

TRANSMUTATION OF HYDROGEN AND HELIUM ATOMS IN NEUTRON IRRADIATED IRON AND TUNGSTEN

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Abstract

Numerical calculations of the hydrogen (H) and helium (He) transmutation atoms production in iron (Fe) and tungsten (W) irradiated by fusion 14.1 MeV neutrons were carried out by using FLUKA and MCNPX codes. This study has demonstrated good agreement between two MC codes for transmutation production ratio. H and He atom production depends on the target depths. The corresponding accumulation of H and He atoms in 16 cm Fe target for full power year (fpy) decreases by 56% atomic parts per million (appm/fpy) in comparison with the initial concentrations. The production of H in Fe depth 16 cm for fpy to 1 MW/m² by FLUKA and MCNPX is about 124.73 appm/fpy, while the amount of He reaches 28.56 appm/fpy. In tungsten for depth 16 cm hydrogen production for fpy 1 MW/m² is 1.40 appm/fpy (FLUKA) and 1.46 appm/fpy (MCNPX), while for He production it is 0.37 appm/fpy by FLUKA and 0.40 appm/fpy by MCNPX.

Key words: radiation effects, transmutation, FW materials, fusion neutron irradiation

Introduction. Iron and tungsten are considered plasma-facing materials in future fusion reactors. The transmutation products are one of the limiting factors of the life of a nuclear fusion power plant [1]. Fusion 14.1 MeV neutrons through inelastic reactions (n, α) or (n, p) create transmutation production in first wall (FW) materials. The nuclear fusion reaction ITER will be based on deuterium-tritium (D-T) interaction where one D nucleus fuses with one T nucleus [2, 3]. At

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present it is known that monoenergetic spectrum associated with the D-T fusion neutrons 14.1 MeV releases significant amounts of H atoms and He as transmutation products, which lead to a degradation of structural materials after a few years of operation [4–6]. In [7] the role of freely migrating point defects in defect cluster evolution during neutron irradiation has been studied using rate equations. Specific requirements for metal breeder blankets have been specified in [8]. The primary techniques used to characterize the behaviour of H and He in materials include TEM, small-angle neutron scattering (SANS), positron annihilation spectroscopy (PAS) [9, 10], and thermal desorption spectroscopy (TDS). All of these techniques have individual limitations.

Purpose of the study. The aim of this study was better understanding of the thermonuclear H and He transmutation in fusion neutron irradiated Fe and W at different target depths. FLUKA [11, 12] and MCNPX [13] codes have been used for performing simulations of H and He atom transmutations in fusion neutron irradiated iron and tungsten. FLUKA calculated results for H and He transmutation atoms have been compared with results of MCNPX. Additional motivation was the interest of transmutation levels production and evaluation of H and He in appm per seconds, per day, and per fpy. Iron has high radiation resistance, high chemical stability, low H isotope retention, and good high temperature mechanical strength especially for fusion applications. Tungsten due to its excellent material properties, the highest temperature melting point 3.695 K of any metal, as well as high thermal diffusivity and low sputtering yield is considered to be one of the important candidates for plasma FW material in fusion plasma reactors.

Computer simulations. The He and H transmutation atom rates have been calculated by using the cross sections and the spectra of neutron computed through the transport code of the Evaluated Nuclear Data Files (ENDF/B-VI) [14]. In our calculations we have taken into consideration initial neutrons with energies of 14.1 MeV. The production rate G in atoms/s can be calculated by using following convolution formula:

$$(1) \quad G = \int [\Phi(E)\sigma_d(E) dE] \text{ atoms/s,}$$

where $\sigma_d(E)$ is the cross-section for H or He production, $\Phi(E)$ is the neutron spectrum. The computer modelling by FLUKA offers the possibility of determining the transmutation production and accumulation of total H and He atoms. Inelastic interactions of primary neutrons and their product particles with the reactor materials lead to a large amount of H and He, also thermal flux in ITER is expected to be 10 MW m^{-2} [15]. In our computer simulations of Fe and W to prevent error due to statistical fluctuations, the primary neutron beam is defined as a cylindrical volume source, emitting neutrons homogeneously. Fe and W targets have been considered a homogeneous continuous medium.

Results. Helium is produced in materials irradiated with high energy neutrons, due to (n, α) -transmutation reaction. In our computer calculations target area of Fe and W for radius $R = 3$ cm is $S = \pi R^2 = \pi \times 3^2 = 28.27$ cm². Fusion neutrons on the Fe or W target surface are $N_s = N_n S = 4.43 \times 10^{13}$ neutrons/cm²s $\times 28.27$ cm² equal to 1.252×10^{13} n/s. Consequently, to 1 MW/cm² neutrons of 14.1 MeV corresponds fluence rate $\varphi = 1.252 \times 10^{13}$ n/cm²s. Neutrons for fpy N_{fpy} are equal to 1.252×10^{13} n/s $\times 3.1536 \times 10^7$ s = 3.95×10^{20} n/fpy, where 3.1536×10^7 s is the time for fpy. An important characteristic of the fusion neutron irradiated Fe and W targets is the production ratio appm/dpa and appm/fpy of the specific H and He atoms. The calculated H and He formation ratio (appm/dpa and appm/fpy) as a function of the different target depths for irradiated with 14.1 MeV fusion neutrons to 1 MW/m² by FLUKA and MCNPX codes for H and He are shown in Fig. 1–4. Hydrogen is typically produced during (n, p) reactions. We found that the existence of H and He atoms is significant to a wide range of fusion irradiated Fe target depths as shown in Fig. 1, 2. A decrease of H production ratio appm/dpa for different depths of neutron irradiated Fe targets calculated by FLUKA and MCNPX has been found (see Fig. 1). The calculated values of the H atoms in neutron irradiated Fe targets for depths 16 cm are almost equal for both codes as well as the calculated values for He production.

Figure 2 shows the H and He production ratio appm/fpy in neutron irradiated Fe targets with different depths. A considerable decrease of H production ratio as a function of the different Fe target depths was found. The H production for depth region from 1 cm to 16 cm in appm/fpy decreased by 56.14% (MCNPX) and

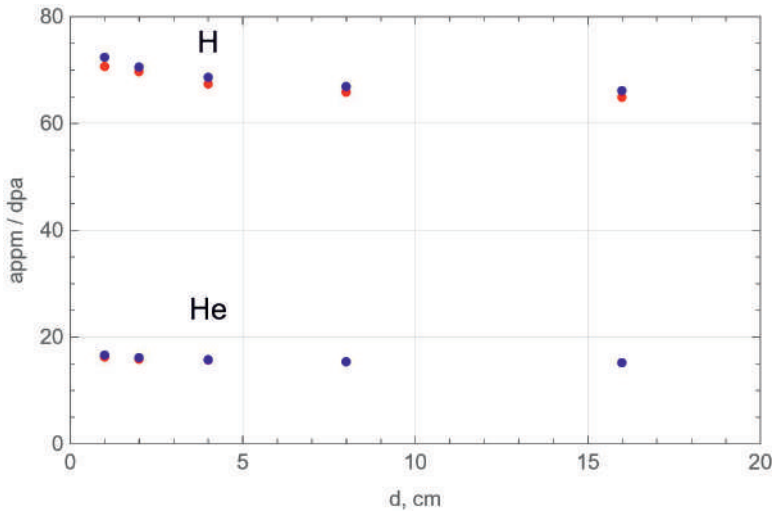


Fig. 1. H and He transmutation production ratio (appm)/dpa as a function of the depth in 14.1 MeV neutron irradiated Fe target for 1 MW/m². The FLUKA points are red, the MCNPX points are blue

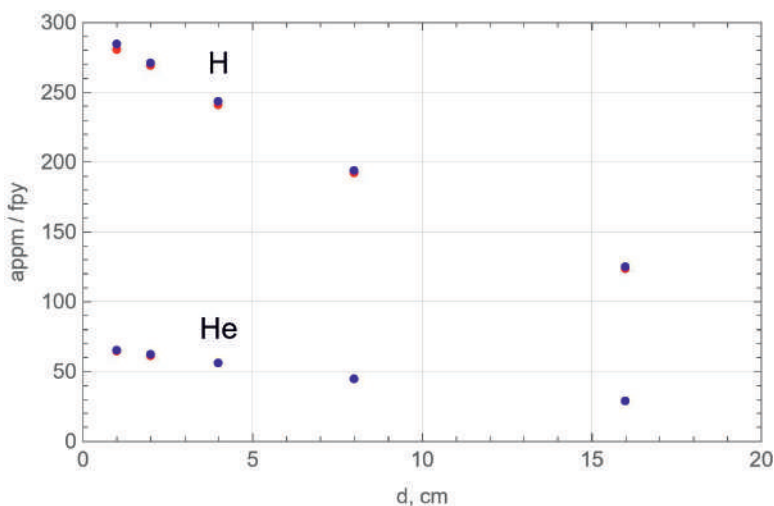


Fig. 2. H and He transmutation production (appm)/fpy ratio as a function of Fe depth irradiated with 14 MeV neutrons for 1 MW/m². The FLUKA points are red, the MCNPX points are blue

by 56.06% (FLUKA) simulations. The calculated results for He decreasing from 1 cm to 16 cm depth in the irradiated Fe targets is 56% (MCNPX) and 55.33% by (FLUKA) (Fig. 2). On the other hand, different correlations between He and H can be seen for different target depths, shown in Fig. 2.

Figure 3 shows H and He atom transmutation production in 14.1 MeV neutron irradiated W targets. A difference is found for H production ratio in appm/dpa

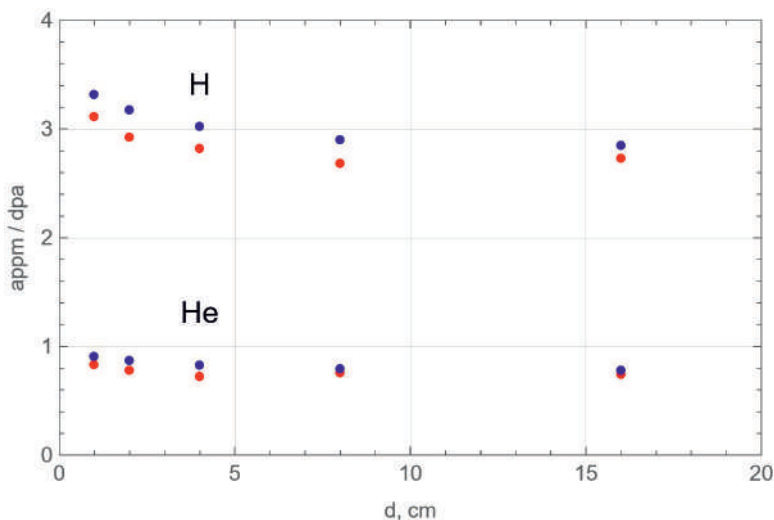


Fig. 3. H and He transmutation production (appm)/dpa ratio as a function of depth of 14.1 MeV neutron irradiated W target for 1 MW/m². The FLUKA points are red, the MCNPX points are blue

for W target depths between 1 cm and 16 cm. The calculated H appm/dpa values are 14.14% (MCNPX) and 12.35% (FLUKA); for He production values are 14.28% MCNPX and 11.02% by FLUKA calculation (Fig. 3). The H and He results are close to the earlier results published in [16,17] if we consider the used volumes [17, 18]. This remarkable result demonstrates that He production in fusion neutron irradiated W is important for the FW and the divertor of fusion power plant.

Figure 4 shows the H and He production ratio for fpy in W targets with different depths. The calculated results by FLUKA and MCNPX for He decrease in target depths from 1 cm to 16 cm in the fusion neutron irradiated W targets are almost the same (Fig. 4). The amount of He in the fusion irradiated W begins to decrease slightly as some of the W atoms are transformed during the irradiation process. This finding agrees well with the calculations of NODA et al. [19]. The level of He production found above is relatively low and may not cause significant structural changes to a W component.

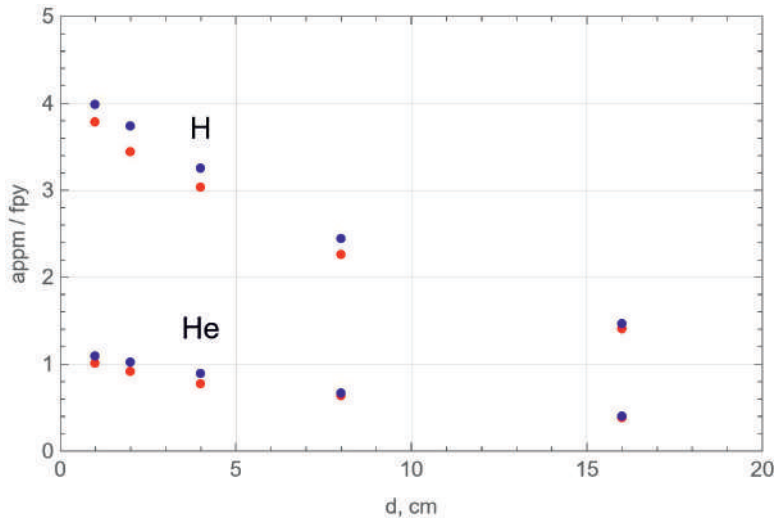


Fig. 4. H and He transmutation accumulation (appm)/dpa ratio as a function of depth of 14.1 MeV neutron irradiated W target for 1 MW/m^2 . The FLUKA points are red, the MCNPX points are blue

Discussion. The 14.1 MeV neutron energy is far above the threshold for n, α (5 MeV) and n, p (1 MeV) reactions in Fe. The variation of the H and He production rates for different depths (Fig. 1, 2) in neutron irradiated Fe targets from 1 to 4 cm appears to be greater by comparing the ratios for target depths 8 and 16 cm. The presented results in Fig. 2 for the H and He production for full power year to 1 MW/m^2 by MCNPX and FLUKA have been the same for H production at around 124.73 appm/fpy in the final depth 16 cm, while for He concentration the amount of He reaches 28.56 appm/fpy. The calculated values for H production in W depth 16 cm for fpy 1 MW/m^2 is 1.46 appm/fpy by MCNPX and

1.40 appm/fpy by FLUKA. The calculated value by MCNPX for He production in W for depth 16 cm is 0.40 appm/fpy and 0.37 appm/fpy by FLUKA. He is essentially insoluble in solids. The difference could be mainly explained by the strong repulsive interaction between H and He in Fe compared to that in W. He created in the fusion neutron irradiated W, takes place in the damage lattice centre of atom position even though H is close to He. The damage volume in Fe is smaller than that in W, because the lattice constant of Fe (2.84 Å) is smaller compared to that of W (3.16 Å). In Fe, the production of He is significant and severe within the first wall of a reactor. Our results predict that in fusion neutron irradiated W, He gas concentrations are rather low to have a serious impact on component lifetime. We found that in neutron irradiated Fe and W there is quite a strong interaction between H and He when the H-He distance is shorter than 2.25 Å due to the strong repulsive interaction between H and He in Fe compared to that in W. The binding energy of H atoms in tungsten is negative (~ -0.06 eV), meaning that H atoms do not cluster together as He atoms in W lattice. We noted that for accumulation of H in W diffusion process is important.

Conclusions. Computer simulations have been performed to determine the accumulation of H and He transmutation atoms in fusion neutron irradiated Fe and W targets by FLUKA and MCNPX codes. The results for maximum calculated transmutation production ratio in Fe by FLUKA for H were 70.60 appm/dpa and for He – 16.17 appm/dpa, while results by MCNPX for H were ~ 72.34 appm/dpa and for He ~ 16.52 appm/dpa. The corresponding transmutation production of H and He atoms in 16 cm Fe target decreases by 56% appm/fpy in comparison with the initial concentrations. This study has demonstrated good agreement between two MC codes – FLUKA and MCNPX for transmutation production ratio to H and He in appm/dpa and for appm/fpy in fusion neutron irradiated Fe and W. The presented FLUKA and MCNPX calculations of irradiated Fe and W show that H and He formation depends on the target depths. In addition, the results represent a necessary input for modelling activities aimed at understanding the expected effects on mechanical and physical properties.

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