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Simulation of displacement cascades in tungsten irradiated by fusion neutrons

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ABSTRACT

Numerical calculations of damage in tungsten irradiated by fusion neutrons were performed using molecular dynamics simulations combined with an embedded atom method potential. The displacement cascade efficiency has been calculated using the ratio of the number of Frenkel pairs determined by molecular dynamics simulations to the number of Frenkel pairs derived from Norgett–Robinson–Torrens formula. The cascade efficiency decreases as the Primary Knock Atoms increases. The Norgett–Robinson–Torrens calculations overestimate the Frenkel pair defect production by a factor of 2. The changes in the cascades dimensions at the early stages after irradiation indicate that the tungsten interstitials are more mobile than the vacancies. We found that the most common types of defects are single vacancies, di-vacancies, vacancy-clusters, interstitials and small number of interstitial clusters containing more than three atoms.

1. Introduction

The purpose of our study is to perform numerical calculations to understand the defect creation processes in tungsten as a result of fusion-induced 14 MeV neutron irradiation. Tungsten and tungsten alloys have high melting temperature, high thermal conductivity and low sputtering erosion. Tungsten is considered as potential plasma facing materials for divertor plates in future fusion power reactors [1,2]. Plasma facing materials have to resist a high neutron flux and a high thermal flux. The thermal flux is expected to be 10 MW m^{-2} in the ITER (International Tokamak Experimental Reactor) [3]. The plasma facing materials will protect the first wall from the high particle flux and transfer the thermal energy away from the first wall surface. The plasma wall interaction with tungsten requires better knowledge in order to model the long term behaviour of the material for understanding the mechanisms and effects of neutron irradiation on the first wall of the fusion reactor. The fusion reaction (d, t) produces 14 MeV neutrons and energetic 3.5 MeV alpha particles. Tungsten has low hydrogen isotope retention. Helium is induced in the tungsten sample by the 14 MeV neutrons through the (n, α) nuclear reaction. In tungsten, helium atoms bind with self-interstitial atoms, vacancies, impurities and hydrogen [4].

Ab initio calculations on intrinsic point defects and He in tungsten have been performed to determine the behavior of self-interstitial atom the vacancy, vacancy-cluster and He in tungsten [5]. The calculated value of 3.11 eV for the vacancy formation energy is different from the experimental value of 4.0 + 0.3 eV as determined by Doppler broadening measurements of the positron annihilation gamma-line [6] in the temperature range from 4.2 to 3462 K. We note that the model calculations [5] were performed for a temperature of 0 K while the experimental results [6] are obtained for temperatures from 4.2 to 3462 K, close the melting point of tungsten. A neutron entering the lattice transfers part of its energy to atoms, called the Primary Knock Atoms (PKA). Irradiation by 14 MeV fusion neutrons produces displacement damage in the form of Frenkel pairs (FP), vacancies, vacancy clusters and dislocation loops. The high energy of PKA created as a result of elastic and inelastic neutron scattering may leave their lattice sites and transfer their energy to other lattice atoms, forming displacement subcascades. It is known that neutron irradiation after long term operation induces changes in the microstructure and thus degrades the mechanical properties. Molecular dynamics (MD) simulation is an excellent tool to probe information for the primary state of damage due to displacement cascades in materials. Typical length scales of MD method are of order of nano-meter and it operates in the pico-second timescale. The molecular dynamic calculations performed by Guinan and Kinney [7] show that in the collision phase the maximum number of defects are formed. A rapid decrease of defect concentration is obtained in the relaxation phase and recombination takes place in the cooling phase, due to the defect migration. Xu et al. [8] performed molecular dynamic simulations of vacancy diffusion in tungsten induced by irradiation. The displacement threshold and recoil energies for vacancy-migration depend on the orientation directions. The recoil atom interacts not only with the nearest neighbor vacancies but also with the next

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near neighbor vacancies. Zhong et al. [9] performed defect production in 20–30 keV self-ion bombardment tungsten by molecular dynamic computer simulations. Their results show good agreement between the computer simulations for vacancy-clusters and interstitial atoms formation obtained in Field Ion Microscopy experiments. Formation of interstitial loops in tungsten [10] by helium ion irradiation has been studied by transmission electron microscopy [TEM] measurements and numerical model calculations of defects accumulation based on the kinetic rate theory. Fikar and Schaeublin [11] perform MD simulations to study the influence of different tungsten inter-atomic potentials on the amount and type of radiation damage. They applied the universal potentials of Biersack and Ziegler [12] and Ziegler–Biersack–Littmark (ZBL) [13] for short-range interactions. For long-range interactions two empirical EAM potentials, namely of Finnis–Sinclair [14] and Ackland–Thetford [15] have been used during the MD simulations. By application of these potentials [12–15] no important difference in the defects produced, the defect number or defect densities has been found. The universal ZBL [13] potential could be used with success in the simulations at small inter-atomic distances less than 0.16 nm. Caturla et al. [16] investigated cascade efficiency and defect distribution in 1.9 GeV proton irradiated tungsten. Their results show that vacancies in tungsten are isolated. There is no vacancy clustering formation for recoil energy of 30 keV. In tungsten at 50 keV a sub-cascade formation has been found. The properties of defects in tungsten containing hydrogen and helium atoms have been investigated by model positron lifetime quantum–mechanical calculations [17]. The hydrogen and helium atoms are trapped in tungsten by lattice vacancies and nano-voids. The presence of hydrogen and helium in the larger nano-voids considerably decreases the positron lifetime. The object of present work was to simulate displacement cascades in tungsten in order to predict the evaluation of defects, by using MD simulations combined with the EAM potential. In addition we calculate the time evolution of the defects in tungsten after neutron irradiation from 5 to 30 ps at a temperature of 300 K for PKA energies 10, 20 and 40 keV. The vacancy and interstitial clustering were also studied as a function of the PKA momentum distribution.

2. Methodology of the simulation

The multi-scale approach [13,18] has been applied in our numerical investigation. Initially we studied the number of displacements per atom (dpa) created by the fusion neutrons. For this purpose we used the NPRIM code [19]. Different approaches are necessary for the simulation of defects in tungsten under irradiation with high energy neutron fluence at about 2.5×10^{22} n/cm^2. The fast neutrons create in tungsten recoils whose kinetic energy is in the range from 1 to 100–200 keV, therefore the methods of molecular dynamic (MD) and kinetic Monte-Carlo (kMC) are applied for calculating damage evolution during the irradiation. Displacement cascades start when PKA receives an energy higher than a few hundreds eV. The produced defects, in fusion materials usually have PKA energies below 100 keV [18]. It is interesting to note that the created displacement cascades are also at the same PKA energy range. At higher PKA energies the crystal structure – the effect of the lattice periodicity of tungsten plays not remarkable role. The multi-particle interactions at higher energies are less important. In our simulations for PKA energies 1–40 keV the modified MD code MDCASK [20] was used for calculation of the radiation induced damage. The simulations have been performed until the end of the cascade phase. The model tungsten structure is bcc with a lattice unit length $a_0 = 3.165$ Å. The size of the simulation domain was chosen according to the PKA energy. The number of atoms in the simulation domain was in the range from 1.2×10^6 up to 1.5×10^6. This corresponds to the sizes of simulation box $90 \times 90 \times 90$ unit cells for PKA energies from 1 to 40 keV. This is enough for accurate presentation of displacement cascades even at their earliest stages of creation. The large amount of atoms included in the simulation and the average time of displacement cascades requires a parallelization of the algorithms with purpose to reduce the simulation time. Fully parallelized calculations were carried out on Core 2 Duo and Core 2 Quad 2.8 GHz processors with 8 Gb RAM. The time required to compute a single cascade depends on the size of simulation domain, the neutron energy, and the inter-atomic potentials. The periodic boundary conditions were assumed for all simulations. We simulated the defect creation and time evolution at 300 K. Additionally, reference calculations at a temperature of 4 K were carried out in order to determine the defects distribution due to the displacement cascades. In MD simulations the quantum mechanical nature is represented by the inter-atomic potentials. The simulation accuracy of defects creation due to the displacement cascades initiated by PKA depends on the quality of inter-atomic potentials used to calculate the inter-atomic forces. On this base, the inter-atomic potential is critical to a realistic simulation of the tungsten structure and the correct calculation of energies associated with the formation of defects. The embedded atom method (EAM) potential for tungsten, developed by Ackland and Thetford [15] as well as Zhou et al. [21] has provided a good potential format for tungsten atoms. The EAM potential for tungsten found in [15] has been applied in our numerical studies. The crystal energy according to the EAM is the sum of pair-wise potential and an energy required to embed an atom into a local electronic medium in which the interaction between the atoms depends on the position of their neighbors. The embedding energy in EAM for local environment of the potential depends on the local electron density and therefore has been successfully used for investigation of the defect structure. We easily adapted the generalized EAM potential for our purpose to calculate defect creation in fusion neutron irradiated tungsten, containing hydrogen and helium. Calculations were performed with initial kinetic PKA energies of 1–40 keV. In the first step of the simulation, the tungsten atoms are placed in their equilibrium position centred at 300 K with an initial velocity. To start the displacement cascade, a tungsten atom becomes a velocity corresponding to the recoil kinetic energy. This atom is the PKA which creates the displacement cascade. The initial positions of PKA were chosen in such a way that the crystal tungsten lattice has the smallest initial energy. The initial direction of the tungsten PKA atoms was selected to be different from the main crystallographic axis in the bcc lattice, in order to avoid channelling. The tungsten atoms and PKA positions in the lattice were recorded at regular intervals of 5 ps. The chosen time step was small to ensure energy and momentum conservation during the MD simulation. The whole simulations were set up to calculate the lattice dynamic up to 30 ps. During the displacement cascade the kinetic energies of the PKA and the displaced atoms are higher than the thermal kinetic energy. The output of the MD results were analyzed, using the atom positions, calculated at 4 K as a reference. Vacancies and interstitials positions were obtained by the space-filling Wigner–Seitz cells method [22]. According to this method for creation of vacancy clusters are taken the first and second nearest neighbor atoms, while for interstitials clusters only the first nearest neighbor atoms. Atoms, which have lees than two lattice constants outside the initial simulation cell were included in the calculations.

3. Results and discussion

A set of atomic displacement cascades in tungsten for a range of the PKA initial energies from 1 to 40 keV has been carried out. The