

DISPLACEMENT OF ATOMS IN FUSION NEUTRON IRRADIATED Fe AND W

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Abstract

FLUKA code has been applied to calculate displacement per atom (DPA) distributions in irradiated Fe and W targets by 2.45 MeV and 14 MeV neutrons. The variations in DPA spectra of Fe and W as a function of target radius, depths and neutron energy are explored. It has been found that DPA depends not only on the depths but also on the size of radius of irradiated targets and neutron energy. FLUKA calculations show that DPA for 14 MeV neutrons in Fe for 1 MW/m² will be 1.49×10^{-7} DPA/s and for full power year (FPY) will be 4.67 DPA/FPY per 1 MW/m². DPA in W for 14 MeV neutrons for 1 MW/m² will be 8.62×10^{-8} DPA/s and for DPA/FPY will be equal to 2.73 DPA/FPY per 1 MW/m², respectively.

Key words: damage energy, displacement per atom, primary knock-on atoms, plasma facing materials, fusion neutrons

Introduction. The physical and mechanical degradation of materials associated with neutron irradiation damage is an important factor for fission and fusion plants operation [1]. From physical point of view, the creation of radiation defects, elastic and inelastic scattering of neutrons are interesting due to the transferring of the target atoms of some kinetic energy [2]. Embrittlement is an important damage effect due to irradiation with neutrons. The Fe, W and their alloys have been considered to be the structural material of the nuclear fusion reactor [3, 4]. Primary knock-on atoms (PKA) can induce a displacement cascade, which leads

to more crystallographic defects in the material [5, 6]. The necessary energy to DPA from its steady state position in a lattice to transfer it in the interstitial position could be above the threshold energy E_d . DPA measure is related to the number of the Frenkel pairs (FP). The DPA cross-section is calculated from the damage energy, using the NORGETT–ROBINSON–TORRENS (NRT) model [5]. The conversion to DPA is performed by modified KINCHIN–PEASE damage model [6] considering the displacement efficiency for higher recoil energies due to recombination and migration of the FP.

Purpose of the study. The main purpose of this paper is to demonstrate the importance of DPA and DPA rates on the atom structure of first wall (FW) materials in fusion reactors. We focus on displacement cascades in the bulk of bcc formation of fusion irradiated Fe and W by 2.45 MeV and 14 MeV neutrons based on FLUKA computer code [7]. The elastic neutron interactions in Fe and W result in DPA [8], creating mono vacancies, vacancy clusters, edge and screw dislocations as well as nano-voids similar to the void formation in austenitic stainless steels. The experimental studies on the void behaviour in the neutron irradiated materials to high doses have been done by transmission electron microscopy (TEM) and positron lifetime spectroscopy (PLS) [9, 10]. PKA has been used for estimation of the average displacements of each atom under irradiation [11]. The PKA collision involves a larger energy transfer and creates a localized cascade of defects that result from the additional atom-to-atom collisions. Inelastic neutron reactions are also important for fusion applications [12].

Computer calculation. DPA numerical results of the simulations served to calculate average and peak damage R_d (DPA/s) [12]. The neutron induced DPA of Fe and W calculated by FLUKA have been used for calculation by the NRT formula in [9]. The NRT DPA-cross section in FLUKA is expressed by the number of times that an atom is displaced for a given fluence φ . MD is a computational method and provides description of atomic interactions in cascades [12]. FLUKA is able to read the information stored in the Evaluated Nuclear Data Files (ENDF) databases [13]. A correlation between the number of FP produced and the initial energy of a PKA has been established [5]. DPA rate can be obtained dividing displacement rate (R_d). The R_d at time t can be calculated by the following formula using the maximum and minimum energy of the incoming particle:

$$(1) \quad R_d = N \int_0^{\infty} \Phi(E) \sigma_d(E) dE \quad (\text{disp/cm}^3),$$

where N is the atom number density, E is the energy-dependent neutron flux per unit energy, and $\sigma_d(E)$ is the energy-dependent displacement cross-section derived from the nuclear data libraries of the transport codes [13]. The thermal flux in ITER [14] is expected to be 10 MWm^{-2} . The average number of calculated PKA

by FLUKA code [9] has been expressed by the following formula:

$$(2) \quad PKA = N \int_{E_d}^{E_{SN}} \Phi(E) \sigma_s(E) dE \quad (1/\text{cm}^3),$$

where N is the atomic number density, $\Phi(E)$ is the neutron fluence, $\sigma_s(E)$ is the energy dependent displacement cross-section for the transfer of energy in excess of E_d (E_d is the averaged threshold energy of atomic displacement) between lattice atoms. The DPA is directly related to the total number of defects or FP. PKA cannot produce atomic displacement if the PKA energy $EPKA < E_d$. The calculation of DPA has been done with a specific E_d value of 40 eV for Fe and 90 eV for W. At neutron energies of 14 MeV the neutron interaction cross section is almost constant. Iron and tungsten target have been considered a homogeneous continuous 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.

Results. In our calculations we selected the initial directions of the PKA atoms to be different from the main crystallographic axis in the bcc lattice, in order to avoid the channelling. A lattice atom must receive a minimum amount of energy in the collision in order to be displaced from its lattice site. Simulations were completed for each of the tested Fe and W targets with the initial energy 2.45 and 14.1 MeV for cylinder with radius 3 cm and 10 cm and the thickness has been changed to 1 cm, 2 cm, 4 cm, 8 cm, and 16 cm. The PKA lead to cascades of atomic displacements, which can subsequently evolve and collapse to produce extended defects such as dislocation loops and voids. The obtained results of DPA for different depths of Fe cylinder targets for 2.45 MeV and 14 MeV neutron irradiation are shown in Fig. 1–2. Figure 1(a) shows distribution of DPA for 2.45

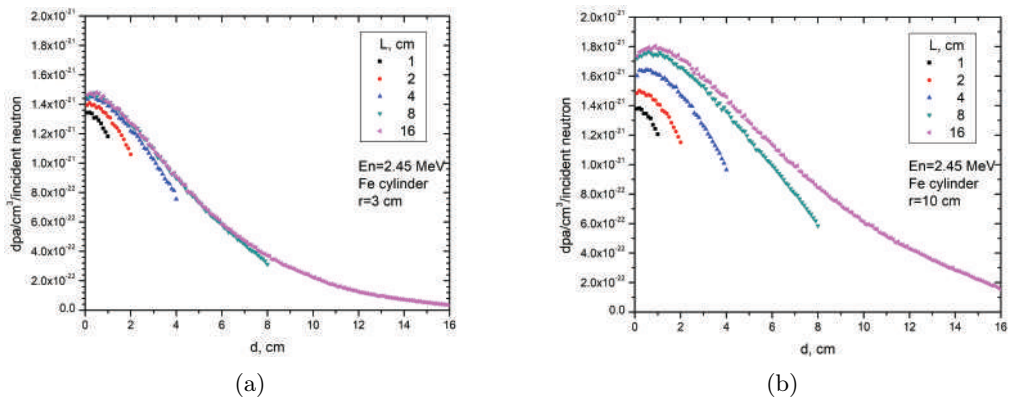


Fig. 1. DPA distribution in Fe irradiated with 2.45 MeV neutrons plotted as a function of target depth a) for radius 3 cm, b) for radius 10 cm

MeV neutron irradiation in Fe cylinder target with radius 3 cm and Fig. 1(b) – for 10 cm with depth from 1 to 16 cm. In Fig. 1(a), a correlation is found between the DPA and Fe target depths for 2.45 MeV neutron irradiated Fe cylinder with radius 3 cm. The calculated DPA values for Fe target with radius 3 cm by 2.45 MeV neutron's change for depth 1 cm from 1.34×10^{-21} to 1.18×10^{-21} DPA/cm³, for 8 cm from 1.54×10^{-21} to 3.11×10^{-22} DPA/cm³, while for 16 cm depth, DPA decreases from 1.46×10^{-21} to 3.37×10^{-23} DPA/cm³. The Fe target with radius 10 cm irradiated by 2.45 MeV neutrons shows differences for various depths from 1 cm to 16 cm. The DPA calculations have been done for Fe densities (7.87 g/cm³).

The plotted results in Fig. 2(a) show DPA values as a function of Fe target depths with radius 3 cm irradiated by 14 MeV neutrons. The DPA change for 1 cm depth from 2.93×10^{-21} to 2.67×10^{-21} DPA/cm³ and for 16 cm depth from 3.06×10^{-21} to 2.51×10^{-22} DPA/cm³, respectively.

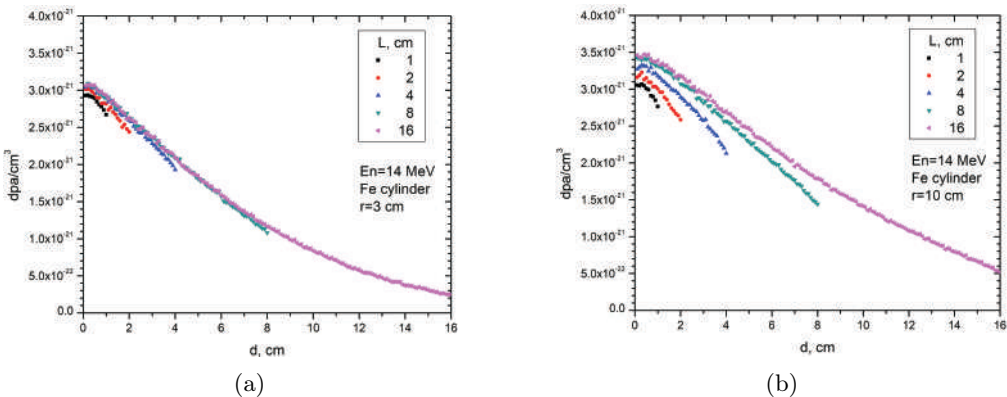


Fig. 2. DPA distribution in Fe irradiated by $E_n = 14$ MeV plotted as a function of target depth, a) for radius 3 cm, b) for radius 10 cm

The DPA results indicate that the damage energy due to the high energy neutron interaction in the Fe lattice change significantly at 8 and 16 cm depth. Figure 2(b) shows the calculated DPA values of Fe targets for radius 10 cm with different depths from 1 cm to 16 cm. The DPA calculated values of neutron irradiated by 14 MeV cylinder W targets with radius 3 cm and 10 cm and different depths are presented in Fig. 3. Our DPA calculation for tungsten targets with radius 3 cm, Fig. 3(a), irradiated by 14 MeV neutrons shows depth changes. We consider in neutron irradiated W target absence of significant contributions from other scattering as well as from (n, 2n) reaction. DPA distribution in W at each depth for radius 10 cm is shown in Fig. 3(b) for cylinder tungsten target irradiated by 14 MeV neutrons.

DPA for 1 cm depth decreases from 9.25×10^{-22} to 8.37×10^{-22} DPA/cm³ and for 16 cm depth from 1.04×10^{-21} to 1.02×10^{-22} DPA/cm³, respectively. DPA calculations have been done for W density (19.30 g/cm³).

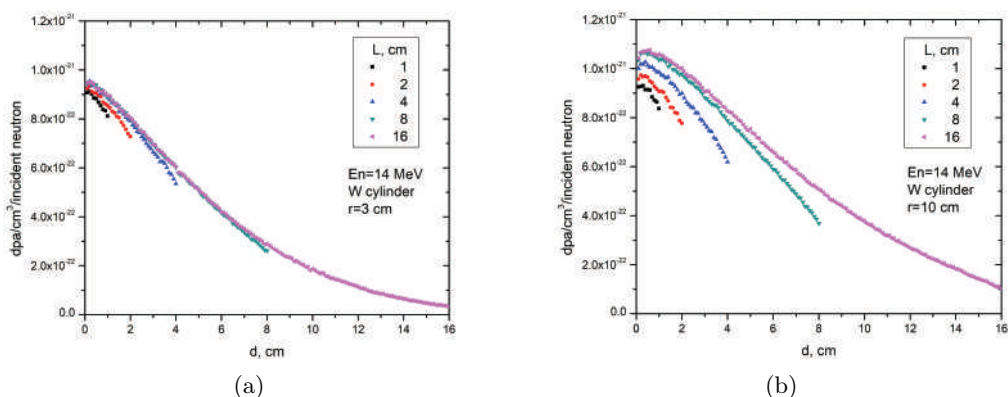


Fig. 3. DPA in W irradiated by 14 MeV fusion neutron plotted as a function of target depth a) for radius 3 cm, b) for radius 10 cm

Discussion. The damage stage depends on PKA energy. It is known that large number of atoms initially displaced, could be returned to perfect crystal positions. We established a decrease in the calculated DPA values for irradiated by 2.45 MeV Fe target with different depth from 1 cm to 16 cm as shown in Fig. 1(a). The differences could be due to PKA recombination at the different depths. The results presented in Fig. 1(b) for irradiated by 2.45 MeV fusion neutrons Fe target with radius 10 cm show also remarkable differences for various depths from 1 cm to 16 cm. The plotted results for 14 MeV fusion neutron irradiation of iron target with radius 3 cm in Fig. 2(a) show DPA as a function of target depths from 1 cm to 16 cm and indicate that the damage energy due to the high energy neutron interaction in the Fe lattice change significantly DPA distributions at 8 and 16 cm depth. The estimated differences in the DPA values for radius 3 cm and depth 4 cm is at about 1.11×10^{-21} DPA/cm³, while for 16 cm depth is 0.55×10^{-21} DPA/cm³. A considerable differences in the DPA calculated values of the Fe targets with radius 10 cm has been established in target with 16 cm depth of the 14 MeV neutron irradiation Fe targets. We establish for 2.45 and 14 MeV fusion neutron irradiation Fe targets existence of similar correlation of DPA distributions for different radius and depths by comparison of the result shown in Fig. 1 and Fig. 2. The DPA calculations for W targets with radius 3 cm, Fig. 3(a) for 1 cm depth shows changes 0.95×10^{-22} DPA/cm³ while for 16 cm is 6.05×10^{-23} DPA/cm³. DPA distribution in W at each depth for radius 10 cm, Fig. 3(b), shows correlation between DPA and target depth, similar to the established correlation for fusion neutron irradiated Fe targets. The differences in the DPA values for fusion neutron irradiated W targets are lower than the corresponding values for Fe. DPA calculations by FLUKA confirm the DPA dependence on the target depths and size of radius of the fusion neutron irradiated Fe and W targets. In summary, a comparison of the number of displacements per unit volume (DPA/cm³) and per

unit time for various depths and radius of 14 MeV neutron irradiated Fe target shows that the calculated value of 2.67×10^{-21} DPA/cm³ is close to the value of Fe NRT-DPA 2.89×10^{-21} DPA/cm³ for 14 MeV [11], but it is different from the value of Fe arc-DPA, which is equal to 8.62×10^{-22} DPA/cm³ for 14 MeV. The W calculated dpa value for 14 MeV neutrons of 8.11×10^{-22} DPA/cm³ is different from the W_{NRT}-dpa value of 1.77×10^{-21} DPA/cm³ as well as from W arc-DPA value [16] which is equal to 3.74×10^{-22} DPA/cm³ for 14 MeV. The NRT and dpa values [16] have been obtained by the Particle and Heavy Ion Transport PHITS programme. The presented FLUKA calculations show that DPA value for 1 MW/m² of 14 MeV neutron irradiated Fe is equal to 1.49×10^{-7} DPA/s and for FPY it is 4.67 DPA/FPY, while DPA for 14 MeV neutrons in W for 1 MW/m² is 8.68×10^{-8} DPA/s and DPA/FPY will be 2.73 DPA/FPY, respectively. It is important to emphasize that the damage distribution is a significant factor in fusion radiation plants. It is much better to use DPA than a neutron fluence value.

Conclusions. This paper describes an approach to calculate DPA and DPA for FPY in fusion neutron irradiated Fe and W by FLUKA code. The following conclusions could be drawn: The used FLUKA code could be successfully applied to evaluate the energy distributions of PKA in fusion neutron irradiated Fe and W targets for DPA calculation. It has been found that DPA depends not only on the depths but also on the size of radius and neutron energy, which result in different damage production rates. The findings will be beneficial for DPA evaluation used for applications of radiation damage in a 2.45 MeV and 14 MeV energy. The calculated DPA data can be used to predict defect formation in FW materials of fusion reactors, since it is currently impossible to realize experiments with irradiation doses up to $\sim 10^{23}$ n/cm² in fusion materials.

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