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RADIATION DAMAGE AND He PRODUCTION CALCULATIONS FOR THE FOURTH SINQ TARGET IRRADIATION PROGRAM, STIP-IV

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ABSTRACT

The fourth SINQ target irradiation program, STIP-IV, was performed in 2004 and 2005. More than 1100 specimens of several tens kinds of materials of interest for various applications such as development of high power spallation targets, fusion reactors and next generation fission reactors were irradiated for two years with a total of 10.87 A·h proton charge on target. Neutronic calculations using MCNPX 2.5.0 were performed in support of this program. The spallation target, and the surrounding facility was thoroughly modeled, with particular care in the modeling of the different target rods. The experimental beam profile on target, obtained by gamma mapping of the $AlMg_3$ beam window, was used in the calculations. Calculations of neutron and proton integral fluences and spectra, energy deposition, dpa and He production were performed. With respect to the STIP-III irradiation program the peak irradiation increased on the average by 25%, due to a narrower beam profile. The maximum displacement on steel samples is of 25 dpa, the maximum helium production is of about 2200 appm.

1. Introduction

The SINQ target irradiation program (STIP) was started in 1996 under a collaboration between the Paul Scherrer Institut (PSI), the Forschungszentrum Jülich (FZJ), Oak Ridge National Laboratory (ORNL), Commissariat à l'Energie Atomique Centre d'Etudes the Saclay (CEA), Japan Atomic Energy Agency (JAEA) and Los Alamos National Laboratory (LANL) [1]. The goal of the program is to study irradiation-induced degradation in the mechanical properties of the target and structural materials in spallation irradiation environments, consisting in a mixed spectrum of high energy protons and spallation neutrons. Specimens of different materials of interest for spallation targets of spallation neutron sources for neutron scattering science as well as accelerator driven systems (ADS) are irradiated. Most of the materials irradiated in the STIP-IV program were steels samples, but also other materials and compounds (i.e. W, Ta, SiC/SiC, CMC, etc.).

The irradiation program is being carried out at the SINQ facility, in operation since 1997 [2]. SINQ spallation targets conventionally consist of solid rod bundles, with the notable exception of the liquid metal target MEGAPIE, which was irradiated in 2006. The specimens are irradiated in a mixed neutron/proton spectrum. For the analysis of the irradiated samples, it is necessary to calculate important irradiation conditions, such as the proton and neutron integral fluences and spectral information, and the heat deposition in the test samples. In this work, these parameters have been determined for the target 6 (STIP-IV) by Monte Carlo calculations using MCNPX, version 2.5.0 [3].

2. The SINQ solid target and STIP-IV irradiation

The goal of the SINQ facility is to produce thermal and cold neutrons which are then used for various experiments. Neutrons are produced by spallation of 575-MeV protons on a target, which is inserted in a heavy water tank of diameter of about 200 cm, surrounded by a H_2O reflecting layer. The maximum proton current on target was of 1.25 mA during the STIP-IV irradiation.

Spallation targets have been constantly improved over the years. The target 6 was irradiated in 2004 and 2005 for a total charge on target of 10.87 A·h. The target consisted of a vertical double cylinder with two shells one inside the other. The diameter of the external cylinder was of 21.2 cm. The thickness of each shell was variable, between 2 and 4 mm. For both shells, at the bottom (at the proton beam entrance) the thickness was of 2 mm, while it was 4 mm elsewhere. The target contained cylindrical rods arranged in layers of 9 and 10 rods each, as shown in Fig. 1. The rod bundle was housed by a 3 mm thick aluminum structure.

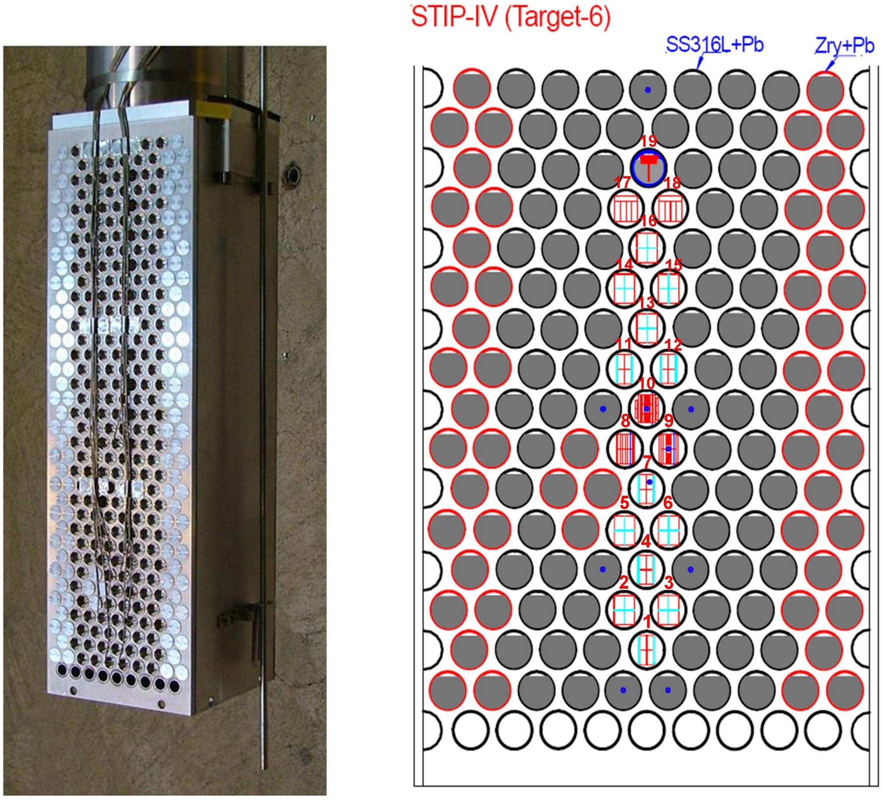

Figure 1. *Left***:** the SINQ target 6. *Right*: schematic representation of the target with the STIP samples. Zircaloy cladding is indicated in red, the steel cladding in black. The lowest row consists of empty $AlMg_3$ tubes. Specimen rods from 1 to 19 are indicated.

The center of the target was shifted by 8 cm downwards with respect to the zero longitudinal position, which corresponds to the center of the cold D_2 moderator placed inside the SINQ heavy water tank.

Each rod was a cylinder with radius 0.54 cm, 13.6 cm long. A total of 37 rows with 351 rods composed the target. There were different types of rods (see also Fig. 2):

1. The majority consisted of Pb rods inside a steel 316L cladding (with 0.5 mm thickness), the volume inside the cladding being filled to 90% with Pb. The lead rod inside the cladding was 11.9 cm long.
2. The lowest row of 9 rods consisted of open $AlMg_3$ cylinders; during operation the D_2O surrounding the target circulated inside.
3. For some of the Pb rods a zircaloy cladding replaced the steel.
4. Finally, several rods filled of specimens for the STIP program (mostly steel specimens) occupied some of the central positions of the target.

There were 19 specimen rods for the STIP-IV program. In Table I geometrical parameters concerning the rod dimensions and spacing are given.

The STIP-IV specimens were of many kinds of materials, with a predominance of austenitic (AISI 316L) and martensitic (such as T91) steels. Other materials, such as Ti, Ni and Si alloys were used, as well as samples of pure Pb and W, etc.

The samples are currently being extracted at the PSI Hotlab and analyzed by the various partners of the collaboration.

Table I. List of geometrical parameters of Target 6. The horizontal pitch is the distance between the center of two rods. Dimensions are in cm.

number of rod planes	37
number of rods per plane	9 or 10
distance between two rods	0.2
horizontal pitch	1.28
vertical pitch	1.10
Pb rod length	11.9
Pb rod radius	0.49
Pb rod cladding material	Steel 316L - zircaloy
Pb rod cladding inner/outer radius	0.49 / 0.54 (steel) - 0.4625 / 0.5375 (zircaloy)
specimen rod cladding material	Steel 316L
specimen cladding inner/outer radius	0.49 / 0.54
cladding length	13.3

3. MCNPX model

The following components of the SINQ facility were included in the MCNPX model:

- SINQ target block, consisting mainly of an iron structure;
- heavy water tank, with the beam inserts, surrounded by a layer of H_2O reflector;
- beam lines up to the exit of the SINQ target block;
- cold D_2 tank;
- the H_2O scatterer;
- the SINQ target itself.

Particular care was put in the modeling of the rod bundle. The actual dimensions of the Pb rods and of the cladding tubes are specified in Table I.

Rather than modeling the detailed structure of the specimens, the specimen rods were modeled as cylinders with mass equal to the total mass of the samples. The material for each specimen rod was specified in the MCNPX input file as a mixture of elements, in agreement with the composition of the specimens in each rod. In Fig. 2 a horizontal cut of the target model is presented. For that rod plane, the four rods on the sides have zircaloy cladding, while the six rods at the center have steel cladding. The two central rods are filled with steel specimens.

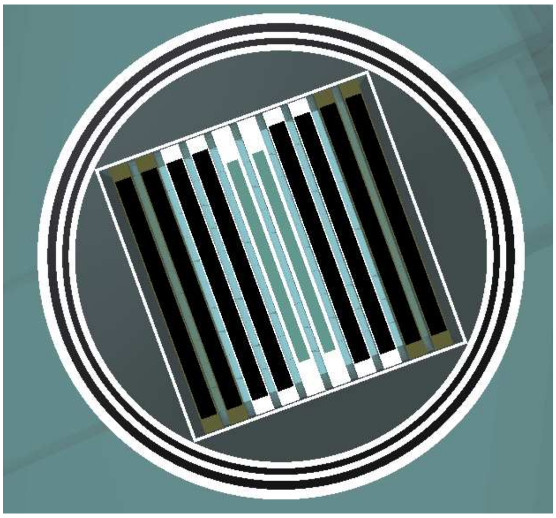

Figure 2. XY cut of the SINQ target, at the longitudinal height of the second layer of specimen rods.

Of particular importance in this work is to input the correct proton beam profile, as it has a great impact on the irradiation of the samples. The proton source distribution was modeled in MCNPX according to the experimental beam profile previously determined from the ^{22}Na γ lines mapping of the beam window (Fig. 3).

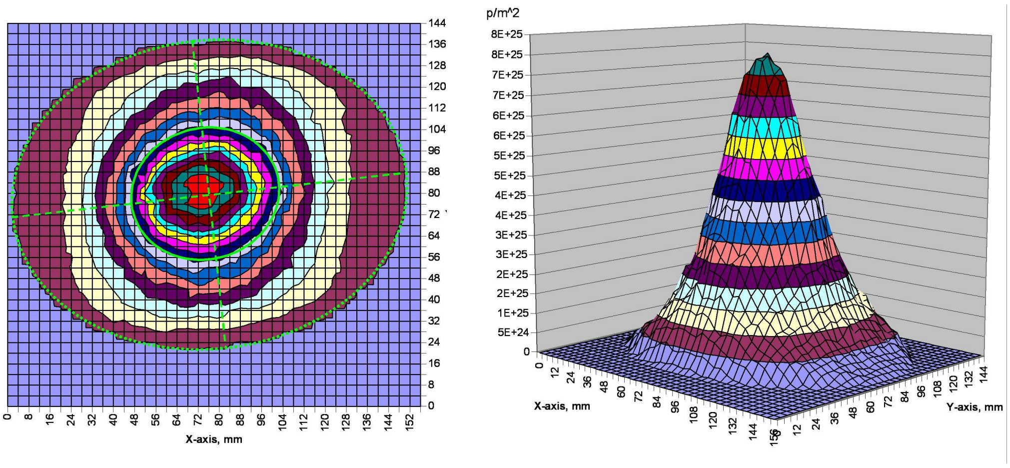

Figure 3. Target 6 experimental beam profile from ^{22}Na gamma counts on the AlMg$_3$ container.

The code MCNPX version 2.5.0 was used, with the standard Bertini-Dresner model for spallation/evaporation. ENDF libraries available in MCNPX were used for low-energy neutron transport. The following quantities were calculated by MCNPX: energy deposition, integral neutron and proton fluences and energy spectra. Calculated neutron and proton spectra were later used for the determination of the radiation damage and of the helium production. Different models were prepared for the specimen rods, in which the material composition of the specimens was changed. In a first calculation, the material composition consisted of a compound with the same elemental mixture as in the actual specimen rods (every rod contained samples of different materials). Additional calculations were performed, in which the composition of a specimen rod was fixed to only one material. In the following section a part of the results, in particular for the steel samples, is presented.

4. Fluxes and energy deposition

Integral proton and neutron fluences were calculated for all the specimen rods. The results along the length of rods 1,7, 13 and 16 (see Fig. 1) are shown in Fig. 4, for a total proton charge of 10.87 A·h of irradiation. The neutron fluence is always greater than the proton fluence and the distribution is wider for neutrons, as expected. It is interesting to observe that the distributions are asymmetric, and integral flux values are higher on one side. This is an effect due to the beam profile used; results obtained with a calculated beam profile showed symmetric distributions.

Neutron and proton energy spectra were also calculated. Results calculated at the center of the same four specimen rods are shown in Fig. 5. The neutron spectra are very similar in all the rods, showing a thermal peak due to neutron moderation in the heavy water tank, besides the fast component, almost independent of the irradiation position.

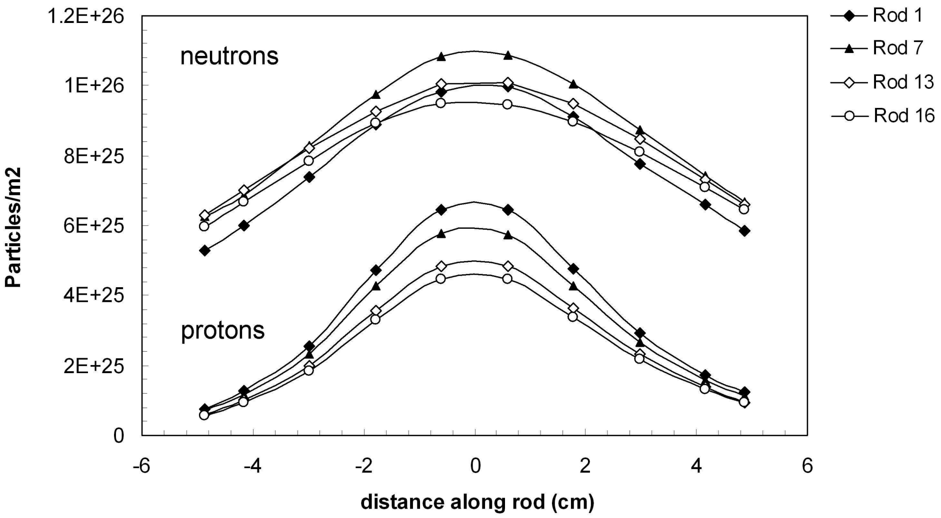

Figure 4. Integrated neutron and proton fluences along the length of four specimen rods in target 6, for 10.87 A·h of irradiation.

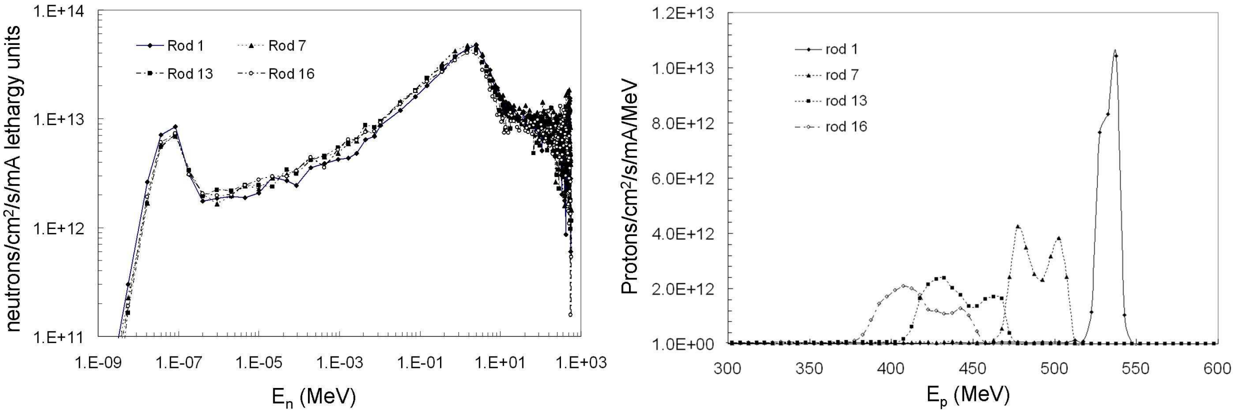

Figure 5. Neutron and proton spectra calculated at the center of four specimen rods.

Total energy deposition was calculated for specimen rods and tubes. Energy deposition for steel tubes for some rods from 1 to 16 are shown in Fig. 6. As expected, the deposited energy decreases due to the decrease of the proton flux and of the average proton energy. Calculation was also performed for single materials in specific rod positions, in this case the energy deposition varies according to the material used.

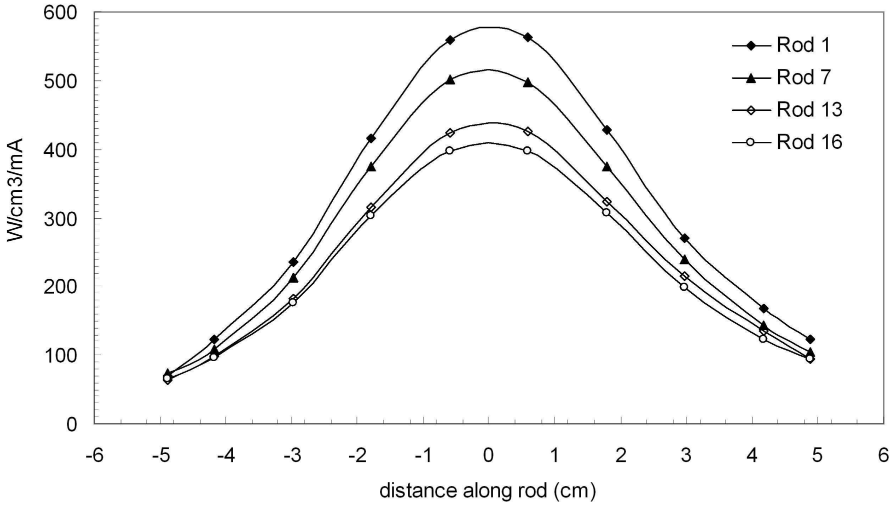

Figure 6. Energy deposition distribution for tubes in several specimen rods.

5. Radiation damage

In order to estimate the radiation damage in the specimens, displacement cross sections for Fe and Cr (the main components of T91) were calculated using two approaches described in Ref. [4]. The first approach consisted in using nuclear models and the NRT model [5]. A second method was used, combining the method of the molecular dynamics and the binary collision approximation model for the calculation of the number of defects in irradiated materials. For protons interactions, elastic and non-elastic components were determined (Fig. 7).

In Fig. 8 the proton and neutrons displacement cross sections for Fe are displayed. In the energy range of interest, i.e. for protons above 1 MeV, the BCA,MD cross sections are about a factor of 3 lower than the NRT cross sections.

For reference, the calculations of the displacements have been made using only the NRT cross sections. Results are shown in Fig. 9. In the left the total displacement, and the contribution from protons and neutrons, calculated for the first 316L specimen rod is shown. Results for four different rods are given in the Fig. 9 (right). The peak total displacement at the center is of about 25 dpa after 10.87 A·h of irradiation.

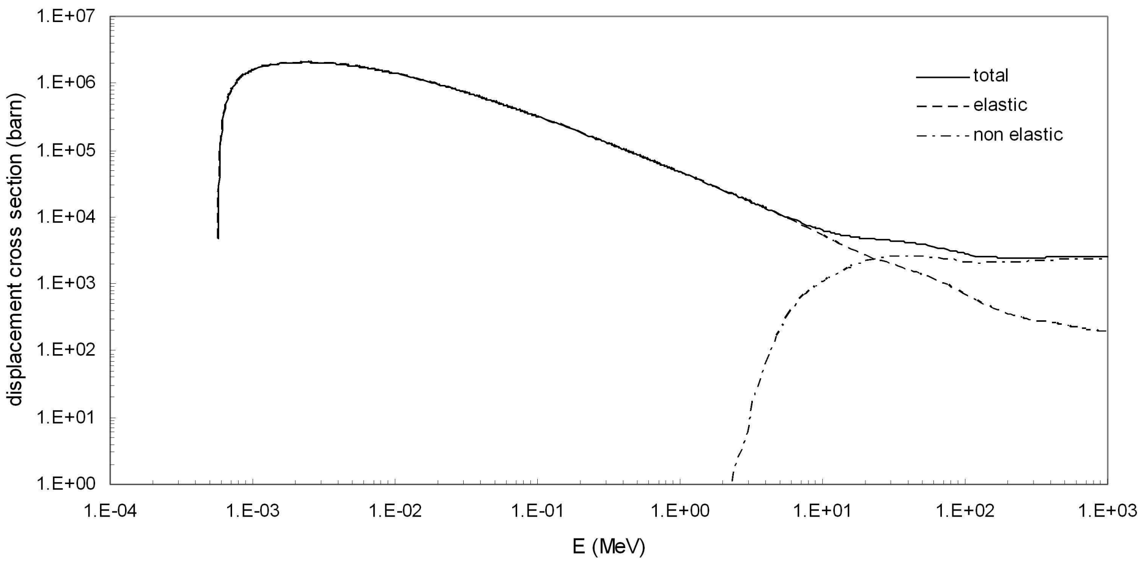

Figure 7. NRT elastic, non elastic and total displacement cross section for protons on Fe.

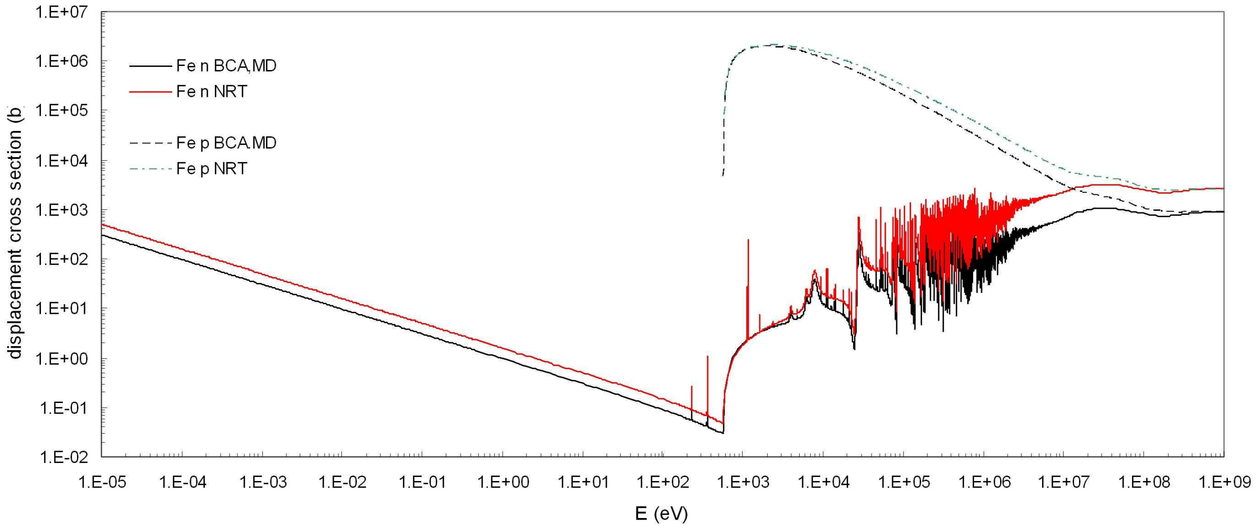

Figure 8. Displacement cross sections for protons and neutrons on Fe, calculated using BCA,MD and NRT models.

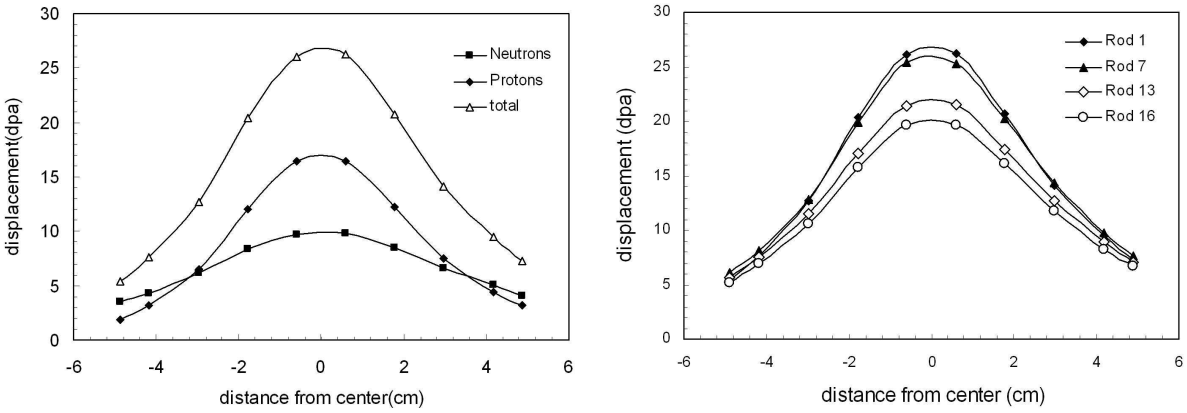

Figure 9. *Left*: calculated dpa in 316L steel specimens in the first rod, for neutrons, protons and total. *Right*: calculated total dpa in four specimen rods with steel samples. NRT displacement cross sections have been used.

6. He production

For an estimate of the He production in steel we used the recently calculated ^{3,4}He production cross sections in ^{56}Fe [6]. The calculation was performed using the CASCADE/INPE code and compared with calculations using ALICE/ASH, and various measurements from the literature in the range from 10 MeV to 3 GeV; they are very close to the values evaluated from the thermal discharge measurements on STIP samples [7]. For neutrons, we used cross sections from Ref. [8]. The He production in four rods containing steel specimens is given in Fig. 10. The neutron contribution is much smaller since the cross section is similar but the neutron energy is much lower (see Fig. 5). The contribution from neutrons is higher in the upper rods (where the proton energy is lower) and at the sides of the rods: in rod 1 the neutron contribution is expected to be between 3 % (center) and 8 % (sides); in rod 17 the neutron contribution is expected to be between 6 % (center) and 15 % (sides). In Fig. 10 also the He production per dpa is shown. The peak value at the center of the rods is close to 90 appm/dpa.

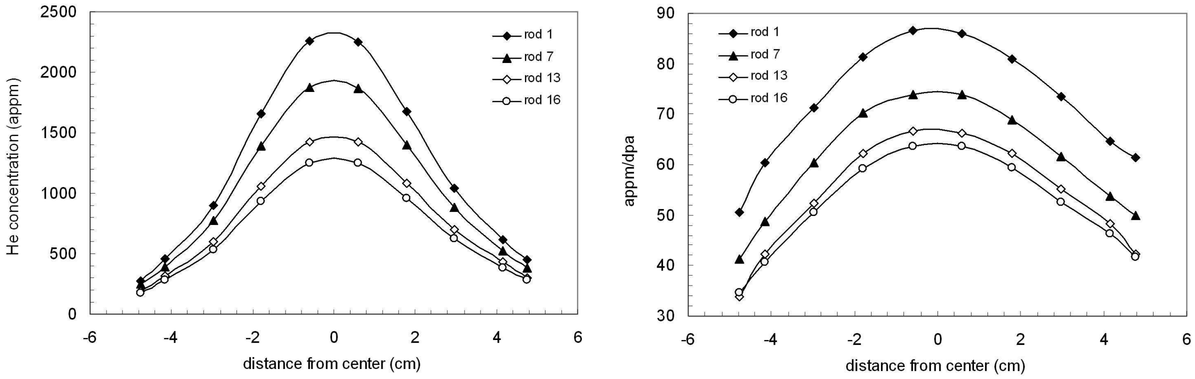

Figure 10. *Left*: He production in steel samples. *Right*: He production per dpa.

7. Conclusions and outlook

A series of Monte Carlo calculations for the fourth STIP irradiation program has been performed using MCNPX. These calculations are in support of the STIP experimental analysis program. Proton and neutron fluences, energy deposition in rods containing specimens have been performed. Calculations of displacement and He production have been performed, using the latest displacement cross sections for Fe, and He proton-production cross sections evaluated using the CASCADE/INPE code. For the two-year irradiation of the samples, a peak value of 26 dpa is reached for the steel samples. He production was also calculated for all the specimen rods. Peak values approaching 90 appm/dpa are obtained, indicating the large differences of a typical proton/neutron mixed spectrum in a spallation target, as compared with a pure neutron environment. The STIP-IV program is thus ideal for studying materials for spallation targets; for fusion applications, a lower He production rate of about 10 appm/dpa would be more appropriate.

A validation of the flux calculations is necessary. Some validation work was done for earlier STIP programs [7], but more information is necessary as the neutron and proton fluences are the starting quantities for damage and helium production calculations. Such validation can be performed by analyzing activation data on available specimens, including distributions along the rods. We are also considering placing activation foils in the next SINQ target which will also contain STIP samples.

8. Acknowledgements

H.P. Linder and Hot-cell Group are acknowledged for their help on gamma measurements of the $AlMg_3$ beam window.

9. References

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