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Interaction of hydrogen and helium with nanometric dislocation loops in tungsten assessed by atomistic calculations

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ABSTRACT

The interaction of H and He interstitial atoms with ½⟨1 1 1⟩ and ⟨1 0 0⟩ loops in tungsten (W) was studied by means of Molecular Static and Molecular Dynamics simulations. A recently developed interatomic potential was benchmarked using data for dislocation loops obtained earlier with two other W potentials available in literature. Molecular Static calculations demonstrated that ½⟨1 1 1⟩ loops feature a wide spectrum of the binding energy with a maximum value of 1.1 eV for H and 1.93 eV for He as compared to 0.89 eV and 1.56 eV for a straight ½⟨1 1 1⟩{1 1 0} edge dislocation. For ⟨1 0 0⟩ loops, the values of the binding energy were found to be 1.63 eV and 2.87 eV for H and He, respectively. These results help to better understand the role played by dislocation loops in H/He retention in tungsten. Based on the obtained results, a contribution of the considered dislocation loops to the trapping and retention under plasma exposure is discussed.

1. Introduction

Tungsten (W) is the material to be used for ITER plasma-facing components (PFCs) [1], selected due to its low sputtering yield, high melting point and high thermal conductivity. However, the impact of neutron irradiation in synergy with high heat flux plasma exposure is still to be assessed with respect to the structural integrity [2] and hydrogen isotope retention [3]. In the ITER divertor, the plasma-facing materials will be exposed to a very high plasma flux ($\sim 10^{24}$ D/m^{2}s) [4] with the ion energies lower than 100 eV, i.e., well below the atom displacement threshold (the energy needed to generate a stable Frenkel pair), and the implantation range will be limited to several nanometers. Subsequently, trapping of hydrogen (H) isotopes and helium (He) will be defined by the natural structural defects and neutron-induced defects. By now, many experimental and computational works have been dedicated to the assessment of trapping due to natural defects, such as vacancies, grain boundaries and dislocations (see e.g. [5–9]).

Under neutron irradiation, besides the conventionally accepted traps, dislocations loops (DL) are to be accounted for because these defects are the primary microstructural features observed directly by transmission electron microscopy (TEM) under in-situ irradiation of W in the ITER-relevant temperature range [10]. Dislocation loops of both types ½⟨1 1 1⟩ and ⟨1 0 0⟩ are formed and their relative fraction depends on irradiation temperature as well as on tungsten purity. In addition to the cascade-producing damage, the dislocation loops have been regularly observed in tungsten under high flux plasma exposure [11] by TEM as well. Presumably, the DLs are formed either as a result of the loop-punching mechanism of H bubble growth or due to sub-surface plastic deformation induced by thermal shock. DLs should exhibit stronger binding as compared to straight screw dislocations, moreover ⟨1 0 0⟩ loops are expected to be stronger traps then ½⟨1 1 1⟩ types. The purpose of this work is to clarify the strength of ½⟨1 1 1⟩ and ⟨1 0 0⟩ dislocation loops as traps for H/He interstitial atoms as well as to investigate possible pipe-type diffusion mechanisms of H/He in the core of the loops.

2. Computational details

Given the need to consider nano-metric sized dislocation loops, as experimentally observed, the work was carried out using classical Molecular Dynamics (MD). Simulations were performed using

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LAMMPS [12]. The embedded atom method (EAM) ("EAM2" version as stated in the original paper) interatomic potential for W-H-He system from [13] was used. This potential uses the second version of the EAM potential for W-W interaction from [14]. Previously, the pure W potential was validated with respect to different properties including the dislocation relevant features (see [15] for a review) as well as the H/He-vacancy interaction has been fitted in the original work [13]. As of now, we are not aware of another W-He-H interatomic model for large-scale calculations wherein both dislocation and He/H features are incorporated and validated using *ab initio* data.

Molecular Static (MS) calculations were performed by means of conjugate gradient algorithm implemented in LAMMPS with relative ($\Delta E_{tot}/E_{tot}$) energy change between relaxation steps of 10^{-10} as a stopping criterion. The size and the crystallographic orientation of the principal axes of the model crystal depended on the type of the loop considered. For the loops with Burgers vector $\langle 1\,0\,0\rangle$, cubic boxes with the axes orientation of x: $\langle 1\,0\,0\rangle$, y: $\langle 0\,1\,0\rangle$, z: $\langle 0\,0\,1\rangle$ were used. The dislocation loop was created by replacing two atomic planes of atoms along x direction with $\langle 1\,0\,0\rangle$ dumbbells within the required dislocation loop radius in the y-z plane. For the loops with Burgers vector $\frac{1}{2}\langle 1\,1\,1\rangle$ the model boxes with the axes orientation of x: $\langle 1\,1\,1\rangle$, y: $\langle -1\,-1\,2\rangle$, z: $\langle 1\,-1\,0\rangle$ were used. The dislocation loop was created by replacing three planes of atoms along x direction with $\langle 1\,1\,1\rangle$ dumbbells within a required radius in y-z plane. The size of the box was varied from 10^4 to 1.5×10^6 atoms depending on the loop size. The lattice constant a_0 was equal to 0.314 nm. The formation energy of the loop was calculated as the difference between the total energy of the system containing the loop and the total energy of the perfect crystal containing the same amount of atoms with the following formula:

$$E_{form} = E_{loop} - N_{at}E_{at} \quad (1)$$

where E_{loop} is the total energy of the system containing the loop, N_{at} is the number of atoms in the system, E_{at} is the energy per atom in ideal bulk material predicted by the potential.

The binding energy of H and He atoms with the loops was calculated by placing the He/H atom in a tetrahedral position close to the loop and relaxing the system. The region around the loop was scanned in this way in order to investigate all possible attractive positions. The value of the binding energy was calculated using the following expression:

$$E_B = E_{GA} + E_{loop} - E_{GAloop} - N_{at}E_{at} \quad (2)$$

where E_{GAloop} is the total energy of the system when a He/H atom is attached to the dislocation loop, E_{loop} and E_{GA} the total energy of the system containing only a He/H atom in a tetrahedral position or only a dislocation loop, respectively. $N_{at}E_{at}$ (same as above) is introduced to respect the particle number balance and to compensate for the different number of matrix W atoms present in the configurations corresponding to E_{GAloop}, E_{loop} and E_{GA} energies.

3. Results and discussion

3.1. Benchmark calculations

In order to calculate the dislocation loop formation energy as well as the He/H atom binding energy it is important to eliminate any artefacts of the calculations related to the limited size of the model system. We tested different box sizes for each of the considered loops. The results are shown in Fig. 1(a). The box size is reported in lattice units. It can be seen that the formation energy decreases with the box size dimension reaching a plateau beyond a certain box size. This behavior is explained by elastic interaction of the loop with its image via periodic boundaries. From these calculations, we chose the box size to minimize the self-interaction and ensure constant formation energy of the loop vs. box size. Typically, it is enough that the loop is surrounded by ~10 a_0 of ideal atomic structure in all directions to accommodate the elastic stress. This is also confirmed by calculating the pressure distribution across the loop habit plane as shown in Fig. 1(b) for the $\frac{1}{2}\langle 1\,1\,1\rangle$ loop done by means of the virial calculation procedure embedded in LAMMPS [16]. As can be seen 80% (higher than 0.06 Mbar) of negative pressure is localized within 1 nm (~$3a_0$)distance from the loop and within 2 nm (~$6a_0$) within the positive pressure part, which substantiates our choice for the dimensions of the MD boxes. The pressure distribution for the $\langle 1\,0\,0\rangle\{1\,0\,0\}$ loop is not shown here but remains qualitatively the same as for the $\frac{1}{2}\langle 1\,1\,1\rangle\{1\,1\,1\}$ loop.

The stability of the nanometric dislocation loops was studied in [17] using the EAM potentials by Ackland [18] and by Derlet [19]. The Authors considered the loops with the Burgers vector $\langle 1\,0\,0\rangle$ and the habit plane {100}, and the Burgers vector $\frac{1}{2}\langle 1\,1\,1\rangle$ with the habit plane {1 1 1} and {1 1 0}. In Fig. 2, we present the formation energy of the DLs calculated here and add data from [17] for comparison. We did not find any significant difference in the formation energy for the $\frac{1}{2}\langle 1\,1\,1\rangle\{1\,1\,1\}$ and the $\frac{1}{2}\langle 1\,1\,1\rangle\{1\,0\,0\}$ loops and thus we report only the formation energy for the $\frac{1}{2}\langle 1\,1\,1\rangle$

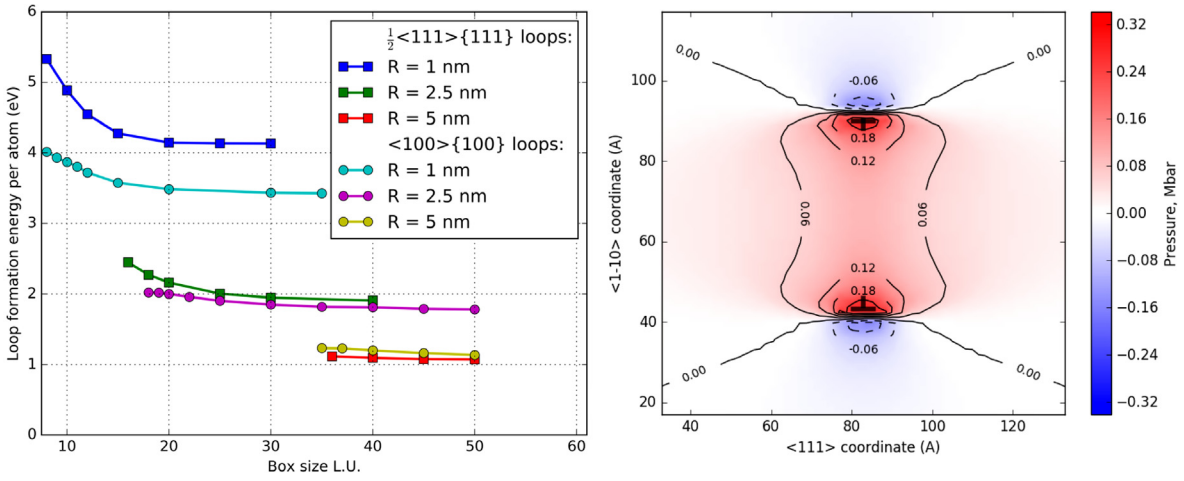

Fig. 1. (a) Loop formation energy per atom depending on the size of the model box given in lattice units (L.U.) (b) pressure distribution around a $\frac{1}{2}\langle 1\,1\,1\rangle$ dislocation loop with 5 nm radius along the Burgers vector. The limits of dislocation loop are marked by the ⊥ and ⊤ symbols. The red area of the colorcode corresponds to compressive and the blue area corresponds to tensile pressure. The contour plot is added for convenience and for the black and white version of the article.

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