Numerical Simulations of Displacement Cascades in Irradiated with Intensive Neutron Flux Iron

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Abstract. Numerical calculations of the radiation defects created in iron irradiated by fast neutrons \( (E > 0.1\) MeV\) were carried out. The total atom damages in iron at a neutron flux of \( 1.4 \times 10^{15} \) n/cm\(^2\)s\(^{-1}\) were determined to be 37.2 displacements per atom (dpa) per full power year (fpy). The helium concentration of 375 appm/fpy was obtained in irradiated iron for the same total neutron flux. A multi-scale numerical model has been developed in order to obtain better values for the neutron damages and the concentration of impurities. Using this approach the concentration of Fe, Mn and Cr isotopes as well as the concentration of helium and tritium has been determined as a result of the fast neutron irradiation.

1. Introduction
Iron is considered as one of the major materials for the first wall of the upcoming new generation fusion prototype reactors ITER and DEMO aimed at demonstrating the technical feasibility of electrical power production by means of (D,T) fusion reaction:

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\ ^2\text{H} + \ ^3\text{H} \rightarrow \ ^4\text{He} (3.5\text{ MeV}) + \ ^0\text{n} (14.1\text{MeV}).
\]

Iron has high radiation resistance, high chemical stability, low hydrogen isotope retention and good high temperature mechanical strength especially for fusion applications. Its function would be the protection of actively cooled wall structures from high heat fluxes in order to sustain the component life time 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. In order to test the iron properties under intensive fast \( (E > 0.1\) MeV\) neutron irradiation numerical as well as experimental studies are necessary. Several nuclear facilities are proposed [1] for experimental studies of irradiation effects on material due to the neutron flux from ITER and DEMO. Another approach relays on numerical simulations of the iron response to the intensive high-energy neutron irradiation. The purpose of our study was the numerical calculation of the damage of Fe sample caused by intensive fusion neutron irradiation. In order to achieve our goal we have used the multi-scale approach [2]. 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. Using Monte-Carlo (MC) simulation we have calculated the atom displacements caused by iron PKA. At the end of the simulation the final position of the atoms involved in damage cascades have been recorded. Finally, 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.

2. Methodology of the simulation

Different approaches are necessary for the simulation of the beryllium behavior under irradiation with high energy ($E > 0.1$ MeV) neutrons and high fluence up to $8 \times 10^{19}$ n/cm$^2$ for various energies and time scales. $^4$He, $^2$H and isotopes like $^{55}$Mn and $^{53}$Cr created by inelastic neutron capture have to be precisely determined. In the present work the initial neutron energy distribution for the simulation was taken from [3]. The typical neutron spectrum of D-T reactor for high energies ($E > 0.1$ MeV) is shown in figure 1.

![Figure 1. Total neutron flux from plasma in D-T reactor.](image-url)

One can see that the sharp neutron peak of the fusion neutrons is located at 14.1 MeV and its intensity is more than one order of magnitude higher than the intensity of the low energy neutrons. One can see on the other hand that the variation of intensity of the neutrons with lower energies is small and they can be considered as a background. One can expect from the spectrum that most of the radiation damages are due to fusion neutrons at 14.1 MeV. That is why in our calculations we have taken into consideration only neutrons with energies up to 14 MeV. We created a computer Monte-Carlo (MC) code based on the Geant4 CERN package [4] to simulate ion and neutron interactions in Fe homogeneous target at high energies ($E > 0.1$ MeV). The processes like neutron elastic and inelastic scattering, neutron capture with and without emission of charged particles were taken into consideration in the Be target. 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. The high precision database for low-energy neutron cross section NDL ver. 3.20 has been used with the purpose to achieve high accuracy of the neutron interaction in Fe. Our computer simulations were carried out for macroscopic cylindrical Be target with diameter of 60 mm and length of 50 mm. The Fe PKA for the damage cascades due to the neutron scattering and capture were considered for small cylindrical volume with diameter of 30 nm and length of 30 nm. It has been aligned with the beam axes and positioned at 1 cm behind the target.
surface. The total neutron fluence used in the simulation was of about $8 \times 10^{19}$ n/cm$^2$ ($E > 0.1$ MeV). Nuclear transmutations which play an important role in helium, deuterium and tritium formation were also taken into account. The interaction of fast neutrons in the Fe target which were taken into consideration in our code can be expressed by following reactions:

$$^{56}\text{Fe} + ^0\text{n} \rightarrow ^{56-\alpha}\text{Fe} + x^0\text{n}$$
$$^{56}\text{Fe} + ^0\text{n} \rightarrow ^{55}\text{Mn} + ^2\text{H}$$
$$^{56}\text{Fe} + ^0\text{n} \rightarrow ^{53}\text{Cr} + ^4\text{He}$$

In figure 2a is shown the total neutron interaction cross section in $^{56}\text{Fe}$ 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 2b are shown the production cross sections of $^4\text{He}$ and $^3\text{H}$ used in our numerical modeling. One could see that the $^4\text{He}$ production has a maximum at the energy of the fusion neutrons which is 14 MeV. The $^3\text{H}$ production has a threshold of 12 MeV and therefore it takes place in the fusion reactor. As a result the concentration of $^3\text{H}$ in the fusion neutron irradiated $^{56}\text{Fe}$ is expected to be several orders of magnitudes lower than the concentration of $^4\text{He}$. The integral cross section for $^4\text{He}$ production is about 200 times lower than the total neutron interaction cross section in $^{56}\text{Fe}$. 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 (figure 3). For this purpose we used the binary collision approximation (BCA) and the SRIM MC code [5] because it relays on the universal pair potential of Ziegler, Biersack and Littmark [6, 7]. The SRIM code allows us to calculate the stopping of the PKA at energies higher than 10 keV/u with accuracy of 10%. In this approach the crystal structure of Fe has been neglected. Iron has been considered as a homogeneous continuous medium. Every PKA from the high energy neutron interaction with Fe atoms was tracked down to its stop in the medium. According to the model, the target atom which is hit by PKA and starts a recoil cascade is identified with its recoiling energy. 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 Fe target vacancies are next items which were recorded.
The number of Frenkel pairs $N_{\text{NRT}}$ produced per cascade can be estimated by the NRT formula [8]:

$$N_{\text{NRT}} = 0.8 E_D / 2 E_d,$$

where $E_d$ is the average displacement energy for all crystallographic directions and $E_D$ is the damage energy which is the fraction of recoil energy that goes into displacement damage, after subtracting the portion dissipated for electron excitation. In our simulation the average displacement energy $E_d$ has been chosen to be 40 eV. The lattice binding energy was taken to be 3 eV equal to the cohesive energy of the Fe crystal. At the end of every cascade the ion type, the PKA energy, the recoil energy and the atom positions have been recorded for further processing.

3. Results and discussion

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 [3]. $^4$He and $^{53}$Cr concentration was calculated to be about 0.4 appm. According to calculations using the NPRIM code [3] it reaches 375 appm/fpy. Those values are in a good agreement with the results, obtained in [1]. 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 4.
Figure 4. Correlation between PKA energy distribution and the total displacements in a cascade after the neutron irradiation.

One could see that most damages are created by PKAs with energy up to 100 keV. 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 [1,9]. 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. This result is in agreement with our numerical calculations. 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 5. It indicates that although the damages are created in a volume of $30\times30\times30$ nm$^3$ the damage extends up to 400 nm. This is due to the large number of displacements in the cascades as well as to the large number of sub-cascades. 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. All defects are attractive trapping centers for He and H atoms and their properties could be studied by means of precise non-destructive experimental techniques like positron annihilation spectroscopy [10] or transmission electron microscopy (TEM) for point defects larger than 2 nm.

4. Conclusions
Numerical simulations of creation of point defects in $^{56}$Fe, irradiated by intensive fast ($E > 0.1$ MeV) neutron fluence up to $8\times10^{19}$ n/cm$^2$ has been performed. The neutron spectrum represents the energy
structure of the fusion neutrons and the 14.1 MeV peak. Neutron interactions with $^{56}$Fe like elastic and inelastic scattering, gamma ray emission and nuclear transmutations have been considered. Our multi-scale numerical model includes two steps. In the first step precise calculations of the PKA energies and positions for Fe recoils have been made. 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. He content was determined to be 0.4 appm which is in agreement with the available experimental measurements and calculations. $^2$H content was estimated to be 7% of the He content. The correlation between the PKAs energy and the damages was established. It was shown that the most vacancies are created by PKAa with energy below 50 keV with maximum around 30 keV. In the second step of our numerical modeling the depth profile of the vacancy distribution in the radiated sample was determined. It shows sharp maximum at the depth where PKAs were created as a result of the neutron irradiation.

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