Hypervelocity Impact of the Icy Droplet on Al Shell at Nanoscale: A Molecular Dynamics Probe

YUAN Quan-zi, ZHAO Ya-pu*

(State Key Laboratory of Nonlinear Mechanics, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China)

Abstract: Large-scale molecular dynamics (MD) simulations are conducted to investigate the hypervelocity impact of the icy droplet on spacecraft Al shell at the atomic level. The velocity of the droplet is set to move at a typical cosmic speed. Part of the kinetic energy of the droplet is converted to thermal energy, resulting in a sudden increase of the temperature. With the increase of the droplet speed, the aluminum plate experiences elastic, plastic deformation, melting and finally be penetrated by the droplet. The formation and dynamic behavior of a debris cloud is observed and investigated in the simulations.

Key words: hypervelocity impact; molecular dynamics; debris cloud; icy droplet

CLC number: O341 **Document code:** A **Article ID:** 1001-5132（2012）01-0094-04

1 Introduction

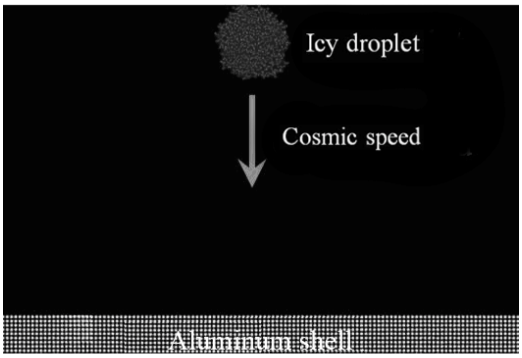
With the fast development of space technology and the increase of human's space activities, the quantity of space debris increases significantly in the last decade. According to the statistics from NASA[1], the approximately estimated population of particles is 19 000 larger than 10 cm; 500 000 between 1 cm and 10 cm; and exceeds 10 000 000 smaller than 1 cm. Owing to their hypervelocity, these space debris would make great threat to the orbit spacecraft. Even the collision of a tiny icy droplet at cosmic speed would result in serious damage on the huge spacecraft. In order to ensure the safety of the spacecraft from the hypervelocity impact, the detailed investigation of the impact and optimization of the structure are necessary[2].

The hypervelocity impact experiments for icy droplet with spacecraft are still extremely difficult to realize till now even in laboratory. So numerical simulations can be complementary powerful tools to explore the extreme conditions as in the hypervelocity impact. The structural dynamic plastic response is controlled by the response number[3]: $Rn \sim (\rho v^2/\sigma_M)(L/l)^2$, where ρ, v and σ_M represent density of the droplet, velocity of the droplet and yield strength of the metal plate, respectively. Here, L and l represent diameter of the droplet and the thickness of the metal shell, respectively. $L \sim l$, which makes the problem independent of the length scale. When space debris impacts on the metal plate, the debris would be compressed adiabatically, and liquefied or even vaporized instantly[4], while the metal plate experiences elastic, plastic deformation and rupture finally[5].

2 Results and discussions

In this article, we investigated from the atomic level the hypervelocity impact of the icy droplet with

Received date: 2011−10−30. JOURNAL OF NINGBO UNIVERSITY (NSEE): http://3xb.nbu.edu.cn
Foundation items: Supported by the National Natural Science Foundation of China (11032001, 11011120245) and by Russian Foundation for Basic Research (11-01-91217).
The first author: YUAN Quan-zi (1983−), male, Beijing, doctor, research domain: solid mechanics. E-mail: yuanquanzi@lnm.imech.ac.cn
Corresponding author: ZHAO Ya-pu (1963−), male, Beijing, doctor/professor, research domain: impact dynamics, physical mechanics. E-mail: yzhao@imech.ac.cn

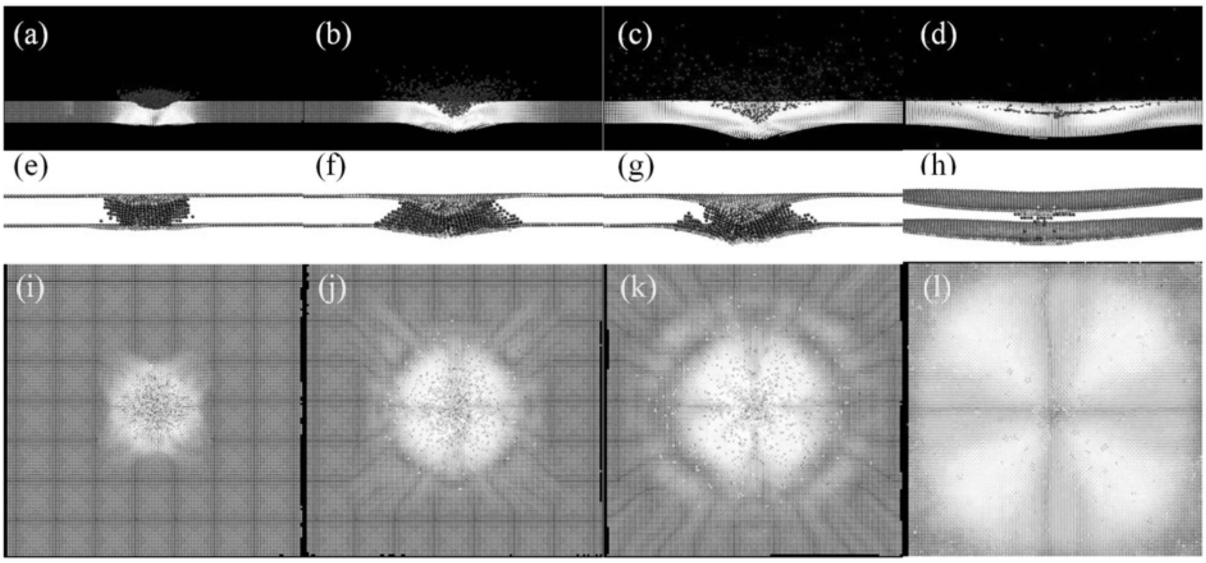


The gray and white balls represent the water molecules and the Al atoms, respectively

Fig. 1　Illustration of the MD simulation domain

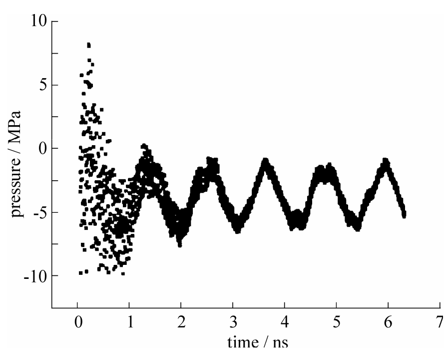
spacecraft Aluminum (Al) shell at nanoscale using molecular dynamics (MD) simulations accomplished in LAMMPS[6]. The simulation domain is illustrated in Fig. 1. The thickness of the Al shell is 2.03 nm. Since the shock-induced yield strength of Al is about 125－150 GPa[7], the corresponding perforation velocity $v \sim \sqrt{\sigma_M / \rho}$ is at the order of 10 km·s^{-1}. Hence, the velocity of the icy droplet (~3.5 nm in diameter) was selected to be typical cosmic speed, i.e., 7.9 km·s^{-1}, 11.2 km·s^{-1} and 16.7 km·s^{-1}, which is a usual speed of space debris.

Fig. 2 illustrate the process of the icy droplet impacting the Al shell at the 1st cosmic speed. Since the kinetic energy of the droplet is less than the yield strength of the shell, the droplet did not perforate the shell. The plastic region accumulated and then released into the Al surface due to the dislocation starvation of



(a)－(d) side view of the impact; gray and white balls represent water molecules and Al atoms, respectively; (e)－(h) the development of the plastic region; (i)－(l) top view of the wave propagation in the Al shell

Fig. 2　The icy droplet impacts the Al shell at the 1st cosmic speed



1st cosmic velocity

Fig. 3　The evolution of the pressure with respect to time

the nano shell (Fig. 2 (e)-(h)). The impact energy spreads in the form of wave. The wave velocity in our MD simulations is about 3.15 km·s^{-1}, which is in accordant with the average theoretical value ~3.20 km·s^{-1}. The impact made the shell vibrate with a period of 2 ns (Fig. 3). Because the impact velocity is much higher than the speed of sound in the Al shell, the shock wave energy accumulated and exerted a tensile force on

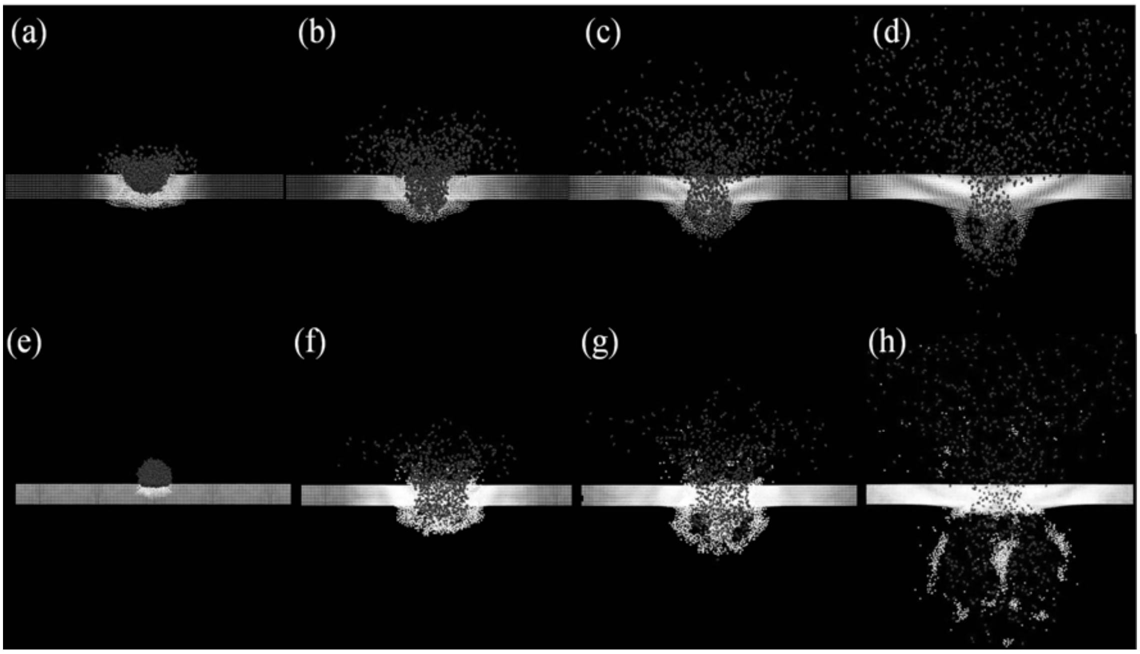


Fig. 4 The icy droplet impacts the Al shell (a)—(d) at the 2nd cosmic speed; and (e)—(h) at the 3rd cosmic speed

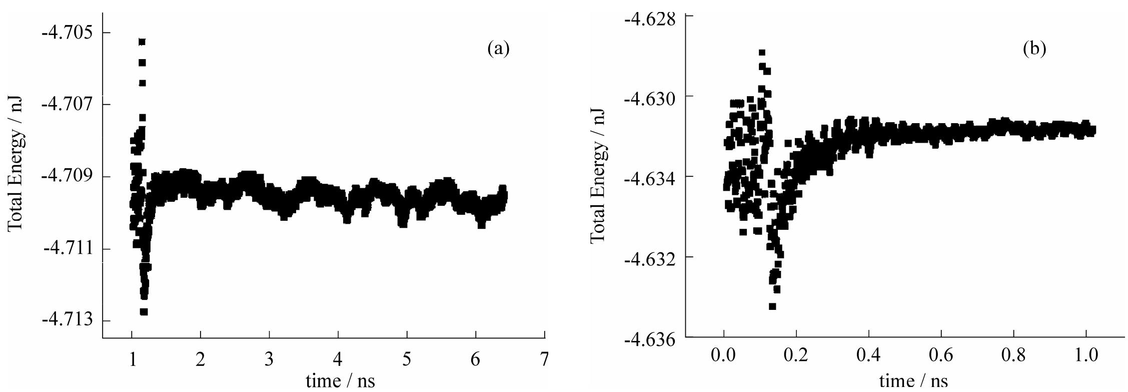


Fig. 5 Total energy with respect to time (a) 1st cosmic speed; (b) 2nd cosmic speed

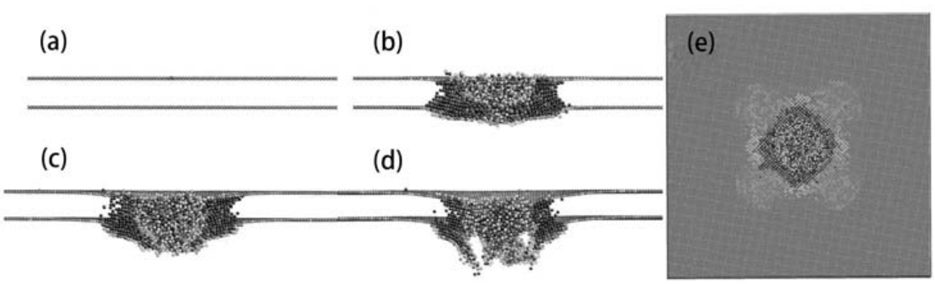


Fig. 6 The development of the plastic region (2nd cosmic speed)

the below surface of the Al shell.

3 Conclusions

In conclusion, we performed the MD simulations to investigate the hypervelocity impact of the icy droplet with spacecraft Al shell at the atomic level. The kinetic energy of the droplet and the yield strength of the shell competed in the dynamic process of hypervelocity impact. The droplet did not perforate the shell at 1st cosmic speed. Most of the plastic deformation was released from the solid surface. The Al shell vibrated almost elastically with a period of about 2 ns. The droplet perforated the shell at 2nd and 3rd cosmic speed (Fig. 4). Part of the deformation would be released in about 0.3 ns (Fig. 5). The plastic region propagated and finally the plate was ruptured (Fig. 6). Accompany with the perforation, a debris cloud would form with its diameter dependant on the impact speed.

We hope our large-scale MD simulation results may help in further understanding the dynamics and mechanisms in the hypervelocity impact for spacecraft.

References:

[1] NASA. Hypervelocity impact technology[EB/OL]. [2011-11-23]. www. nasa. gov.

[2] Yuan J, Qu G, Sun Z, et al. Optimization methodology for shield structure against space debris[J]. Journal of Astronautics 2, 2007, 28(2):243-248.

[3] Zhao Y P. Suggestion of a new dimensionless number for dynamic plastic response of beams and plates[J]. Archive of Applied Mechanics, 1998, 68(7):524-538.

[4] Engel O G. Crater depth in fluid impacts[J]. Journal of Applied Physics, 1966, 37(4):1798-1808.

[5] Yu T X, Zhang L. Plastic bending: Theory and applications[M]. Singapore: World Scientific Pub Co Inc, 1966.

[6] Plimpton S. Fast parallel algorithms for short-range molecular-dynamics[J]. Journal of Computational Physics, 1995, 117(1):1-19.

[7] McQueen R, Fritz J, Morris C. Shock waves in condensed matter-1983[M]. Amsterdam: North Holland Physics Publishing, 1984.

冰滴在宇宙速度下与航天铝壳结构超高速撞击的分子动力学模拟

袁泉子, 赵亚溥*

(中国科学院力学研究所 非线性力学国家重点实验室, 北京 100190)

摘要: 采用大规模分子动力学模拟, 从原子层次探索了冰滴高速撞击航天铝壳结构的动态过程. 冰滴的速度设置为典型的宇宙速度. 在高速撞击时, 部分动能转化为热能, 使得撞击点附近迅速升温. 随着撞击速度的提高, 铝壳经历了弹性变形、塑性变形、冲击融化，最后被穿透的过程. 在分子动力学模拟中, 清楚地观测了碎片云的形成和动态行为.

关键词: 超高速撞击; 分子动力学模拟; 碎片云; 冰滴

(责任编辑　史小丽)