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Molecular dynamic simulation of tungsten ablation under transient high heat flux

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ABSTRACT

Molecular dynamic (MD) method is used to simulation the tungsten ablation under transient high heat flux generated by energetic ions. A model including 363,600 W atoms was built based on Finnis–Sinclair potential. The results show that the ablation threshold is much lower than the one of boiling. So the ablation effects might be underestimated if using energy threshold of boiling instead of that of ablation. Particle size distribution of ablation products follows a power decay law with an exponent around −2.5, which does not affect by the incident heat flux. The transverse velocities of particles obey normal distribution, and a stream speed is added to the random movement for the longitudinal velocity. As the ablation start up, the recoiled impulse can induce shock wave in remained target, which is supported by experimental pressure wave measurements.

1. Introduction

Thermal ablation induced by transient high heat flux (HHF) during the transient events is a main erosion form of the plasma facing materials (PFMs) in TOKAMAK. It may produce lots of dust; in turn influence the plasma discharge status. On the other hand, it may also damage plasma facing components (PFCs), especially divertor. Therefore, the kinetic and dynamic properties of the ablation products and the thermal dynamic effects of ablation on the PFCs are deeply concerned in the plasma–surface interaction research [1–4].

There are many research papers related to ion beam induced ablation using the thermodynamic quantities of boiling under standard pressure instead of the ones of ablation in their numerical calculation or simulation. However, these two processes are quite different. Boiling is a process which release gas from liquid. The boiling point can be reached by a quasi-steady heating process under constant pressure. Thermal ablation occurs when an intense heat flux loaded on the target at high power density, at a temperature lower than the boiling point. It is far from quasi-steady process. Ablation is a complex appearance, which can include multi thermal dynamic courses occurring subsequently or simultaneously, depending on parameters of both heat flux and target materials. The ejected plume often consists of various particles: charged particles (plasma), neutral single atoms or molecules (gas), small clusters, droplets, and even debris. It is necessary to learn the kinetic parameters and mass distributions of these particles to figure the ablation dynamic process out. However, there are certain difficulties to do experimental measurements directly. Molecular dynamic (MD) method is an applausive way to describe the basic dynamic process. Although the MD results cannot be directly compared with experimental results, they can provide a certain consistency in tendency. Here MD simulation is done on a simple model to gain further understanding of the processes that occur during transient thermal ablation of tungsten.

2. MD modeling and calculation

A single crystal system including 363,600 ($60 \times 60 \times 50$ cells) tungsten atoms was built based on Finnis–Sinclair potential [5]. The thickness of primary heat loading layer on the top part of the crystal was defined as 3.17 nm (10 lattice length) referred to the project range of He ions with kinetic energy less than 1 keV.

The initial temperature of the system was 300 K. A pulse width of 100 fs was taken for heat flux loading time, because of the limitation of calculation ability. It is not far from the reason for that 100 fs corresponding to the minimum magnitude of the electron–phonon coupling time. After the transient heat load, we let the system developing freely, and observe what happens. The relaxation time is 100 ps to getting ejected particles distinguishable. From

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27.8 J/m^2 to 434.1 J/m^2, various incident pulsed energy densities were examined. Considered the electronic heat conduction, the energy deposition depth profile was roughly considered as a step shape in our work. In fact, we also checked the heat source with right-angled trapezoid shape. It does not bring distinguished difference to the system relaxation results. So we chose the simple one for higher computational efficiency.

Fig. 1 is a snapshot of an ablation process simulated by means of MD. The ablation depth, kinetic parameters of the ablation products, the stress development and propagation were counted and analysis statistically.

3. Results and discussion

3.1. Energy flux threshold of ablation

As the pulsed energy density increasing, there are coming to a threshold of ablation. Fig. 2 shows that the pulsed energy density threshold is about 120 J/m^2 in the case of our simulation. This value will increase with the heat pulse duration, for heat conducting effect getting more obvious.

Boiling point is often used to estimate the mass loss of materials under transient heat load. But if ablation occurs, the critical energy density would be much lower. Fig. 3 gives the ablation depth dependence on the pulsed energy density. It can be found that ions pulse with pulsed energy density of 148 J/m^2 can ablate tungsten of 1.8 nm. However, in case of evaporation in adiabatic process under the standard pressure, by counting the sensible heats in solid state and liquid state, the latent heats of melting and boiling, the total pulsed energy density needed to fully vaporize the same amount of tungsten can be estimated as 188 J/m^2. In fact, the transient heat loading course is not strictly adiabatic, so the critical pulsed energy density for fully vaporizing should be even higher. If considering the heterogeneous of real material, the ablation threshold will be even lower. So using the boiling point instead of the ablation threshold could underrate the severity of ablation.

3.2. Ablation depth

The ablation depth is related to the mass loss and the life of PFC. From Fig. 3, it is found that the dependence relation between ablation depth and energy density is not linear, but logarithmic. It can be expressed as

$$d = l \cdot \ln\left(\frac{F}{F_{th}}\right) \tag{1}$$

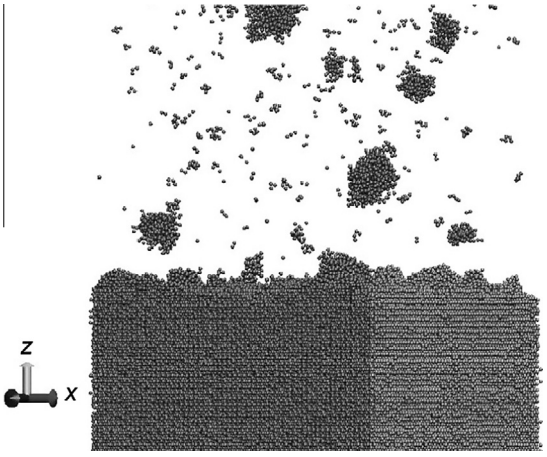

Fig. 1. Snap shot of MD simulated tungsten ablation process induced by intense transient ion beam pulse.

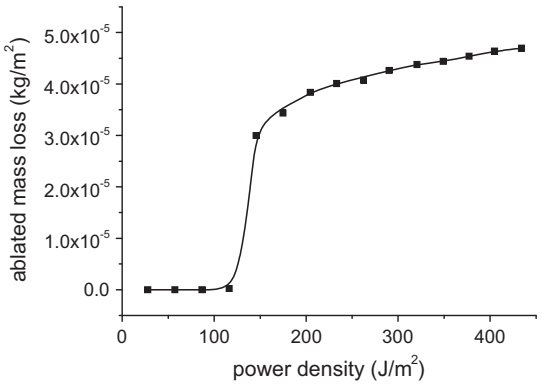

Fig. 2. Ablation mass loss vs. incident transient heat flux.

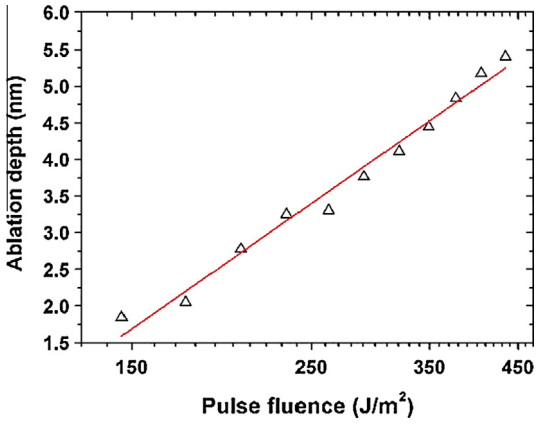

Fig. 3. Ablated depth vs. incident transient heat flux.

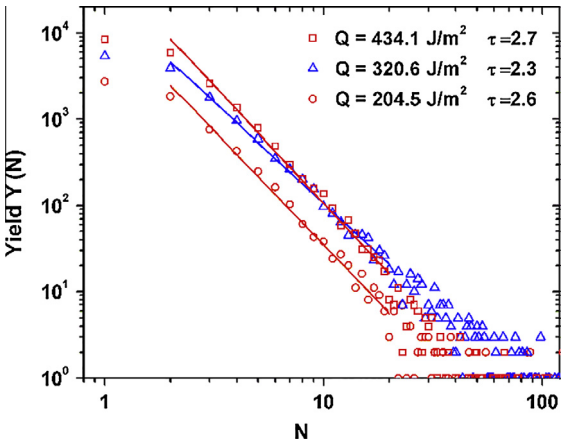

Fig. 4. Particle size distributions of ablation products. Cluster yield appears power law relationship to cluster size with minus power $-\tau$. Q is pulse energy of the high heat flux.

where d is ablation depth, F is heat flux, F_{th} is ablation threshold, and l appears as a fitting constant. In the case of laser ablation [6,7], the l represents the laser penetration depth. Here, it can be regarded as a characteristic depth of heat conduction affected zone.

In Fig. 3, l = 3.35 nm, is very close to the pre-set heat deposition range in our model, 3.17 nm. It implies that the ablation depth can be deeper than the heat deposition range, since ablation process is not strictly adiabatic. However, it is not far from adiabatic, because the difference between l and the heat deposition range is tiny.