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Dynamics simulation of ejection of metal under a shock wave

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Abstract

In this paper, the dynamic process of ejection from a metal surface groove under a shock wave is investigated by molecular dynamics simulation combined with a hybrid tight-binding-like potential. By taking 'snapshots' and analysing the pressure, we classify reflection rarefaction waves and second-uploading compression waves propagating in the material, and find one negative-pressure region and one high-pressure region induced by two wave series. The velocities of both the ejected atom and the free surface of the groove increase with the angle of the groove. When the half-angle of the groove is more than 60°, there is no ejected body, and this result is consistent with experiment.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Metal under shock-loaded conduction can exhibit complex phenomena depending on the varying properties of the material and initial shock conduction. In particular, if a metal target is shocked, target material can be emitted from the surface as the shock interacts at the surface; this is called ejection. In the last two decades, the dynamics of ejection has attracted the attention of both experimental and theoretical physicists [1–10]. One aspect concerns the stability of the surface during dynamic loading. Another aspect relates to the inertial confinement fusion (ICF) driven by a laser. To understand these phenomena, many experimental techniques such as holography and visible 'shadowgraphy' have been developed [6–8]. But there are few papers on theoretical studies.

The defects on the surface leading to ejection are usually in the form of pits, scratches or machine marks [9]. In this paper, we present systematic microscopic investigations of the ejection process by molecular dynamics (MD) simulations on the model of a surface groove, which describes machined surfaces and surfaces with scratches. A hybrid potential [11, 12] combing the Molière potential with a tight-binding (TB) potential [13, 14], which includes the many-body effects and can reproduce satisfactorily many bulk and surface properties of pure Cu metal, is used to describe the interactions among copper atoms.

This paper is organized as follows. In section 2, the method of numerical computation is discussed and the calculated model is specified. The results of the calculations are discussed in detail in section 3 and brief conclusions are given in section 4.

2. Basic theory

2.1. Interaction potential

The many-body atomic interactions use a hybrid potential [11, 12] combing the Molière potential with a TB potential. The potential energy of atom i in the hybrid potential contains two components, written as E_b^i and E_b^i, respectively, where E_b^i is an attractive energy, which is the same as that in the TB potential, i.e.,

$$E_b^i = -\left[\sum_{j\neq i} \xi^2 \exp(-2q(r_{ij}/d_0 - 1))\right]^{1/2}. \tag{1}$$

However, the repulsive pair potential E_r^i is a combination of the repulsive part in the TB potential with the Molière potential given as follows:

$$E_r^i = \sum_{j\neq i} V_r(r_{ij}). \tag{2}$$

And

$$V_r(r) = \begin{cases} A\exp[-p(r/d_0 - 1)] & r \geqslant r_1 \\ A_0 + A_1 r + A_2 r^2 + A_3 r^3 & r_1 \succ r \succ r_2 \\ B_m(0.35\mathrm{e}^{-0.35r/a_f} + 0.55\mathrm{e}^{-1.2r/a_f} + 0.10\mathrm{e}^{-6.0r/a_f})/r & r \leqslant r_2 \end{cases} \tag{3}$$

where r_{ij} is the distance between the atom i and atom j and d_0 is the nearest-neighbour distance. The parameters in the hybrid potential are obtained from fitting the body modulus and coherence energy.

2.2. Calculated model

The lattice constant of face-centred cubic Cu is 3.44 Å. For calculations on the problem in two dimensions, the crystal surface Cu(001) is chosen. In the present work a shock 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 shock direction. The initial velocity U_p of the flying slice was varied from 1 to 8 km s^{-1}. We sum over 500 000 atoms or so in the model. The model structure is shown in figure 1. It is big enough for studying the ejection process. The time step t is chosen as 0.001 ps.

3. Results and discussion

First of all, we calculated the ionic velocity $\vec{u}$ behind the wave surface and the velocity $\vec{D}$ of the shock wave propagating in Cu. $\vec{D}$, $\vec{u}$ satisfy a linear relationship. And the fitting parameter λ is 1.45, which is in agreement with the experimental value 1.5 [16]. This supports the rationality of our potential and calculated model.

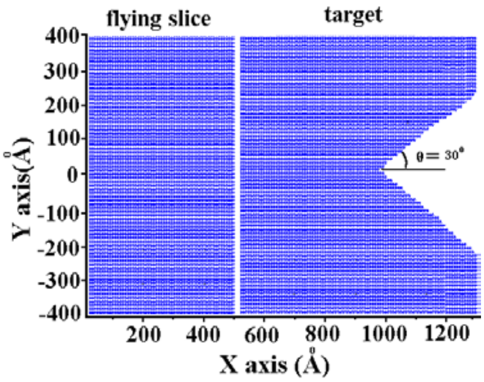

Figure 1. The initial calculated model 1, $\theta = 30°$ (θ is the half-angle of the groove).

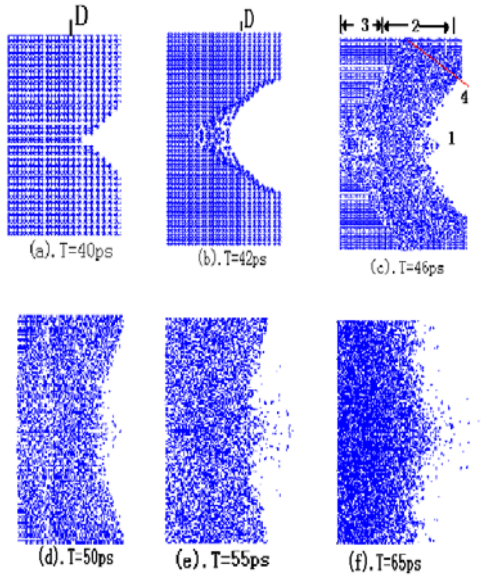

Figure 2. A snapshot of the location of target atom for model 1 with a groove half-angle equal to 30°; only atoms within 150 Å of the top of the groove are included in the figures. *D* represents the wave surface.

To explain the ejection from a groove surface, the observed process of ejection when a half-angle of groove equal to 30° is shown in figure 2. For clarity, only atoms within 150 Å distance with the top of the groove are included in those figures. The flying slice pumps on the target, and the shock wave forms and propagates in the target and flying slice. It is seen in figure 2(a) that shock wave surface arrives at the groove top at about 40.0 ps. Then, in figure 2(b) (at $t = 42.0$ ps), the groove free surface begins to move toward region 1; simultaneously the reflection rarefaction wave propagates in the metal. Because of the time difference of the shock wave reflecting on the groove free surface, the rarefaction wave pattern looks the same as that of the groove. At about 46.0 ps (figure 2(c)), in the front of moving free surface, some atoms move at higher velocity than the groove free surface. It should be specifically mentioned that metal can evidently be divided into two different regions. In region 3, there is one atom-sparse region. It will turn out that it is a negative-pressure region, from the following pressure analysis. Region 2, the nearest neighbour of the sparse region, is an atom-dense region. This shows that, behind a rarefaction wave there propagates a compression wave whose wave angle is nearly perpendicular to the groove surface. We call it the second-uploading wave. At about 50.0 ps (figure 2(d)), the dissociation of the ejected atom from the free surface becomes

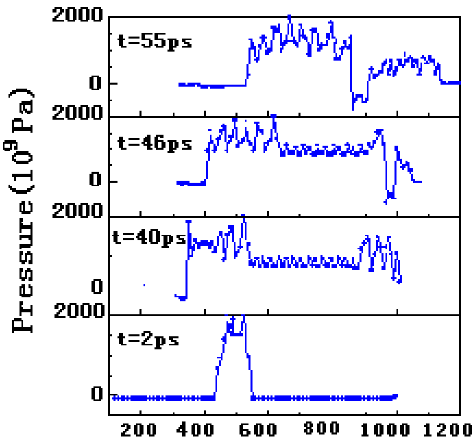

Figure 3. The pressure versus position r for the calculation box along the line $Y = 0$ at different times for model 1.

pronounced. Subsequently, the ejected body continues to dissociate from the free surface in region 1 (figures 2(e), (f)), but the number of ejected atom is not added. In general, the whole process can be divided into four phases:

(a) shock wave uploading and propagating into the target and flying slice,
(b) the groove free surface moving out and the rarefaction wave forming,
(c) jetting and the second-uploading compression wave forming,
(d) the ejected body forming and dissociating from the free surface.

In order to investigate the effect induced by ejection, the pressure $P(r)$ of a small box region along line $Y = 0$ is calculated; the area of box is 26 Å × 26 Å, and $P(r)$ is defined as [17]

$$P(r)v = P_T(r)v + P_E(r)v = Nk_BT + \frac{1}{2}\left\langle \sum_{i=1}^{N} \vec{r}_i \cdot \vec{F}_i \right\rangle$$

where r is the centre position of the calculated box, N the number of particles in the chosen region, k_B the Boltzmann constant, $\vec{r}_i$ the distance between atom i and the centre position of box, $\vec{F}$ the total force acting on atom i. Because the negative and positive pressure are not shown in the same isobar graph, we show pressure versus position r of the box at different times; see figure 3. At $t = 2.0$ ps, one high-pressure part at $r = 500$ Å shows that the shock wave forms and propagates into the flying slice and target. At $t = 40.0$ ps, the width of the high-pressure part is added to $r = 1000$ Å, and the shock wave arrives at the top of the groove. At $t = 46.0$ ps, negative-pressure part is nearly at $r = 980$ Å. The negative-pressure region is due to time difference for the shock wave reflecting on the groove free surface. Propagating rarefaction wave will induce lateral stress. Under lateral stress, atoms will move laterally, and form negative-pressure regions. The nearest neighbour of the negative-pressure part is a high-pressure part at $r > 1000$ Å. It contributes to the compression wave. At $t = 55.0$ ps, the negative-pressure region arrives at $r = 870$ Å. The existence of a negative-pressure region shows that ejection probably produces micro-damage in material.

We also study the effect on the groove of different half-angles. There is no ejected body when the half-angle is more than 60°.

The velocities of the ejected body and groove free surface are two important parameters. We study the dependence of the two velocities on the different groove models and initial shock waves. The calculated results show that the average velocities of the ejected atom and free surface increase with the groove half-angle and the initial velocity of flying slice. This conclusion also accords with other theoretical results [9].

4. Summary

In this paper, we study the surface ejection of metal Cu under a shock wave. The mainly conclusion is as follows. After ejection, two different wave series propagate in metal: one is the reflection rarefaction wave; the other is the compression wave inducing by jetting. Because of the time difference for the shock wave reflecting on the groove surface, the rarefaction wave produces a negative-pressure region in the metal. And a second-uploading compression wave induces a high-pressure region. Meanwhile, we find that the velocity of ejection and that of the groove free surface increase with the half-angle of the groove. When the half-angle of the groove is more than 60°, the ejection does not occur. In general, MD simulation is a good tool for study the interaction between a shock wave and a surface, and we have used it to provide insight into the process of ejection.

References

[1] Asay J R, Perry F C and Mix L P 1976 *Appl. Phys. Lett.* **29** 284
[2] Barness J K *et al* 1974 *J. Appl. Phys.* **45** 727
[3] Borodulin S A *et al* 1976 *Sov. Phys.–Solid State* **18** 1644
Meyer K A and Blewett P J 1972 *Phys. Fluids* **15** 753
[4] Walsh J M, Shreffler R G and Willing F 1953 *J. Appl. Phys.* **651** 24, 349
[5] Warnes R H 1979 *Bull. Am. Phys. Soc.* **24** 720
[6] Freeman J R *et al* 1977 *Nucl. Fusion* **17** 223
[7] Perry F C and Mix L P 1974 *Appl. Phys. Lett.* **24** 624
[8] Elias P 1986 *Shock Waves in Condensed Matter-1985* ed Y M Gupta (New York: Plenum)
[9] Asay J R 1976 SAND 76-0542
Asay J R 1978 SAND 78-1256
[10] Sorenson D S *et al* 1997 CONF-9706119
[11] Lee Rongwu and Pan Zhengying 1996 *Phys. Rev.* B **53** 4156–61
[12] Yue Y, Ho Y K and Pan Z Y 1998 *Phys. Rev.* B **57** 6685–8
[13] Rosato V, Guillope M and Legrand B 1989 *Phil. Mag.* A **59** 321
[14] Loisel B, Gorse D and Pontikis V 1989 *Surf. Sci.* **221** 365
[15] Wang Jihai and Zhang Jing-Lin 1989 *Chin. J. Comput. Phys.* **6** 53
[16] Duvall G E and Fowles G R 1963 *High Pressure Physics and Chemistry* vol 2, ed Bradley (New York: Academic)
[17] Haile J M 1992 *Molecular Dynamics Simulation* (New York: Wiley)