ANNEX 4

MD simulation of the Helium bubbles formed in Beryllium under Helium bombardment

E. V. Votyakov and S. C. Kassinos
Computational Science Laboratory UCY-CompSci, Department of Mechanical and Manufacturing Engineering, University of Cyprus, 75 Kallipoleos Str., Nicosia 1678, Cyprus

INTRODUCTION

Beryllium is a candidate plasma-facing material in future fusion reactors and it is important to assess Be walls sputtering in the H-He plasma. Molecular Dynamics (MD) is a widely recognized simulation technique, which supplies the detailed picture of all the atoms by solving equations of motion. Near a decade ago, Ueda et al. had proposed a pairwise interatomic potential for Be, He, H and D atoms, and performed few MD studies [1, 2] with the aim τo calculate sputtering yields in series of independent single MD experiments. In this study, we have carried out a cumulative series of sputtering MD experiments with the goal to study a formation of He bubbles in the Be-substrate. Specifically, when the incident He dose exceeds a threshold, a bubble of He atoms is formed in the Be subsurface region due to Van-Der-Waals interaction. Following its initial formation, the bubble starts to either grow up or break down. While the latter is advantageous, because the He bubble evaporates with minimal destruction, the process nevertheless leaves interatomic defects in the MD cell. These defects are crucial for the subsequent accumulation of the He atoms in the Be wall. When size of the He bubble reaches the spanwise size of the MD cell, so, many bonds between internal Be atoms are destroyed, it is observed so called "peeling" effect, characterized by simultaneous removal of several Be atomic layers above the bubble. This process releases the bubble; further He bombardment repeats the phenomenon for the next Be layers.

METHOD

MD simulations were performed with the freely distributed code LAMMPS [4]. An incident atom was placed at a random position above the Be(001) face at the height 1.83 nm. The initial velocity vector, $v_i = (v_x; v_y; v_z)$, of the atom was taken as $v_x = v_i \sin\theta\cos\varphi$, $v_y = v_i \sin\theta\sin\varphi$, $v_z = v_i \cos\theta$, $v_i = (2m_iE_i)^{1/2}$, where E_i and m_i are respectively the energy and mass of the incident atom, and θ and φ are respectively the polar and azimuthal incident angles. The incidence angles θ and φ were selected randomly on the surface of the unit sphere according to the Marsaglia algorithm [5]. Time interval between successive collisions was 5 or 10 ps. The time integration step was $0.5\text{x}10^{-4}$ ps in the first 1ps after issue of the incident atom, and then 10^{-3} ps, when main collisions in the substrate have passed and we observed substrate relaxation. This flexible time step allowed proper dissipation of the kinetic energy of the incident atom. Shrink-wrapped boundary conditions were imposed in the vertical *z*-direction with two most bottom Be planes fixed. To define horizontal boundary conditions, we used (i) fixed walls with the Langevin thermostat (LT); (ii) fixed walls with Berendsen thermostat (BT); and (iii) periodic boundary conditions (PBC). Other parameters are given in Table 1. The incident energy (E_i), the size of the MD cell (l_xxl_yxl_z), and the temperature (T) were varied in the range E_i=25, 50, 100, 150, 200 eV; (l_x x l_y x l_z) = (9x5x39) , (17x9x19) and (34x20x20); T=750, 1000, 1250K.

RESULTS

The typical He-Be results, shown in the figure below, have been obtained in the year 2011, and, during the year 2012, we have observed the same results for the larger MD cells, other BC, temperature and incident energy. The objective of the experiments in 2012 was to clarify the effect of the boundary conditions and size of the MD cell on the He bubbles behavior.

The plot in Fig. 1 shows the number of He atoms accumulated by the Be crystal (red line, the number of the incident minus number of the reflected He atoms), and the number of Be atoms sputtered into vacuum (blue line) as a function of the incident He atoms. At first, one observes almost linear dependence both of the He and Be atoms. The slope of the line is a single sputtering rate, which is close to the Ueda's MD results [1,2]

When the Be substrate accommodates a threshold number of He atoms, they evaporate, and the red line sharply drops down. This process repeats many times, in each cycle the size of the evaporated He bubble can be either small (near 4000 incident He atoms) or big (near 3000 and 6000). With each cycle, the Be substrate accumulates additional internal damage, so that in subsequent cycles it can accommodate larger He bubbles than before. Finally, when the size of the He bubble reaches the borders of the MD cell, so that most the Be internal bonds appears to be broken, one can see a dramatic rise up on the blue curve accompanied by a drop down in the red line. This means that finally the He bubbles is released through splitting off the Be upper atomic layers. It is

illustrated by the MD snapshot on the right of Fig. 1. One can see in the snapshot the moment when the upper Be layers are separated from the bulk upon the action of the big He bubble (intermediate layer). One can also see few smaller bubbles below, which will eventually grow during the subsequent He bombardment.

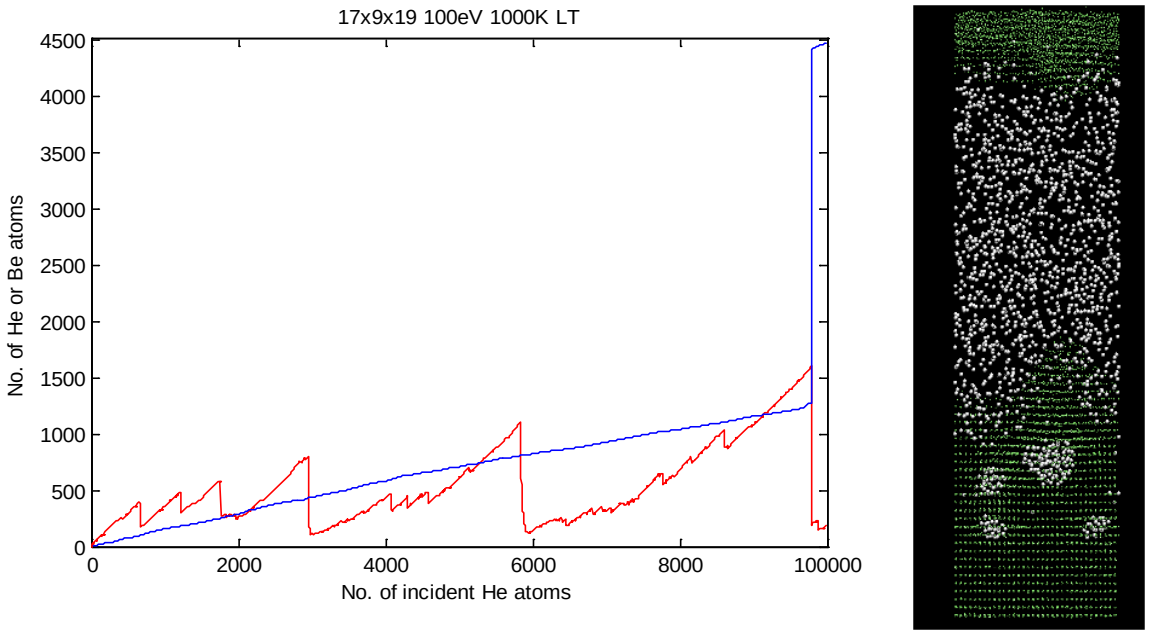

Fig. 1: Cumulative sputtering effect. The red line shows the total number of He atoms absorbed in the Be crystal as a function of the total number of incident He atoms. The blue line shows the total number of Be atoms sputtered.

The time to reach the saturation of the Be-cell by the He atoms depends on the incident He-fluxes. In the MD simulation, the frequency of issuing He-atoms towards the Be-surface is unrealistically high; otherwise, because of limited computational power, the simulation is not feasible. As a result, the simulated incident fluxes are in 5-6 orders of magnitude higher than in reality. If, during the time gap between adjacent He-Be collisions, the MD Be-cells can reach equilibrium, then, the difference in the theoretical and experimental incident fluxes is inconsequential and one may rely on the theoretical results. Thus, in 2012 our MD simulations were directed to clarify whether the observed He-bubble formation is artificial due to necessary use of high He-fluxes in the simulation or not. If shown to be artificial, one could argue that the peeling effect could not happen in reality. Otherwise, one needs to take special care when using Be as a plasma-facing material.

By checking the destruction of the Be-surface at various BC, and size of the MD-cell, we have found that the “peeling” process starts at almost constant ratio between the number of He-atoms accommodated by the Be-cell and the total number of Be-atoms. The time to reach destruction scales linearly with the size of the MD-cell. This indicates that the cell destruction starts at the same fraction of the broken interlayer bonds. Under realistic conditions, these broken Be bonds might be recovered because of the low incident doze and larger time between the adjacent He collisions. If one neglects the recovering process, then, the lifetime of the real Be surface can be estimated from the time when the Be real crystal reaches He saturation shown in the current MD experiments.

CONCLUSION

Systematic MD experiments have been performed for large MD cells and various and boundary conditions. The general atomic scenario, which was suggested earlier for Be swift erosion, has been confirmed.

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