International Journal of Mechanical Sciences 86 (2014) 54–59

Contents lists available at ScienceDirect

International Journal of Mechanical Sciences

journal homepage: www.elsevier.com/locate/ijmecsci

Molecular dynamics simulation on plasma phase transition of aluminum single crystal under extreme conditions

Yuanyuan Ju [a], Qingming Zhang [a,*], Fenglei Huang [a], Zizheng Gong [b], Guangfu Ji [c]

[a] State Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology, Beijing 100081, China
[b] National Key Laboratory of Science and Technology on Reliability and Environment Engineering, Beijing Institute of Spacecraft Environment Engineering, Beijing 100094, China
[c] Laboratory for Shock Wave and Detonation Physics Research, Institute of Fluid Physics, China Academy of Engineering Physics, Mianyang 621900, China

ARTICLE INFO

Article history:
Received 22 January 2014
Received in revised form
21 February 2014
Accepted 27 February 2014
Available online 19 March 2014

Keywords:
Hypervelocity impact
Electron force field
Effective core pseudo-potential
Plasma phase transition
Molecular dynamics

ABSTRACT

The electron force field is a new molecular dynamics method which combines the quantum mechanics and the classical molecular dynamics and has the ability of computing systems with electrons explicitly over multi-picoseconds time scales and 10^4 atoms space scales. The effective core pseudo-potential method is introduced in order to overcome the problem that the electron force field is only suitable for the system containing s electrons while is incapable to solve the system including p and d electrons. The plasma phase transition of aluminum single crystal under static extreme conditions and hypervelocity impact is investigated by exploring the electric force field in conjunction with the effective core pseudo-potential method. The typical snap of plasma phase transition and the relationship between the ionization percent and temperature under static extreme conditions are obtained. The micro-structure of the shock front in the aluminum single crystal is presented in detail, and the ionized electrons appear in the compressed region. The Hugoniot relationship is obtained by simulating the shock processes under various shock wave velocities, and the simulated results agree well with the experimental data. The characteristic of plasma induced by the hypervelocity impact is also studied based on the ionization percent. The results show that the ionization percent increases with the shock strength and the reflect wave has a negative effect on the ionization of the electrons. The current study indicates that the electron force field in conjunction with the effective core pseudo-potential method has a good ability of computing the plasma phase transition of material under static extreme conditions and hypervelocity impact.

© 2014 Elsevier Ltd. All rights reserved.

1. Introduction

Understanding material properties and performance under extreme conditions, including static extreme conditions and dynamic conditions, becomes an absolute requirement for their design, application and optimization. It is a challenge to describe the plasma phase transition under static extreme conditions theoretically and experimentally. The reason is that the plasma under static high pressure and temperature lies in between the cold matter described well by ground state quantum mechanics [1,2], and the hot matter described well by classical plasma models [3]. Plasma phase transition induced by hypervelocity impact is an important physical response induced by dynamic loading acting on solid material, involving a number of subjects such as impact dynamics, solid state physics, plasma physics and high pressure physics [4–7]. The electromagnetic radiation associated with the plasma may cause interference or even complete failure on the electronic equipment of the orbit spacecraft [8–11]. In 1963 Frichtenicht and Slattery firstly reported the plasma generated by hypervelocity impact [12]. Since then, the plasma phase transition induced by hypervelocity impact and associated electromagnetic effects have attracted a large number of researchers. Harano conducted the hypervelocity impact experiment on solar cell array structure and detected the electron temperature and density using Langmuir probe [13]. Crawford et al. conducted the hypervelocity impact experiments to explore the properties of plasma and electromagnetism [14–17]. Close et al. detected the plasma signal generated by hypervelocity impact using Van de Graaff dust accelerator accelerating iron projectiles quality of 10^{-16}–10^{-11} g to speeds of 1–70 km/s to impact targets made of different materials and with different amount of charge [18–21]. However, the plasma phase transition of materials under extreme

* Corresponding author. Tel.: +86 1068915837; fax: +86 1068914284.
E-mail address: qmzhang@bit.edu.cn (Q. Zhang).

http://dx.doi.org/10.1016/j.ijmecsci.2014.02.027
0020-7403/© 2014 Elsevier Ltd. All rights reserved.

conditions, especially induced by hypervelocity impact, has not been understood clearly. Simulations at atomic even electronic level can stimulate the further understanding for the phenomena.

Born approximation considers nuclei at ground state as classical particles, since the electrons are much lighter than the nuclei, the electron wave functions and energy are functions of the nuclear coordinates [22]. In order to calculate the time evolution of the nuclei movement, the time-independent Schrodinger equation is required to solve at each time step. This method is very slow, so the classical molecular dynamics (MD) method based on the potential function reflecting the atomic interaction is usually employed. However, Born approximation cannot meet the computing need in many cases, such as the excited electrons at certain extreme conditions. In order to describe the physical and chemical phenomena more widely, especially the excited electrons, the electron force field (eFF) is proposed [23–26]. The eFF is a new molecular dynamics method which combines the quantum mechanics and the classical molecular dynamics and has the ability of computing systems with electrons explicitly over multi-picoseconds time scales and 10^4 atoms space scales. Unfortunately the eFF is only suitable for the system containing s electrons. It is difficult to solve the system including p and d electrons for the eFF. In order to overcome the limitation, the effective core pseudo-potential (ECP) method is introduced. The ECP method simplifies the multi-electrons into the valence electrons and describes the Pauli repulsion energy between the nuclear electrons and valence electrons with a pseudo-potential [27].

In the current study, the plasma phase transition of aluminum single crystal under static extreme conditions and hypervelocity impact is investigated by exploring the eFF in conjunction with the ECP method. Under static extreme conditions the typical snap of plasma phase transition and the relationship between the ionization percent and temperature are presented. The micro-structure of the shock front in the aluminum single crystal and the Hugoniot relationship are obtained, and the characteristic of the plasma induced by hypervelocity impact is also discussed.

2. Methodology of the simulation

2.1. Momentum equation

The electron wave function in the eFF is simplified as follows: the single electron is described by the spherical Gaussian wave packet, and the location $\mathbf{x}$ and size s of the packet varies with time respectively; the multi-electrons are described by the Hartree product of the single electron Gauss wave packet [23,24]

$$\Psi(\mathbf{r}) \propto \prod_j \exp\left[-\left(\frac{1}{s^2}-\frac{2p_s}{s}\frac{i}{\hbar}\right)(\mathbf{r}-\mathbf{x})^2\right]\exp\left[\frac{i}{\hbar}\mathbf{p_x}\mathbf{r}\right], \tag{1}$$

where $\mathbf{x}$, $\mathbf{p_x}$, s, p_s represents the position, translational momenta, size, and radial momenta of the spherical Gaussian wave packet, respectively.

Submitting the wave function into the time-dependent Schrodinger equation, the Hamiltonian equation of motion with simple forms can be obtained [25–27]

$$\dot{\mathbf{p}}_\mathbf{x} = -\nabla_x V, \dot{\mathbf{x}} = m_e^{-1}\mathbf{p_x}$$
$$\dot{p}_s = -\partial V/\partial s, \dot{s} = (3m_e/4)^{-1}p_s, , \tag{2}$$

where m_e represents the mass of electron, and V represents the potential energy of the system.

The Eq. (2) shows that the position and size of the electrons comply with the classical molecular dynamics, and can evolve with time independently. Therefore, the eFF can be used to simulate the non-adiabatic dynamics of materials under extreme conditions over long time-scale and large space-scale.

2.2. Energy expression

In the eFF the nucleus is regarded as a point charge and the electron as spherical Gauss wave packet. The total energy is a function of the nucleus position R, electron position x and size s, it can be expressed as [28,29]

$$E = E_{nuc\cdot nuc} + E_{nuc\cdot elec} + E_{elec\cdot elec} + E_{Pauli} + E_{ke}, \tag{3}$$

where $E_{nuc\cdot nuc}$, $E_{nuc\cdot elec}$, $E_{elec\cdot elec}$ represents the electrostatic interactions between nuclei, nucleus and electron as well as electron and electron, respectively. These three terms of energy correspond to the potential function in the classical force field. E_{Pauli} represents the Pauli repulsion energy, and E_{ke} represents the electron kinetic energy. These two terms of energy reflect the quantum effect. The above five terms of energy can be specifically expressed as [30]

$$E_{nuc\cdot nuc} = \frac{1}{4\pi\varepsilon_0}\sum_{i<j}\frac{Z_iZ_j}{R_{ij}}, \tag{4}$$

$$E_{nuc(i)\cdot elec(j)} = -\frac{1}{4\pi\varepsilon_0}\sum_{i,j}\frac{Z_i}{R_{ij}}Erf\left(\frac{\sqrt{2}R_{ij}}{s_j}\right), \tag{5}$$

$$E_{elec(i)\cdot elec(j)} = \frac{1}{4\pi\varepsilon_0}\sum_{i<j}\frac{1}{R_{ij}}Erf\left(\frac{\sqrt{2}R_{ij}}{\sqrt{s_i^2+s_j^2}}\right), \tag{6}$$

$$E_{Pauli} = \sum_{\sigma_i=\sigma_j} E(\uparrow\uparrow)_{ij} + \sum_{\sigma_i\neq\sigma_j} E(\uparrow\downarrow)_{ij} \tag{7}$$

$$E_{ke} = \frac{\hbar^2}{m_e}\sum_i \frac{3}{2}\frac{1}{s_i^2}, \tag{8}$$

where Z represents the charge of nucleus, R_{ij} represents the distance between the nuclei in Eq. (4), the nucleus and the electron in Eq. (5) and the electrons in Eq. (6).

Compared with the quantum mechanics to solve the time-dependent Schrodinger equation, the eFF can save calculation cost obviously and meanwhile ensure the computational accuracy. In quantum mechanics, such as *ab initio*, N^4 (where N represents the number of electrons) operations are required to compute the energy of the simplest anti-symmetric wave function which is capable to describe the multi-electrons accurately. In eFF the energy of single-term Hartree product is computed, which requires only N^2 operations. The Pauli repulsion is added on to approximate the energy difference between the anti-symmetric wave function and the Hartree product wave function which does not consider the anti-symmetry of the multi-electrons wave function [28–30].

2.3. Effective core pseudo-potentials

The eFF is only suitable for the system containing s electrons while is incapable to solve the system including p and d electrons. In order to solve the problem, researchers introduced the ECP method which simplifies the multi-electrons into the valence electrons and describes the Pauli repulsion energy between the nuclear electrons and valence electrons with a pseudo-potential [27]. The simplification results in the significant reduction of the electrons number and the obvious improvement of the computation efficiency.

Download English Version:

https://daneshyari.com/en/article/783475

Download Persian Version:

https://daneshyari.com/article/783475

Daneshyari.com