Simulation of defects in fusion plasma first wall materials

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Abstract. Numerical calculations of radiation damages in beryllium, alpha-iron and tungsten irradiated by fusion neutrons were performed using molecular dynamics (MD) simulations. The displacement cascades efficiency has been calculated using the Norgett–Robinson–Torrens (NRT) formula, the universal pair-potential of Ziegler–Biersack–Littmark (ZBL) and the EAM inter-atomic potential. The pair potential overestimates the defects production by a factor of 2. The ZBL pair potential results and the EAM are comparable at higher primary knock-on atom (PKA) energies (E > 100 keV). We found that the most common types of defects are single vacancies, di-vacancies, interstitials and small number of interstitial clusters. On the bases of calculated results, the behavior of vacancies, empty nano-voids and nano-voids with hydrogen and helium were discussed.

1. Introduction

The paper is devoted to numerical calculations of cascade effects due of 14 MeV neutron irradiation and the defect creation processes in fusion materials. The purpose of this study is to perform numerical calculations to understand the defect creation processes in beryllium, alpha-iron and tungsten as a result of fusion 14 MeV neutron irradiation. The fusion reaction (D, T) produces 14 MeV neutrons and energetic 3.5 MeV alpha particles.

\[
\text{D-T Fusion Reaction: } D + T \rightarrow ^4\text{He} + n
\]

Alpha particle (He nucleus):
\[20 \% \text{ of reaction energy}\]
Neutron:
\[80 \% \text{ of reaction energy}\]

In the last years the study of the evolution of radiation defects in tungsten under fusion neutron irradiation increased, due to the requirements of fusion reactor technology. Beryllium alpha-iron, tungsten and tungsten alloys are considered as one of the major materials for the first wall of the upcoming new generation fusion prototype reactors [1] ITER (International Tokomak Experimental Reactor) and DEMO aimed at demonstrating the technical feasibility of electrical power production by means of (D,T) fusion reaction. 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 [2]. The plasma facing materials will protect the fist wall from high particle flux and they will transfer the thermal energy away from the first wall surface. The reason for the selection of Be is the low effect on plasma...
contamination due to the low Z, low radiative power losses, good oxygen gettering ability, absence of chemical sputtering in comparison with carbon and the possibility of in situ repair of damaged surfaces. On the other hand in the fusion reactor beryllium could play an important role as a neutron multiplier to sustain tritium breeding. This is especially important for the present design of the solid breeder blankets of the DEMO reactor [1] since the resulting low energy neutron flux spectrum necessary for tritium breeding via \(^4\text{Li}(n, n')\ ^4\text{He} + \ ^3\text{H}\) reaction is due to beryllium neutron moderation. Iron is considered as one of the major materials for the first wall of the upcoming new generation fusion prototype reactors. Its function would be the protection of actively cooled wall structures from high heat fluxes in order to sustain the component lifetime and the plasma compatibility. Another reason for the selection of Fe would be its ability to produce only stable or very short lived Mn and Cr isotopes due to nuclear transmutations caused by fusion neutrons. Additionally iron and the stainless steel are widely used low cost materials which would significantly lower the costs of the first wall (FW) blanket. Several nuclear facilities are proposed [2] for experimental studies of irradiation defects on material due to the neutron flux from ITER and DEMO. Another approach relays on numerical simulations of the beryllium response to the intensive high-energy neutron irradiation. The validation of the performed defect simulations for vacancies and interstitials in first wall fusion materials could be done by experimental transmission electron microscopy (TEM) or positron annihilation spectroscopy measurements (PAS). TEM cannot be used for investigation of nano voids smaller than 2 nm, while PAS allows the local investigation of single vacancies di-vacancies and nano-voids smaller than 2 nm.

2. Methodology of the simulation

Different approaches are necessary for the simulation of defects in fusion materials under irradiation with high energy neutron fluence at about 2.5×10\(^{22}\) n/cm\(^2\). The method of molecular dynamic (MD) and kinetic Monte-Carlo (kMC) could be applied for calculation of the damage evolution of PKA down to 10 keV. The fast neutrons create recoils, whose kinetic energy is in the range from 1 keV to 1–2 MeV. In order to achieve our goal we have used the multi-scale approach [3]. Most of the produced defects in fusion materials posses PKA energies below 50 keV [4]. 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 plays not remarkable role. We created a computer Monte-Carlo code based on Geant 4 CERN package to simulate ion and neutron interactions in homogeneous target at high energies (E > 0.1 MeV). High-precision Geant4 NDL ver. 3.20 database for neutron interaction cross sections (up to 20 MeV) was used. The PKAs (primary knock-on atoms) were calculated in 30×30×30 nm\(^3\) volume on the neutron beam axis. SRIM calculations using ZBL [5] potential were carried out to determine the defect distribution. Initially we studied the number of displacements per atom (dpa) created by the fusion neutrons. For this purpose we used the NPRIM code [6]. The pair-potential that depends only on the atomic separation of two atoms can be used for defect calculations. At higher energies (>100 keV) we applied the universal pair-potential of ZBL for calculation of defects creation in fusion materials. In our simulations for energies below 50 keV the modified MD code MDCASK [7], was used for calculation of the radiation induced damage. The time required to compute a single cascade depends on the size of simulation domain, the neutron energy, and the interatomic potentials. 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 4.32×10\(^5\) up to 1.5×10\(^6\). This corresponds to sample sizes from 60 to 90 inter-atomic distances in all directions. 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 4K were carried out in order to determine the defects distribution due to the displacement cascades. The embedded atom method (EAM) potential, developed by Daw and Baskes [8] has provided a good potential format for metal atoms. 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 neighbours. The embedding energy in EAM for local environment of
the potential depends on the local electron density and therefore has been successfully used to solve problems like surface structures and defect states. We easily adapted the generalized EAM potential for our purpose to calculate defect creation in fusion neutron irradiated beryllium, alpha-iron and tungsten, containing hydrogen and helium.

Using Monte-Carlo (MC) simulation we have calculated the atom displacements caused by fusion materials PKA. At the end of the simulation the final position of the atoms involved in damage cascades have been recorded. The statistical methods were applied to calculate the atom displacements and the number of the produced vacancies and interstitials as a function of the PKA energy for the created isotopes. The processes like neutron elastic and inelastic scattering, neutron capture with and without emission of charged particles were taken into consideration in the Fusion materials matrix. The low energy processes like gamma ray and secondary electron emissions as well as all types of electromagnetic interaction of charged particles and photons with matter were included in the present calculations. Nuclear transmutations which play an important role in helium, deuterium and tritium formation were also taken into account. The number $N$ of Frenkel pairs produced per cascade has been estimated by the NRT formula [9].

$$\text{NRT} = \frac{0.8E_{PKA}}{2E_d},$$

where $E_{PKA}$ is the initial PKA energy and $E_d$ is the displacement energy for the creation of a stable Frenkel pair.

3. Results and discussions

First we have simulated the interaction of neutrons with macroscopic Be target at high energy ($E > 0.1$ MeV). For this purpose the fusion neutron spectrum data was taken from the experiment as an input for the simulation. In the present work the initial neutron energy distribution for the simulation was taken from [5]. The total number of primary events used in the simulation was $2 \times 10^9$ which resulted in a neutron fluence of about $1.6 \times 10^{20}$ n/cm$^2$ ($E > 0.1$ MeV). Nuclear transmutations were also taken into account [10]. The $^7$Li production has threshold of 12 MeV and therefore it takes place in the fusion reactor. If we scale the result for the neutron flux of $1.3 \times 10^{15}$ n/cm$^2$/s expected for the DEMO first wall (FW) [2] our data are in agreement with the available ones in the literature [11,12] although our results are obtained by different procedure. It is well known that the main parameter which carries the information about the radiation resistance of the material is the dpa (displacement per atom). It has been established that this parameter reaches the value of 30 dpa/fpy (dpa per full power year of operation) for iron irradiated by fast neutron fluxes up to $1.3 \times 10^{15}$ n/cm$^2$/s [13]. The results for dpa cross section vs. various neutron energy are shown in figure 1.

![Figure 1. dpa cross section for a typical deuterium-tritium reactor for different types of neutron interactions as a function of the neutron energy](image)

Important process is the neutron capture in Be with gamma ray emission. Its magnitude is relatively small but it is important for the tritium production. Our calculations show that the threshold for the $(n,n^0)$ induced dpa is about 2 MeV and for the $(n,n^0)$ is about 1 MeV. The dpa due to elastic...
scattering was present at the whole energy range \((0.1−14 \, \text{MeV})\) in the present simulation. The dpa cross sections for \((\text{n,n}^0)\) grow rapidly up to about \(4 \, \text{MeV}\), after that they reach saturation. The next step in our computer simulations was to carry out nano-structural damage calculations using the results from the described high-energy neutron interactions. For this purpose we used the binary collision approximation (BCA) and the SRIM MC code [14] because it relays on the universal pair potential of ZBL [5, 15]. In this approach the crystal structure of Be has been neglected. Beryllium has been considered as a homogeneous continuous medium. For each cascade we consider the displacement collisions, vacancy production, replacement collisions and interstitial atoms, as described below. The number of displacement collisions records how many target atoms were set in motion in the cascade with energies above their displacement energy which is specified at the input. The Be target vacancies are next items which were recorded. The stopped recoil atom can take position at some distance from its vacancy. When after inducing a displacement cascade it leaves the target, the sum of interstitials will be less than the number of vacancies by the loss of that atom. In our computer simulation both Be and He PKA could induce displacement cascades. In the simulation the average displacement energy \(E_d\) has been chosen to be 40 eV. The lattice binding energy was taken to be 3.32 eV equal to the cohesive energy of the Be crystal. Tritium created by neutron irradiation of Be behaves as trapped ones. The implanted tritium never diffuses into the bulk of the material and becomes trapped at ITER operating temperatures [16]. According to calculations [17, 18] the total tritium inventory in the beryllium first wall armor due to implantation, diffusion, trapping, and breeding after 12000 pulses will be of 100−250 g [16]. Tritium could be well localized in bulk Be at ITER and DEMO temperatures but the tritium concentration could increase locally due to trapping of tritium by single vacancies and vacancy clusters (nano-voids). These types of defects are due to the large amount of displacement damage cascades as a result of intensive neutron irradiation. We have shown that for neutron fluences \((E > 0.1 \, \text{MeV})\) up to \(2.5 \times 10^{22} \, \text{n/cm}^2\) the damage level reaches the value of 11 dpa/fpy. This value is in agreement with that found in [19, 20]. It was established in our calculations that the total damage of 0.06 dpa for neutron fluence of \(1.6 \times 10^{20} \, \text{n/cm}^2\) scales well with already reported results for \(2.5 \times 10^{22} \, \text{n/cm}^2\) [6]. As discussed in [21] the smallest He gas bubbles with sizes in the range of 1−4 nm appear when the annealing temperature was 500 °C. Helium was not found at temperatures below 400 °C. They concluded that the He atoms were trapped in subatomic complexes. According to [21] the defects in neutron irradiated Be should be interstitials and dislocation loops although they can be distributed throughout the structure non-uniformly.

![Figure 2. Cascades length as a function of the energy of PKA for Be(left) and He (right)](image-url)

The neutron irradiation of beryllium over the temperature range up to 500 °C leads to formation of radiation-induced plane defects. The cascades length distribution for both Be and He PKA is presented in figure 2. In the Figure it is seen that He recoils have higher initial kinetic energy but they cause approximately 2−3 times less dpa. We have established that the calculated number of the replacement collisions which lead to recombination of vacancies and self-interstitials was only 1.8 % compared to the total number of displacements. This result indicates that high-energy recoils generate atomic collision cascades in Be in which a fraction of the defects recombine during the cooling phase.
The calculated results of the Be sub-cascades as a function of the PKA energy are shown in figure 3. They indicate a correlation between PKA energies and the number of sub-cascades. It is seen in figure 3, that PKA with higher energies produce large number sub-cascades. It is seen that Be PKA energies in the range 20–120 keV have higher probability to induce sub-cascades. Obviously the most probable number of sub-cascades is around 50. Similar results are discussed in [15, 21, 22]. The authors pointed out that for PKA with energy higher than some critical value in the range of 10–40 keV the formation of sub-cascades is more probable. Our simulation results show that low energy cascades (\(E < 100\) keV) are responsible for about 70 % of the defects production.

**Figure 3.** Correlation between the number of Be PKA sub-cascades and the energy.

The distribution of vacancies created by beryllium atom displacements and helium atoms created by neutron capture in Be is shown in figure 4. The crystal structure of Be was not taken into account for the calculation of the Be dpa in the present model. It has been used the pair potential of ZBL [5].

**Figure 4.** Distribution of vacancies and helium created by beryllium recoil the domain size is 60×30×30 nm³.

It is seen from figure 4 that large amount of helium atoms are stopped outside of the single vacancies or vacancy clusters after the ballistic phase of the cascades. The He atoms we considered as interstitials which contribute to the interstitial clusters concentration. The solution of this problem has
been done by using the methods of gas diffusion in solids, the kinetic Monte-Carlo (kMC) approach [23] and the kinetic rate-theory [24]. Experimental data of the He and T kinetics in neutron irradiated Be were presented in [25]. Most of the He atoms precipitated into bubbles and are released during abrupt of pores at 1500 K. The explanation of He nucleation in bubbles and its release at high temperatures was done in [25]. The same authors applied the kinetic-rate theory for calculation of the time evolution of the He concentration in bulk and in bubbles. This is an important macroscopic property which gives information about the He migration in the Be sample 2000 seconds after the displacement cascade.

We apply the multi-scale approach [26] to study the damages in Fe lattice caused by intensive fusion neutron irradiation. First we have simulated the interaction of neutrons with macroscopic iron target at high energy ($E > 0.1$ MeV). For this purpose the fusion neutron spectrum data was taken from the experiment as an input for the simulation. We have recorded the initial energy and position of iron primary knock-on atoms (PKA) and of all isotopes created in the nuclear reactions at the output of the calculation. The obtained results allowed us to calculate the concentration of Fe, Mn and Cr isotopes as well as the concentration of helium and deuterium and used it as an input for the next step in our simulation.

In figure 5(a) is shown the total neutron interaction cross section in $^{56}$Fe taken from the ENDF/B database and used in our simulation. The resonance structure is dominant for the neutron interactions at energies lower than 3 MeV. At neutron energies higher then 5 MeV up to 14.1 MeV the neutron interaction cross section is almost constant and has the value of about 5 barn. In figure 5(b) are shown the production cross sections of $^4$He and $^3$H used in our numerical modeling. The integral cross section for $^4$He production is about 200 times lower than the total neutron interaction cross section in $^{56}$Fe. Therefore one could expect that the most of the created defects are due to Fe recoils as a result of neutron elastic and inelastic collisions.

The next step in our computer simulations was to carry out structural damage calculations using the results from the described high-energy neutron interactions. Every PKA from the high energy neutron interaction with Fe atoms was tracked down to its stop in the medium. For each cascade we consider the displacement collisions, vacancy production, replacement collisions and interstitial atoms, as described below. The number of displacement collisions records how many target atoms were set in motion in the cascade with energies above their displacement energy which is specified at the input.
Our SRIM-based calculations show that the damages, produced by fast neutron fluence up to $8 \times 10^{19}$ n/cm$^2$, correspond to 0.151 dpa. The total damages of 37.2 dpa/fpy were calculated using the NPRIM code [5]. $^4$He and $^{53}$Cr concentration was calculated to be about 0.4 appm. According to calculations using the NPRIM code [5] it reaches 375 appm/fpy. Those values are in a good agreement with the results, obtained in [13]. The $^2$H and $^{55}$Mn concentrations were determined to be about 7 % of the He concentration. In order to investigate the influence of the energy distribution of the $^{56}$Fe PKAs, created as a result of fusion neutron induced nuclear reactions, we have calculated the total number of defects in displacement cascades as a function of the PKAs energy. The result is shown in figure 6. Most probable cascades have between 50 and 150 displacements. We have found that they are well concentrated in the PKA energy range up to 10 keV. The maximal damage is caused by PKAs with energy around 30 keV. PKAs with higher energies could produce more displacements but the number of such cascades is small probably due to the fact that the most efficient energy transfer in $^{56}$Fe occurs at lower energies. If the PKA has enough energy it can produce secondary recoils which could initiate additional cascades.

In our simulation we obtained values for the number of such sub-cascades as a function of the PKA energy. The results indicate that $^{56}$Fe PKA energies up to 50 keV have higher probability to induce sub-cascades. We determined that the most probable number of sub-cascades is around 150. Similar results are discussed in [12,13]. We established that low energy cascades ($E < 100$ keV) are responsible for about 90 % of the defects production. In our simulation we investigated the vacancy and self-interstitial recombination due replacement collisions. We found that the number of recombination processes was about 2.5 % of the total number of displacements. In the last step in our multi-scale model calculation we determined the depth profile of the vacancy distribution inside the $^{56}$Fe sample. The result is shown in figure 7. It indicates that although the damages are created in a volume of $30 \times 30 \times 30$ nm$^3$ the damage extends up to 400 nm.

The distribution has a sharp maximum in the area where PKAs are created as a result of the neutron interactions. As we already shown this fact can be explained with the large probability of the damage creation due low energy PKAs. The small maximums in the distribution indicate the presence of sub-cascades.

Tungsten has low hydrogen isotopes retention. Helium is induced in the tungsten sample by the 14 MeV neutrons through the $(n, \alpha)$ nuclear reaction. Irradiation by 14 MeV fusion neutrons produces displacement damage in the form of Frenkel pairs i.e. self-interstitial atoms and vacancies. The high energy Primary knock-on atoms (PKA) in tungsten created as a result of elastic and inelastic neutron scattering may leave their lattice sites and transfer their energy to other lattice atoms thus forming...
displacement cascades. In the present work we use MD simulations combined with EAM potential to study defects formation in the presence of displacement cascades in tungsten. In addition we calculate the time evolution of the defects in tungsten after neutron irradiation from 5 ps to 30 ps at a temperature of 300 K. The PKA energies, range from 10 keV to 40 keV.

The EAM potential for tungsten found in [27] has been applied in our numerical studies. Calculations were performed for PKA with initial kinetic energies of 10, 20, 35 and 40 keV. The initial positions of PKA were chosen in such a way that the crystal lattice has the smallest initial energy. The initial directions of the tungsten PKA atoms were 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 whole simulations were set up to calculate the lattice dynamic up to 30 ps. The output of the MD results were analyzed, using the atom positions, calculated at 4K as a reference. Vacancies and interstitials positions were obtained by the Wigner-Seitz cell method [5]. We calculated the number of displacement atoms (dpa) in tungsten for Full Performance Year in unit dpa/FPY as a function of fast neutrons ($E > 0.1$ MeV) irradiation at a neutron fluence of $2.5 \times 10^{22}$ n/cm$^2$. A value of 2.85 dpa/FPY has been determined. When compared to beryllium and iron which are 11 and 30 dpa/FPY, respectively, we find that tungsten has the greatest radiation resistance against the fusion neutron irradiation among the candidates for first wall materials. This could be due to the large value of the crystal lattice bonding energy of tungsten. In order to investigate more precisely the radiation resistance of tungsten we calculated the density of stable Frenkel pairs created by PKA with different initial energy and momentum orientation. The number of created Frenkel pairs due to the displacement cascades is first determined by the NRT formula [9]. In our model for $E_d$ we used the value of 90 eV found in [10]. At the next step we compare our results for tungsten obtained by SRIM [12] and MD calculations using ZBL and EAM potentials [27]. The cascade efficiency is defined as the ratio between the number of Frenkel pairs, calculated by MD or SRIM models and the theoretical number of Frenkel pairs in the displacement cascade determined by the NRT formula.

![Figure 8. Frenkel pairs as a function of PKA energy in tungsten at 300 K.](image)

The cascade efficiency obtained by SRIM based on binary collision approximation shows large deviation for lower PKA energies ($E < 50$ keV) relative to the one of the MD with EAM potential results. The binary collision approximation overestimates the damages by factor of 2 at energies below 30 keV. Note that both models predict lower concentration of damages compared to the NRT formula [9]. Similar results have been obtained by Caturla et al [28], although they apply different method. We calculated by our MDCASK the number of stable Frenkel pairs as a function of the PKA energy 30 ps after the displacement cascade at temperature of 300K. The results are shown in figure 8.
A remarkable similarity is found between the cascade dimensions and PKA energy for (100), (010) and (001) lattice directions for vacancies. These results are similar to ones reported earlier for copper [29]. The differences exist in the cascades dimensions for tungsten which are generally 30% lower. The time evolution of the cascade dimensions for PKA energies from 20 keV to 40 keV is shown in figure 9, for vacancies and interstitials. In the case of vacancy calculation the interstitials and interstitial clusters are removed before the simulation. We start the simulations with the 10 keV cascade in tungsten as shown in figure 9. It is seen that there is a variation in the dimensions for vacancies at about 10% for time of 25 ps after the irradiation. The variation of the cascade dimensions in the case of interstitial is more prominent especially at lower energies. This is probably due to the high vacancy mobility and recombination, during the first stages of the displacement cascades in tungsten. Similar behaviour has been reported in [34, 35] although the interatomic potential and the simulation procedure have been different. On the other hand one can expect formation of single vacancies and di-vacancies, but not larger vacancy-clusters (nano-voids). The rise of the interstitial dimensions at 25 ps could be explained with the formation of sub-cascades which are difficult to be separated. The formation of sub-cascades leads to larger damage volumes compared to the case of a single cascade. We established that the formation of sub-cascades starts at PKA energy of 20 keV. Sub-cascades are dominant at energy of 40 keV. Our calculations using the Wigner-Seitz method show that in the early stages of the cascade the dominant are vacancies, interstitials and interstitial-clusters containing more than 3 atoms. The interstitial and interstitial clusters formation is about 2 times higher than those of vacancies at the same time scale.

**Figure 9.** Time dependence between the cascades dimensions evolution time for vacancies and interstitials for PKA energies from 20 to 40 keV in tungsten at 300 K.

4. Conclusions

Numerical simulations of creation of point defects in beryllium, alpha-iron and tungsten irradiated by intensive fast ($E > 0.1$ MeV) neutron fluence up to $8 \times 10^{20}$ n/cm$^2$ has been performed. Neutron interactions with first wall fusion materials like elastic and inelastic scattering, gamma ray emission and nuclear transmutations have been considered. The calculated damage of 0.06 dpa for Be was
compared to the available data and a good agreement was found. He content was determined to be 168 appm. $^7$Li content which is important for the tritium production was estimated to be 5 % of the He content. The probable cascade length for Be is between 100 and 150 dpa. The simulation results show that 70 % of the damages occur at Be PKA energies below 100 keV. The number of sub-cascades increases with the PKA energy and reach saturation at about 110 keV. The sub-cascade number is 50 for PKA energies close to 50 keV. The results indicate that the damages caused by He atoms are about 3 times less than damages caused by Be PKA. The final Be and He atoms distribution confirm that the most likely defects are single vacancies, divacancies and vacancy clusters. String-like small nanovoids with 5 and more vacancies are present but they are rare.

Point defects in $^{56}$Fe, irradiated by intensive fast $(E > 0.1 \text{ MeV})$ neutron fluence up to $8 \times 10^{19}$ n/cm$^2$ has been performed. The calculated damage of 0.151 dpa and 37 dpa/fpy was compared to the available data in the literature and a good agreement was found. 4He content was determined to be 0.4 appm. $^2$H content was estimated to be 7 % of the $^4$He content. The correlation between the PKAs energy and the damages was established. It was shown that the most vacancies are created by PKA with energy below 50 keV with maximum around 30 keV.

The damages produced by displacement cascades in tungsten, irradiated with intensive neutron flux have been calculated to be 2.85 dpa/FPY for a neutron fluence of $2.5 \times 10^{22}$ n/cm$^2$. The displacement cascades efficiency calculated by using the theoretical NRT formula is suitable only for rough estimation of the damages. The pair potential overestimates the defects production by a factor of 2. At higher PKA energy $(E > 100 \text{ keV})$ the ZBL pair potential results and the EAM are comparable. The results for 3-dimensional cascades structure indicate that cascades are extended in the direction of PKA momentum. The cascade dimensions at lower energies at the early stages after the irradiation indicate that the interstitial volume is about 2 times larger than the vacancies volume. The created defects are single vacancies, di-vacancies, interstitials and interstitial clusters containing more than 3 atoms.

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