A Molecular Dynamics Study on the Dust-Plasma/Wall Interactions in the EAST Tokamak*

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Abstract The interactions between the W nano-dust and deuterium plasma at different locations of the EAST tokamak are simulated using a molecular dynamics code. It is shown that nano-dust particles, with the radius, R_d, ∼5 nm, can exist for at least several nano-seconds under the interactions from the ions without being ablated in some specific places of the tokamak edge plasma, while those with R_d ≥25 nm may be ablated if the plasma temperature $T\sim$ 50 eV and density $n\sim10^{19}$ m^{-3}. In addition, the collisions of tungsten nano-dust grains with a tungsten wall at 100 m/s or 1000 m/s impinging speeds are simulated. It is demonstrated that the dust will stick to the wall, and the collision will not cause substantial damage to the wall, but it may be able to cause partial destruction of the dust grains themselves depending on their incident speeds.

Keywords: dust, plasma-material interaction, fusion, tokamak

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1 Introduction

Dusts, small particles with sizes between several nanometers and several hundred micrometers, are commonly found in magnetic fusion devices [1∼7]. The composition of these particles is almost the same as those of the plasma-facing components (PFCs), although dust grains may contain some hydrogen isotopes from the fuel and some radioactive elements of wall materials from the neutron bombardment. According to this fact, dust grains are supposed to be formed due to various plasma-surface interaction processes, such as wall material sputtering by plasma, flaking of deposited layers, melting, brittle destruction, arcing, and due to impurity coagulation in cold contaminated plasma regions. In the past few years, many of these processes have been observed [2,7].

Recently, more and more attention has been paid to the issues of dust generation, dynamics and transport in magnetic fusion devices. The increasing interest of this subject may be attributed to impurity transport, tritium retention, potential explosion and radiological hazard of dust accumulation during high power long pulse discharges. Moreover, dust particles, when entering the core plasma, have been observed to terminate discharges in the LHD, which is a long pulse superconducting stellarator [8].

In most regions of magnetic fusion devices, the plasma is so hot and dense that dust particles will be heated and then ablated. Nevertheless, theoretical studies have shown that in some regions where the plasma temperature, T, is below 10 eV and plasma density, n, is within the range of $10^{12}\sim10^{14}$ cm^{-3}, dust can grow [9]. It was also clearly demonstrated experimentally that dust indeed can grow during the discharges [10], which was actually the same as theoretically predicted, and consequently nano-scale dust grains can be formed.

Up to the present, most of the theoretical and simulation studies have focused on the carbon dust issues. However, in order to improve the performance of the EAST plasma discharge, PFCs in the divertor region will be changed into tungsten (W)/CrZrCu heat sinks in 3∼5 years [11]. Since the EAST is a long pulse superconducting tokamak, the W dust production would be substantial, leading to various operational or safety issues.

In this study, we simulate the behavior of W nano-dust in edge plasma, especially the dust-plasma interaction, using the molecular dynamics (MD) method. These simulations may be used to predict the state of the dust in the plasma of the EAST tokamak. Finally, we can see that the ion flux has a limited impact on the W nano-dust in edge plasma, which may give rise to the collisions between dust and the wall, and cause damage or adhesion to the wall.

2 Simulation model of dust-plasma interaction

Our simulations are all performed with a parallel version of molecular dynamics code LAMMPS, an acronym for Large-scale Atomic/Molecular Massively Parallel

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Simulator. To simulate the dust ablation, we need to model the dust-plasma interaction processes. In these processes, the particles from the plasma, including electrons and ions of hydrogen isotopes or wall materials, collide with the dust, usually negatively charged, transferring the heat and momenta to the grain. The grain is either vaporized or remain intact, depending on the temperature and density of the plasma. And the hydrogen ions trapped in the dust grain become hydrogen atoms. Accordingly, there are four kinds of interactions in our simulation model, which are W−W/W^{m-}, W−H, W^{m-}−H^+ and H^+− H^+, where the W^{m-} is tungsten ions on the surface of the dust, as we neglect the heat transfer from electrons, considering the case of dusty plasmas, i.e., the dust grains are kept intact in the plasma with low ion temperature T_i and high electron temperature T_e. The interaction model is shown in Fig. 1, the W nano-dust, i.e., the green ball, is set in the center of the box, and some small ions represented by the colorful particles move around the grain at thermal speeds. The length of the simulation box is 1 μm, and micro-canonical ensemble (NVE) for dust grain and canonical ensemble (NVT) for the plasma ions are used respectively in our simulations. Periodic boundary conditions are used, time-step is 0.5 femto-second for both plasma and dust grains.

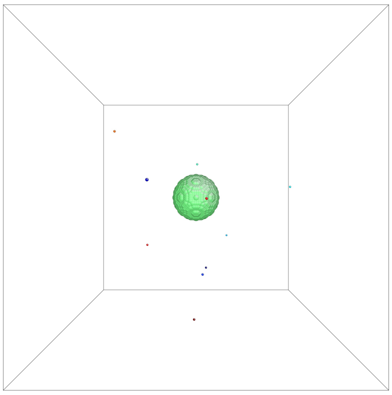

Fig.1 Simulation model of dust-plasma interactions (color online)

Although we do not consider the impact from the electrons due to their small mass compared to the ions, they are able to contribute a lot to the charging processes of the dust grains, which are quite important in dust-plasma interactions. The charge of the dust, Z_d, can be calculated according to the Orbit Motion Limited model analytically in our simulation model. The quantity $Z_\mathrm{d} = R_\mathrm{d}T_\mathrm{e}$ (R_d is the radius of the dust grain) at the equilibrium state is expressed as a function of $T_\mathrm{i} = T_\mathrm{e}$ and relative speed between the dust and the plasma flow. For this case, where $T_\mathrm{i} = T_\mathrm{e}$ and the relative speed is equal to zero, $Z_\mathrm{d} = 1739 \times R_\mathrm{d}(\mu\mathrm{m})T_\mathrm{e}$. For example, in the case of $R_\mathrm{d} = 5$ nm and $T_\mathrm{e} = 20$ eV, we have $Z_\mathrm{d} = 173.9$.

For W−W/W^{m-} and W−H systems, we employ the modified analytic bond-order potentials (BOP) developed by LI et al. to describe them [12]. This bond-order potential is a 3-body one, and quite sophisticated, such that we would not list its expression here, but details of the potential including the equations and parameters can be found in Ref. [12].

For W^{m-}−H^+ and H^+ systems, the combination of the long-range Coulomb potential and the short-range the BOP is used to describe their interactions, since there are W ions on the surface of the dust grain. The Ewald summation technique is used to deal with the long-range interactions.

In our simulation, we only consider dust grains of a spherical shape. Moreover, the crystal structure of the tungsten is body-centered cubic (bcc) with a lattice constant of 0.3165 nm. Dust particles of a fixed initial size are set at rest, exposed to the plasma whose velocity obeys the Maxwell speed distribution at a certain temperature. Initial radius of dust particles, R_d, is selected to be about 5 or 25 nano-meters. The ranges of plasma temperature and density in this simulation are 5∼400 eV and $10^{18} \sim 10^{19}$ m^{-3}, respectively. The above selections about the plasma parameters are based on the conditions of edge plasma in the EAST tokamak. In this situation, the Debye length can be expressed as

$$\lambda_\mathrm{D} \equiv \sqrt{\frac{\epsilon k_\mathrm{B}T}{ne^2}} \approx 69.0\sqrt{\frac{T}{n}}, \tag{1}$$

the unit of T here is K. Taking into account the plasma conditions in EAST, the order of magnitude of the Debye length is about a few μm or tens of 10 μm, i.e., $\lambda_\mathrm{D} \sim 10^{-5}$ m, which is much larger than the dimensions of the simulation model, hence the Debye screened potentials can be replaced by the Coulomb potentials approximately. In addition, the expression of the ion cyclotron radius is

$$R_\mathrm{i} \equiv \frac{v_{\perp,\mathrm{i}}}{\Omega_\mathrm{i}} \approx 9.47 \times 10^{-7}\frac{\sqrt{AT}}{ZB}, \tag{2}$$

where $\Omega_\mathrm{i} = ZeB/m_\mathrm{i}$ is the ion cyclotron frequency, $v_{\perp,\mathrm{i}} = (2k_\mathrm{B}T/m_\mathrm{i})^{1/2}$ is the ion thermal speed perpendicular to the magnetic field, **B**, which is about 3 T. Ion cyclotron radius of plasma in EAST is about several hundred micrometers, i.e., $R_\mathrm{i} \sim 10^{-4}$ m, which is much larger than the diameter of the dust grains in our simulation as well. For this reason, **B** does not appear explicitly in the simulation, since the magnetic field has little influence on the dust-plasma interactions here.

3 Results of dust-plasma interaction

Firstly, we set the radius of the dust grain to be 5 nm. As shown in Fig. 2, the plasma density is about 10^{18} m^{-3}, and two kinds of plasma temperature, T, are considered, which are 10 eV and 50 eV. The temperature of the nano-dust, T_d, is chosen to be 500 K initially; however, it immediately oscillates and later fluctuates around the equilibrium temperature for the remaining time of the simulation. This sudden oscillation in the dust temperature may be attributed to the fact that the dust grain had not been completely equilibrated before the interactions with ions, when we artificially assigned the velocity by the Maxwell distribution. It suggests that the ions of deuterium plasma do not transfer the thermal energy, and thus do not cause significant damage, to the dust grain, since the nano-dust losses some of the thermal energy and becomes more stable instead. So it is inferred that the dust grain keeps its shape intact, when $n = 10^{18}$ m^{-3} and $T = 10 \sim 50$ eV. Considering the conditions of the plasma in the scrape-off layer (SOL) of the EAST, $n \sim 10^{18}$ m^{-3} and $T < 50$ eV, are almost covered by the parameters we listed above, we can conclude that the dust grain is unlikely to be ablated in the SOL of EAST in several nano-seconds.

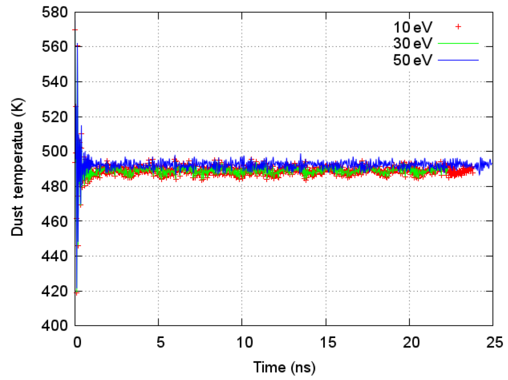

Fig.2 Temporal evolution of the dust temperature, when $n \sim 10^{18}$ m^{-3} (color online)

Figs. 3 and 4 show the temporal evolution of the dust temperature at different plasma temperatures, when $n \sim 10^{19}$ m^{-3}. The initial temperature of the dust is also 500 K, and as shown in Fig. 3 when $T = 10$ eV or 50 eV striking similarities are found in comparison to Fig. 2 which displays the development of T_{d} when $n \sim 10^{18}$ m^{-3}. In other words, the dust grain does not absorb the substantial thermal energy from the ions, and hence still keeps its entire shape. Given the conditions of the divertor plasma in EAST, $n \leq 10^{19}$ m^{-3} and $T \leq 50$ eV, are contained in the parameters of the simulation that we list in Fig. 3, the dust is supposed to exist in the divertor chamber of EAST without destruction.

However, when $n \sim 10^{19}$ m^{-3}, $T = 400$ eV, which are the parameters of the pedestal in the plasma edge during the H-mode confinement in EAST, as shown in Fig. 4, the dust temperature jumps to more than 14000 K immediately, which is much greater than the melting point of tungsten at 3695 K. It suggests that the dust grains may be ablated, and some of the atoms may gain enough kinetic energy to escape from the grain. Fig. 5 displays the interaction processes, where the red and green particles represent the dust and ions respectively, the upper one shows the initial state, and the lower one stands for the state when $t = 0.5$ ps. As displayed in Fig. 5, the ablation occur.

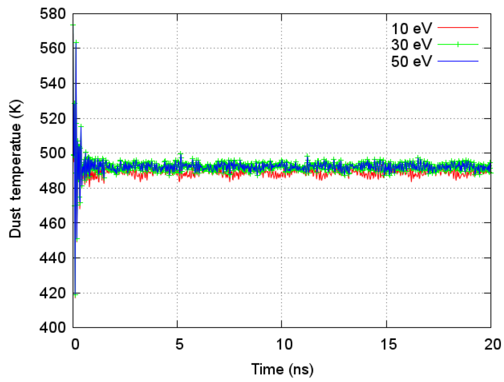

Fig.3 Temporal evolution of the dust temperature, when $n \sim 10^{19}$ m^{-3} (color online)

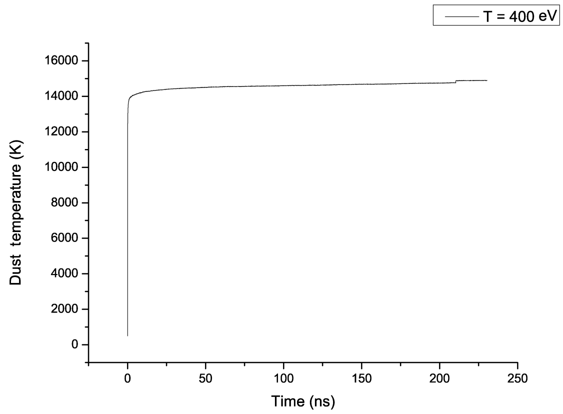

Fig.4 Temporal evolution of the dust temperature, when $n \sim 10^{19}$ m^{-3}, $T = 400$ eV

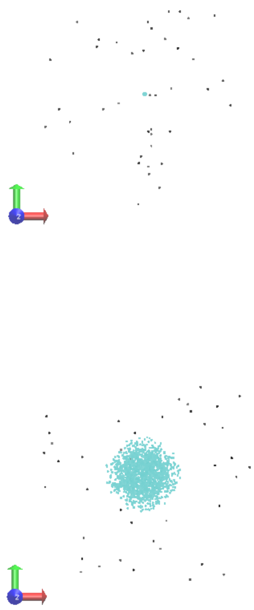

Fig.5 The ablation processes of the dust grains, when $n \sim 10^{19}$ m^{-3}, $T = 400$ eV. The black and cyan particles represent the plasma ions and dust atoms, respectively, the upper one shows the initial state, and the lower one stands for the state when $t = 0.5$ ps (color online)

Now we change the radius of the dust grains to about 25 nano-meters. As shown in the Fig. 6, when $n \sim 10^{19}$ m^{-3}, T=10 eV, the dust still keeps the shape intact. The upper picture in Fig. 6 displays the initial state of the dust-plasma interaction, and the lower one corresponds to the state when $t = 0.5$ ps. It is inferred that the dust can still endure this harsh condition in plasma without being vaporized.

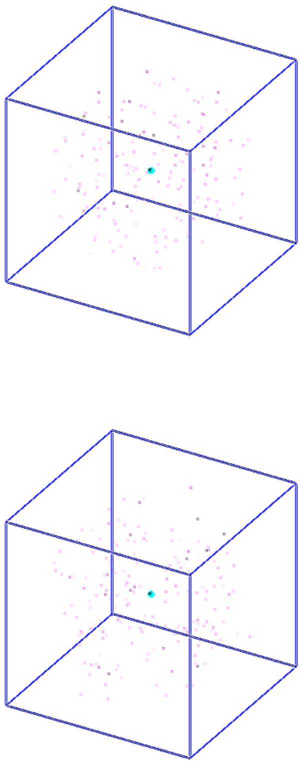

Fig.6 Illustration of the dust-plasma interactions when $R_{\rm d} = 25$ nm, $n \sim 10^{19}$ m^{-3}, $T = 10$ eV. Red and green particles represent ions and dust, respectively. The upper one is the initial state $t = 0$, the lower one corresponds to the state $t = 0.5$ ps (color online)

However, when the plasma temperature rises up to 50 eV, the dust grain becomes unstable and is quickly ablated. As shown in Fig. 7, the upper one illustrates the initial state, and the lower one corresponds to the state when t= 0.5 ps. All the simulations above indicate that the dust would be destroyed by the hot ions from the plasma, when $T \sim 50$ eV, $n \sim 10^{19}$ m^{-3}, which is consistent with the results in Ref. [9].

According to the simulation model, the ablation results from the collisions between the ions and dust grain directly. So whether the ablation occurs is determined by the energy transfer function $P_{\rm c}$ due to these collisions, which are proportional to the plasma density n, plasma temperature T and the square of dusts radius $R_{\rm d}$, i.e. $P_{\rm c} \sim nR_{\rm d}^2F(T)$, where the $F(T)$ is a function of the plasma temperature. The ablation may be attributed to the increase of energy transfer function resulting from the rise of these parameters in our previous simulations.

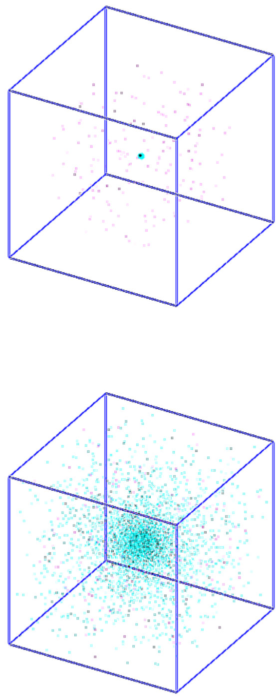

Fig.7 Illustration of the dust-plasma interactions when $R_{\rm d}$= 25 nm, $n \sim 10^{19}$ m^{-3}, T=50 eV. Red and green particles represent ions and dust, respectively. The upper one is the initial state t=0, the lower one corresponds to the state t=0.5 ps (color online)

4 Modeling of dust-wall collisions

As shown in section 3, nano-dust can exist in the edge plasma of the EAST for quite a long time. Since some dust particles can reach a very high speed ~1000 m/s, these grains may have a substantial influence on the wall due to the dust-wall collisions. In order to evaluate the possible effects of these interactions on both the dust and the wall, we performed numerical simulations using molecular dynamics code for them as well. With this method, we simulated impacts of tungsten spherical dust particles, $R_{\rm d}$ = 5 nm, on a at tungsten target at a speed of 100 m/s or 1000 m/s, and at an angle of 45° to the surface normal. In the present simulations we neglected thermal effects, assuming a constant temperature of the dust and the target at 500 K. External forces, such as electric force, did not present in the simulations.

Fig. 8 demonstrates that a tungsten dust particle at a low incident speed 100 m/s, being adhered to the wall in a good shape, causes no significant damage to either the nano-dust particles or the wall. When impinging on the wall at a high impact speed of 1000 m/s, the tungsten dust is partially deformed and destroyed due to shear stresses developed during the oblique collision, but the collision does not cause substantial damage to the wall either, as seen in Fig. 9. We can, consequently, suspect that such nano-dust, impacting on wall surfaces, may enhance the formation of deposition layers, since they can stick to the surface without causing much damage, and thus give rise to more significant erosion and re-deposition in the following plasma-wall or dust-wall interactions.

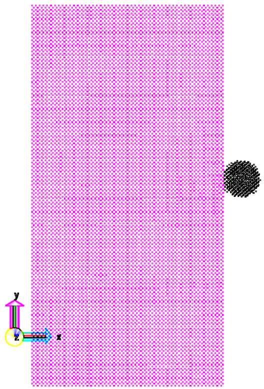

Fig.8 Simulated collision between a tungsten dust grain of $R_{\rm d} = 5$ nm and the tungsten target at speed of 100 m/s, at an impact angle of 45° (color online)

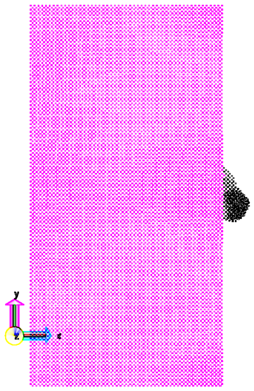

Fig.9 Simulated collision between tungsten dust grain of $R_{\rm d} = 5$ nm and tungsten target at a speed of 1000 m/s, at an impact angle of 45° (color online)

Some investigations are shown in Ref. [7]. Although the size of the dust, the simulation method, and the composition of the dust and wall materials are quite different from our simulations, we can still find that our results are consistent with those of Ref. [7] in general.

5 Conclusion

In this work, the interactions between the W nano-dust and deuterium plasma at different locations of the EAST tokamak are simulated using a molecular dynamics code. It is shown that nano-sized dust particles, whose radii are not greater than 5 nm, can exist for at least several nano-seconds, under the interactions from the ions, without being ablated in some specific place of the tokamak such as the divertor chamber, scrape-off layer, plasma edge and pedestal. Meanwhile, nano-dust with a radius of about 25 nm may be easily vaporized due to the dust-plasma interaction when the plasma temperature is higher than 50 eV.

Additionally, the collisions of tungsten nano-dust grains with a tungsten wall at 100 m/s or 1000 m/s impact speeds are simulated. It is demonstrated that neither the high speed impact nor the low one can cause significant damage to the wall, but the dust grain may be partially destroyed during the collisions depending on their incident speeds and can stick to the wall.

All these effects are important for illustrating the nano-sized dust transport in a tokamak, and may present potential relations between the dust and the erosion and re-deposition processes. However, since we do not consider the in uence from the electron flux in our simulation, the life-time of the nano-dust may be overestimated. Therefore, further studies should be conducted to investigate the critical temperature and density for the ablation of dust particles.

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