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Molecular dynamics simulations of interactions between energetic dust and plasma-facing materials

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ABSTRACT

The interactions between dust and plasma-facing material (PFM) relate to the lifetime of PFM and impurity production. Series results have been obtained theoretically and experimentally but more detailed studies are needed. In present research, we investigate the evolution of kinetic, potential and total energy of plasma-facing material (PFM) in order to understand the dust/PFM interaction process. Three typical impacting energy are selected, i.e., 1, 10 and 100 keV/dust for low-, high- and hyper-energy impacting cases. For low impacting energy, dust particles stick on PFM surface without damaging it. Two typical time points exist and the temperature of PFM grows all the time but PFM structure experience a modifying process. Under high energy case, three typical points appear. The temperature curve fluctuates in the whole interaction process which indicates there are dust/PFM and kinetic/potential energy exchanges. In the hyper-energy case in present simulation, the violence dust/PFM interactions cause sputtering and crater investigating on energy evolution curves. We further propose the statistics of energy distribution. Results show that about half of impacting energy consumes on heating plasma-facing material meanwhile the other half on PFM structure deformation. Only a small proportion becomes kinetic energy of interstitial or sputtering atoms.

1. Introduction

Over the past few years progress towards the understanding of dust behaviors in fusion devices has been significant through experiments, modelling and model validation in it [1–3]. Many plasma processes such as flaking of blisters [4], volume polymerization [5], cracking development [6], arcing [7], brittle destruction [3] and surface melting [9] even ELM and disruption events [10,11] contribute to the production of dust particles. Dust particles increases the operation difficulties of plasma since the dusts can contaminate the core plasma [12]. The contamination can increase the amount of impurity concentration in plasma or even lead to disruption [13,14]. Dust particles can also worsen the operation safety of fusion devices, including the risk of exploding and tritium leaking. As a result dust generation and its transport have been attached great importance to.

Because of the dust-PFM (plasma-facing materials) interaction associated with the life time of PFM and impurity generations, it is also a crucial issue in fusion science. Impacting velocities, angle, materials of dust, number of impacting dust, etc. are the factors influencing dust-PFM interaction. Although some studies are being performed for the interaction, it remains a major unsolved problem. One of the reasons is lacking of diagnose methods on dust-PFM interaction process. To the author's knowledge, few effective diagnose techniques can investigate dust-PFM interaction at present. Our knowledge on the interaction is mainly from numeric simulation results, such as finite element method or molecular dynamics [15–17]. Moreover, previous dust studies basically focus on carbon dust owing to the widely use of carbon plasma-facing materials (such as CFC or graphite) [18,19]. However, the characteristics of carbon and metal dust are quite different. Carbon materials are active in hydrogen's isotopes which is used as fusion fuel [14,21–25]. The chemical erosion is the primary erosion mechanism for carbon materials. But metal materials are more stable in hydrogen environment (especially tungsten) thus the physical sputtering caused by heavy ions or dust particles becomes a more important erosion process than chemical erosion comparing to carbon PFM. As metal materials will be used in ITER, the research on metal dust-PFM interactions has become necessary and urgent.

The rest of this paper is organized as follows. Section 2, we briefly overview the molecular dynamics (MD) simulation methods. In

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Section 3, we present dust-PFM interaction process and investigate the effect of tungsten (W) dust particles impacting into W surfaces. Finally, we summarize our results and provide concluding remarks in Section 4.

2. Methods

The interactions between dust particle and PFM surface were simulated with classical molecular dynamics (MD) employing many-body interatomic potentials implemented in the LAMMPS code (Large-scale Atomic/Molecular Massively Parallel Simulator) [26]. Both of the materials of dust particles and surface are W. The embedded atom method (EAM) potential, namely the Finnis–Sinclair (FS) potential [27] is used to describe the W–W interactions.

The total energy of FS potential is

$$U_{FS} = U_N + U_P \tag{1}$$

M. W. Finnis and J. E. Sinclair wrote U_N as a sum over all atoms of a cohesive function [27]:

$$U_N = -A\sum_i \sqrt{\rho_i} \tag{2}$$

where

$$\rho_i = \sum_j \phi(R_{ij}) \tag{3}$$

here

$$\phi(R_{ij}) = \frac{(R_{ij}-d)^2 + \beta(R_{ij}-d)^3}{d} \tag{4}$$

when $R_{ij} \le d$ and $\phi(R_{ij})$ equal to zero elsewhere. R_{ij} is the distance between two specific atoms labeled by i and j. For W, d = 4.400224 Å, A = 1.896373 eV, β = 0.

The pair-potential part U_P is expressed as

$$U_P = \frac{1}{2}\sum_{ij} V(R_{ij}) \tag{5}$$

where

$$V(R_{ij}) = (R_{ij}-c)^2(c_0 + c_1 R_{ij} + c_2 R_{ij}^2) \tag{6}$$

when $R_{ij} \le c$ and equal to zero elsewhere. For W, the values of c, c_0, c_1, c_2 are 3.25 Å, 47.1346499, −33.7665655 and 6.2541999, respectively [27].

FS potential is too "soft" for high pressure cases, so the ZBL pair-potential U_{ZBL} is applied to improve the compressibility. The ZBL potential is in the following form [28]:

$$U_{ZBL} = \frac{1}{4\pi\epsilon_0}\frac{Z_i Z_j e^2}{R_{ij}}\psi\left(\frac{R_{ij}}{a}\right) \tag{7}$$

The first part of U_{ZBL} is Coulomb repulsive term with Z_i, Z_j as the number of protons in i and j atom, respectively, e as the electron charge and ϵ_0 as the permittivity of vacuum. The second part is the ZBL universal screening function, with $a = 0.8854a_0/(Z_1^{0.23} + Z_2^{0.23})$ and a_0 = 0.529 Å as the Bohr radius. The screening function is

$$\psi(x) = 0.1818e^{-3.2x} + 0.5099e^{-0.9423x} + 0.2802e^{-0.4029x} + 0.02817e^{-0.2016x} \tag{8}$$

In order to combine the FS and ZBL parts smoothly, the actual potential used in present research is the combination of ZBL and FS potential, the form is

$$U = (1 - h(R_{ij}))U_{ZBL} + h(R_{ij})U_{FS} \tag{9}$$

The $h(R_{ij})$ function is

$$h(R_{ij}) = \frac{1}{1 + e^{-A_F(R_{ij}-r_C)}} \tag{10}$$

The parameter r_C is 1.6 Åand A_F is 12 Å^{-1} in present case.

The structure of W material is body-center cubic (BCC) and the lattice constant a=3.165 Å. The size of dust particles is 541 atoms/dust. The size of PFM in x-, y- and z- directions are 180, 180 and 160 times of lattice constant length a, respectively, which has been tested enough for the simulation. z- direction is the normal direction of PFM and x- and y- directions are perpendicular to it. According to the report from FTU, the velocity of dust particles can be over 10 km/s [29,30]. The mechanism is stated in Section 3.1.3. So in present research three typical impacting energies are selected: E_{im} = 1, 10 and 100 keV/dust. The counterpart velocities are 1.5 km/s, 4.5 km/s and 15 km/s. This velocity range should be enough to cover most of the dusts. The distance between dust bottom and PFM surface is 1 Åat the very start of simulation (t = 0). We have discussed the angle dependence of dust impacting in reference [16] whose results showed that the incident angle is not significantly influence the consequence of collision. The accumulating effect of multiple dust impacting has also been discussed in [16]. So in present we only consider the normal and single-dust impacting case. The dropping point of dust is randomly selected. The automatically adapting time step is applied in present MD simulation. The time step ranges from 10^{-3} to 1 fs in order to make sure the moving distance of every atoms less than 0.1 Åin each step. The purpose of doing this is to avoid possible strange but unphysical phenomenon due to overlong moving distance of atoms in one simulation step. The temperature of system is 300 K. The shape of tungsten clusters is spherical in the present simulation. Periodical conditions are applied in x- and y- directions. Several parallel simulations have been performed to make sure the confidence of the results.

3. Results

3.1. Energy evolutions

We investigate the temporal evolution of three average energies of PFM atoms: kinetic energy $\langle E\rangle$, potential energy $\langle U\rangle$ and total energy $\langle T\rangle$. These energies are defined as follows:

$$\langle E(t)\rangle = \frac{1}{N_{PFM}}\sum_i^{N_{PFM}} E_i(t) \tag{11}$$

$$\langle U(t)\rangle = \frac{1}{N_{PFM}}\sum_i^{N_{PFM}} U_i(t) \tag{12}$$

$$\langle T(t)\rangle = \langle E(t)\rangle + \langle U(t)\rangle \tag{13}$$

here N is the total number of PFM atoms, E_i, U_i and T_i are the kinetic, potential and total energy of atom i.

As we have confirmed that the velocity of mass-center of PFM is zero, $\langle E\rangle$ shows the temperature of PFM atoms. $\langle U\rangle$ is closely related to the distance between atoms thus sensitive to the PFM structure. For W whose cohesive energy is 8.9 eV, the average potential energy for the atoms in lattice is -8.9 eV. When PFM is compressed or stretched, $\langle U(t)\rangle$ increases. In present research, no tensile force acts on PFM. So the increasing of $\langle U(t)\rangle$ presents the compression of PFM. The decrease of $\langle U(t)\rangle$ implies the releasing of pressure. In the equilibrium state, the increase of $\langle U(t)\rangle$ means certain atom is sputtered (because for single atom U_i = 0 > −8.9 eV) or PFM surface is modified (because U_i of the atoms on surface is greater than that of in lattice). Similar method is applied in reference [31] to study the bombardment of Au cluster on Au target.

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