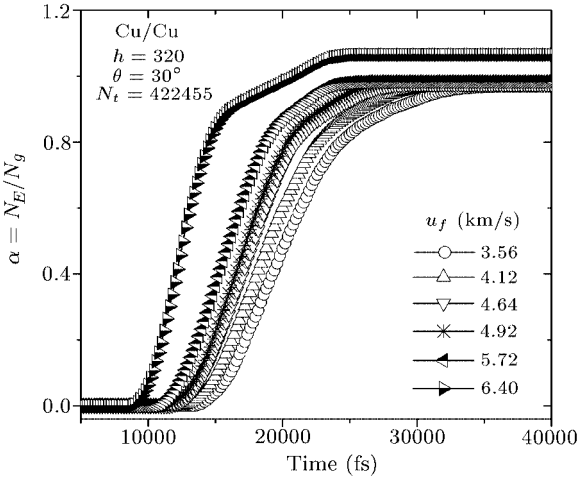

Fig. 1. The evolution of the ejected mass coefficient α $(= N_E/N_g)$ depending on simulated time in different impact velocities for metal Cu.

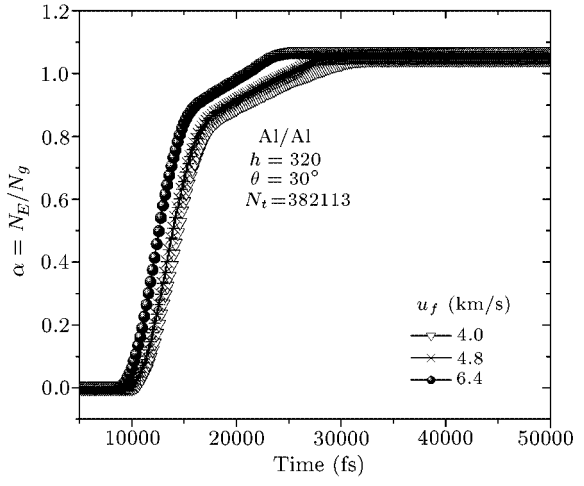

Fig. 2. Evolution of the ejected mass coefficient α $(= N_E/N_g)$ depending on simulated time in different impact velocities for metal Al.

In order to investigate the effect of ejection dependence on the half angle of groove with depth 320 Å,

we observed the evolution of the ejected mass coefficient $\alpha = N_E/N_g$ in the constant impact velocity $u_f = 4.0\,\mathrm{km/s}$ (i.e., at constant shock strength). The ratio N_E/N_g of the particles of ejection from the grooves with the half-angle dependence on simulated time for metal Al is shown in Fig. 3. Note that the ejected mass coefficient decreases with the increasing half-angle of groove and it has significantly decreased when the half-angle of groove is equal to 60° or more.

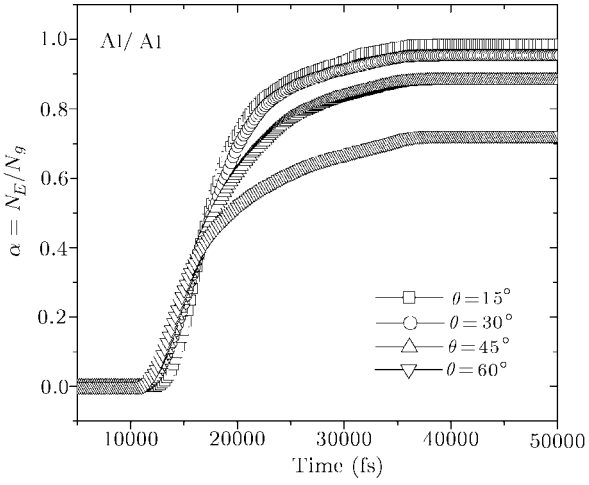

Fig. 3. Evolution of the ejected mass coefficient α (= N_E/N_g) at constant shock strength in different half-angles of groove for metal Al.

The evolution of the ejected mass coefficient depending on the simulated time in impact velocity 4.64 km/s and the half-angle of groove 30° with different depth h for metal Cu is given in Fig. 4. Note that the ejected mass coefficient α decreases with the increasing groove depth.

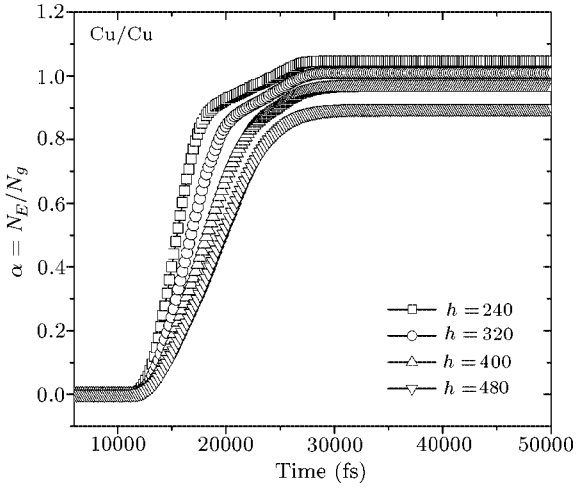

Fig. 4. Evolution of the ejected mass coefficient N_E/N_g depending on the simulated time at constant impact velocity in different groove depths for metal Cu.

To monitor the evolution of ejected particles from the groove with 30° half-angles and 320 Å depths in impact velocity 4.92 km/s for Cu and in impact velocity 4.8 km/s for Al, respectively. The size distribution of ejected particles (clusters of atoms) for these particular snapshots are analysed using the cluster multiple labelling technique[17,18] based on the equilibrium distance r_0 of approach of the two atoms are shown in Figs. 5 and 6, respectively. We find that the ejected cloud for this snapshot consists of 2116 atoms in 983 clusters for Cu and of 1263 atoms in 416 clusters for Al. In order to analyse the size of ejected particles, all the data were fitted to the $N^{-1.94}$ power-law distribution for Cu, or the $d^{5.82}$ relation to particle diameter. Ignoring the largest four clusters ($N > 40$ atoms), the remaining data closely fits the $N^{-1.57}$ power-law distribution for Al, or the $d^{4.71}$ relation to particle diameter. The size distribution of the ejected particles, moving ahead of the free surface, fit well to a power

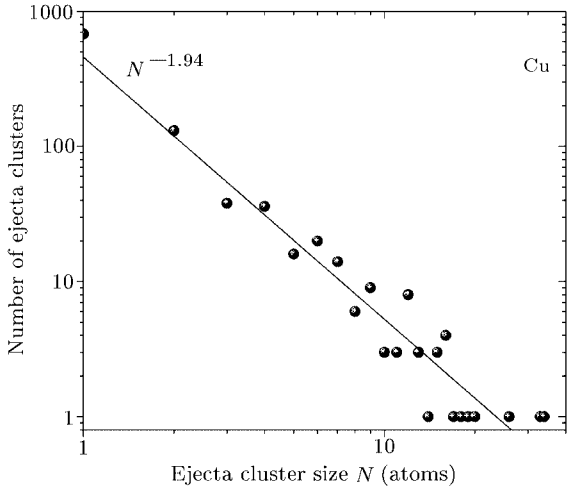

Fig. 5. Ejecta particle size distribution 24 ps after shock loading of a Cu ⟨100⟩ perfect crystal with $u_f = 4.92\,\mathrm{km/s}$. The solid line represents a fit to clusters.

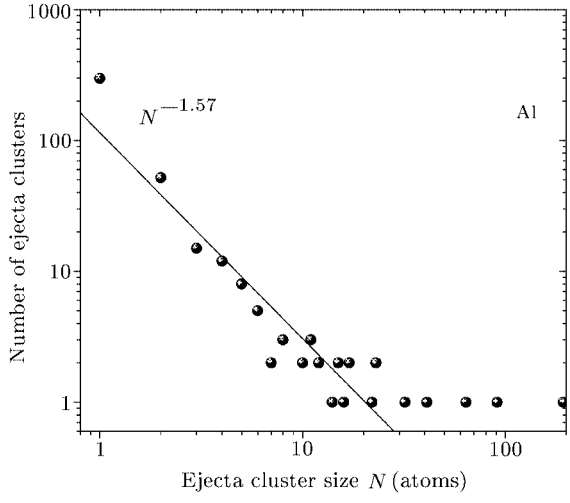

Fig. 6. Ejecta particle size distribution 22 ps after shock loading of an Al ⟨100⟩ perfect crystal with $u_f = 4.8\,\mathrm{km/s}$. The solid line represents a fit to $N < 40$ clusters.

scaling law $N(r) \sim r^b$, where b is constant, which is dependent on the material. This type of the scaling law is found in percolation theories.[19] Many phenomena in nature involve fragmentation from very large (planets) to very small (nuclei) scale system. A model that has been used successfully to describe the fragment size distribution is based on percolation theory. For example, fragmentation of heavy nuclei resulting from high-energy nucleus-nucleus interactions are described well using this theory. Percolation theory predicts simple power laws. The resulting micro jets can fragment into particle cluster. Then it will be described well using this theory.

The dynamic process of ejection from the metal Cu and Al surface groove under a shock wave has been studied by using large-scale non-equilibrium parallel molecular dynamics simulations. It is found that the ejected mass coefficient is decreased with the increasing half-angle or the depth of groove, and its maximum is approximately equal to 1 below the melting temperature and above the critical shock strength. The ejected mass coefficient is significantly decreased when the groove half-angle is approximately 60° or more, and above the melting region the ejected mass coefficient is largely enhanced but is not increased by several orders of magnitude. The size distribution of ejected particles (cluster for atoms) has a power-law form (i.e. $N^{-1.94}$ for Cu and $N^{-1.57}$ for Al), it is in agreement with the characteristic of percolation theory. The present results indicate that the surface roughness is the determinative factor in Cu and Al ejecta production. The implication of these results is being further studied.

References

[1] Asay J R, Mix L P and Perry F P 1976 *Appl. Phys. Lett.* **29** 284

[2] Asay J R 1976 *Material Ejection from Shock-Loaded Free Surface of Aluminum and Lead* (Sandia Report) SAND76-0542

[3] Asay J R and Bertholf L D 1978 *A Model for Estimating the Effects of Surface Roughness on Mass Ejection from Shocked Materials* (Sandia Report) SAND78-1256

[4] Holian B L, Germann T C, Maillet J B and White C T 2002 *Phys. Rev. Lett.* **89** 285501

[5] Dai L H, Yan M and Shen L T 2004 *Chin. Phys. Lett.* **20** 921

[6] Werdiger M, Arad B and Hens Z 1996 *Laser Particle Beams* **14** 133

[7] Sorenson D S, Minich R W, Romero J L, Tunnell T W and Malone R M 2002 *J. Appl. Phys.* **92** 5830

[8] Chen J, Jing F Q, Zhang J L and Chen D Q 2002 *J. Phys: Condens. Matter* **14** 10833

[9] Cao X L and Mo Z Y 2004 A new scalable parallel method for molecular dynamics based on cell-block data structure: parallel and distributed processing and applications *ISPA'2004* (Berlin: Springer) LNCS 3358, p 757

[10] Cao X L, Mo Z Y, Zhang J L and Chen Q F 2004 *Chin. J. Comput. Phys.* **21** 377

[11] Holian B L and Lomdahl P S 1998 *Science* **280** 2085

[12] German T C, Holian B L, Lomdahl P S and Ravelo R 2000 *Phys. Rev. Lett.* **84** 5351

[13] Kadau K, German T C, Lomdahl P S and Holian B L 2002 *Science* **296** 1681

[14] Germann T C, Hammerberg J E and Holian B L 2004 *AIP Conf. Proc.* **706** 285

[15] Holoian B L et al 2002 *AIP Conf. Proc.* **505** 35

[16] Girifalco L A and Weizer V G 1957 *Phys. Rev.* **114** 687

[17] Hoshen J and Kopelman R 1976 *Phys. Rev.* B **14** 3438

[18] Hoshen J, Berry M W and Minser K S 1997 *Phys. Rev.* E **56** 1455

[19] Stauffer D 1985 *Introduction to Percolation Theory* (London: Taylor and Francis)