# Investigation of radiation damage of copper using MCNP-4C2 and TRIM 98.01 codes

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**Abstract.** The work is focused towards the radiation damage of the first wall material of International Thermonuclear Experimental Reactor (ITER). There were performed Monte Carlo (MC) simulations by MCNP-4C2 and TRIM 98.01 codes to design the experimental part for Positron Annihilation Spectroscopy (PAS) measurements of neutron treated material of ITER first wall based on Cu-alloys. MC simulations by MCNP-4C2 code have been performed to determine the distribution of neutron fluence and primary-knock out- atoms (PKA) creation and to predict the probable activation of Cu sample. Considering our boundary conditions of the calculations, the helium production was 2.413E-03 atoms/(source neutron·cm$^3$), and the hydrogen production was 1.324E-02 atoms/(source neutron·cm$^3$). Calculated activity of the specimen is of about 20.5 MBq. The TRIM 98.01 code was used for the simulation of defects creation (vacancies, voids) in pure Cu by hydrogen H of 95 keV, only. The aim was to find out the distribution of protons in the defined depth. The main defects production was identified in the region of about 400-800 nm. Data obtained from computer simulations were compared with experimental data from PAS technique and are useful also for irradiation experiment preparing currently in FZ Rossendorf in the TUD neutron laboratory.

## 1. Introduction

Material resistance to the high neutron load is one of the crucial questions for the fusion technology. The aim of the work is to present the results of the three dimensional Monte Carlo calculation of the nuclear parameters in the Cu specimen, which are useful for understanding of results of the next experiment - Positron Annihilation Spectroscopy measurement which offers a view at radiation damage measure in the investigated material under the influence of the high energy neutron load [1, 2, 3].

## 2. Approach based on Monte Carlo method

Computational codes (MCNP, TRIM) used in our work are based on the Monte Carlo method, in which the individual probabilistic events that comprise a process are simulated sequentially. The probability distributions governing these events are statistically sampled to describe the total phenomenon. The statistical sampling process is based on the selection of random numbers. Particle transport by MC method consists of actually following each of many particles from a source throughout its life to its termination in some terminal category (absorption, escape, etc.). Probability distributions are randomly sampled using transport data to determine the outcome at each step of its life. Fig. 1 shows the random history of a neutron incident on a slab. Numbers between 0 and 1 are selected randomly to determine what and where interaction takes place, based on the rules (physics) and probabilities (transport data) governing the process and materials involved. If this neutron history is complete then more and more such histories are followed, the neutron and photon distributions become better know. The quantities of interest are tallied along with estimates of the statistical precision (uncertainty) of the results.

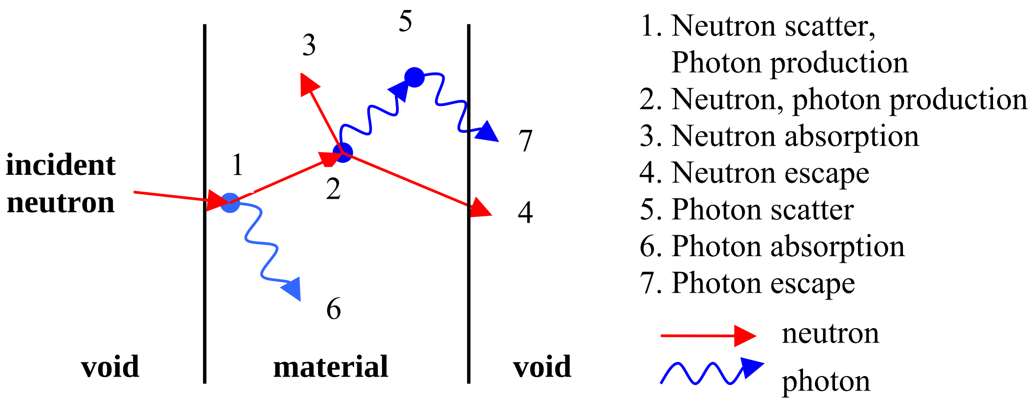


*FIG. 1. Random history of a neutron incident in a slab.*

The generalized-geometry, continuous energy, coupled neutron/photon/electron Monte Carlo transport code MCNP-4C2 [6] has been used in the three-dimensional neutron/photon calculation. The nuclear data used are based on the continuous-energy data libraries ENDF60, RMCCS and ENDL85.

## 3. Calculation model

The geometry of the copper specimen has been modeled for 3-D neutronics/photonics calculations. MCNP model of the specimen is given in the Fig. 2.

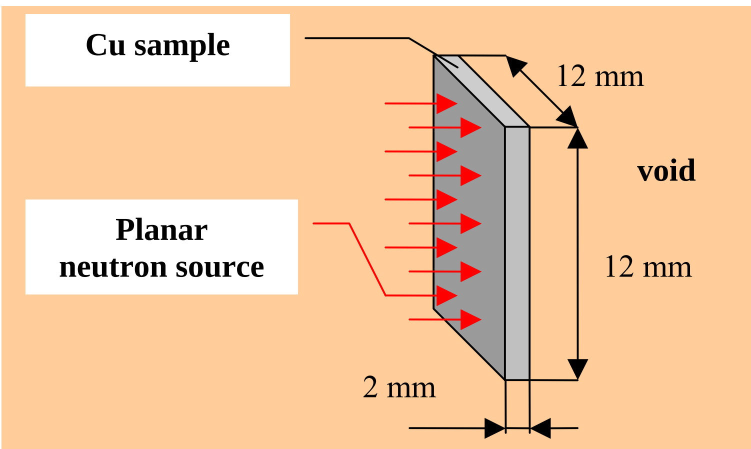


*FIG. 2. Model of Cu specimen for MCNP calculations.*

Geometrical model of the investigated specimen consists of the slab with dimensions 12 x 12 x 2 mm. Model of the specimen has been divided into 40 layers which create elementary cells with thickness 0.05 mm to provide detailed spatial distribution of the nuclear parameters. The shape of the modeled specimen correlates with the shape of samples used in the intended experiment - Positron Annihilation Spectroscopy (PAS) measurements.

Source model consists of the planar neutron source, which is located on a boundary surface. Energy of the mono-energetic source neutrons is 14.1 MeV, which corresponds to energy of the neutrons produced in International Thermonuclear Experimental Reactor (ITER).

Material model consists of the pure copper, which is one of the best candidate materials for the first wall of ITER. Material characteristic is given in the Tab. I. [4].

TABLE I: MATERIAL CHARACTERISTICS OF THE SPECIMEN.

| Material | Mass density ($g/cm^3$) | Isotope fraction (%) | |
|---|---|---|---|
| Cu | 8.93 | $^{63}Cu$ | 67.17 |
| | | $^{65}Cu$ | 30.83 |

## 4. Nuclear parameters in the specimen

Calculated nuclear parameters include distribution of neutron fluence, nuclear reactions, photon production, gas production, nuclear heating, number of primary knock-out atoms (PKA) and induced activity.

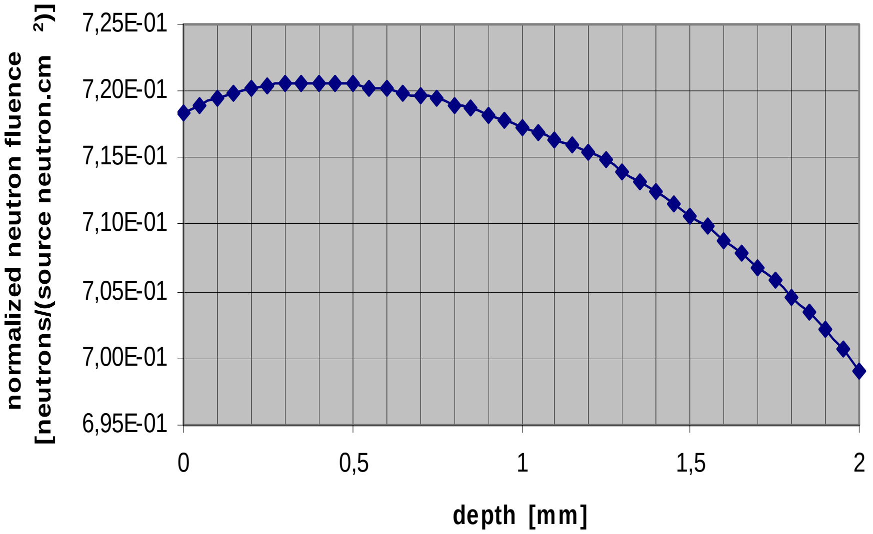


*FIG. 3. Distribution of neutron fluence in the specimen.*

Distribution of neutron fluence normalized per source neutron in the specimen is given in Fig. 3 and distribution of creation of the primary knock-out atoms normalized per source neutron in the layers with thickness 50 μm in Fig. 4. The decreasing of neutron fluence and number of PKA in the surface region is caused by Cu sample-vacuum boundary. The average normalized neutron fluence in the specimen is 7.139E-01 neutrons/(source neutron·$cm^2$) and unnormalized neutron fluence is 2.205E12 neutrons/$cm^2$. The total normalized number of PKA is 8.76E-02 atoms/(source neutron·$cm^3$) and unnormalized number of PKA is 2.706E11 atoms/$cm^3$, which has been determined by number of scatters on the copper atoms in neutron energy range from 1.289 keV to 14.1 MeV, where energy of 1.289 keV is the minimal neutron energy necessary to displace the atom from the crystal lattice node point and thus to create the PKA (Treshold energy of about 40 eV). The total particle production in the specimen is given in Tab. II. The unnormalized values of the nuclear parameters have been calculated according to the following irradiation conditions and neutron source parameters – 14.1 MeV neutron irradiation in duration of 203 min and neutron fluence of 2.145E12 neutrons/$cm^2$. The conditions of the neutron irradiation have been taken from the irradiation experiment performed by Institut für Kern- und Teilchenphysik, TU Dresden, Germany [5]. The calculated average heating number is 3.760E-02 MeV/collision. Considering the irradiation conditions the total nuclear heating in the investigated specimen is 4.985E-04 J. The heat transfer from specimen to surrounded vacuum was not considered.

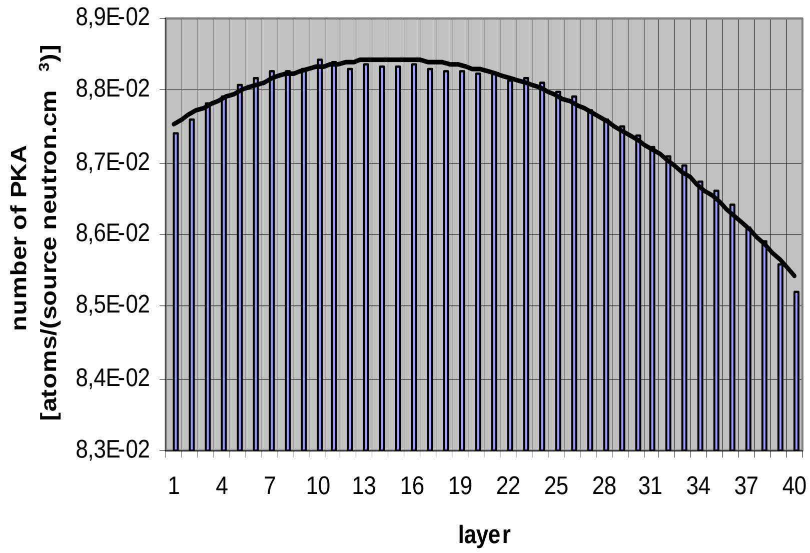


*FIG. 4. Distribution of primary knock-out atoms in the specimen.*

TABLE II: PARTICLE PRODUCTION IN THE SPECIMEN.

| Particle | Total normalized production in the specimen [1/(source neutron·cm$^3$)] | Total unnormalized production in the specimen (1/cm$^3$) |
|---|---|---|
| Photon | 2.539E-01 | 7.842E11 |
| Proton | 1.324E-02 | 4.090E10 |
| Deuterium | 5.578E-04 | 1.723E09 |
| $^3$He | 2.002E-07 | 6.184E05 |
| Alpha | 2.414E-03 | 7.456E09 |

The results of the calculation of nuclear reactions on the $^{63}$Cu, $^{65}$Cu isotopes of the Cu sample are given in Tab. III. The values are normalized per source neutron and volume. The results of these reactions are isotopes Cu, Ni, Co and their decay products. The probable activation of the alloy sample is shown in Fig. 5. The accuracy of all calculated results is better than 0.1%.

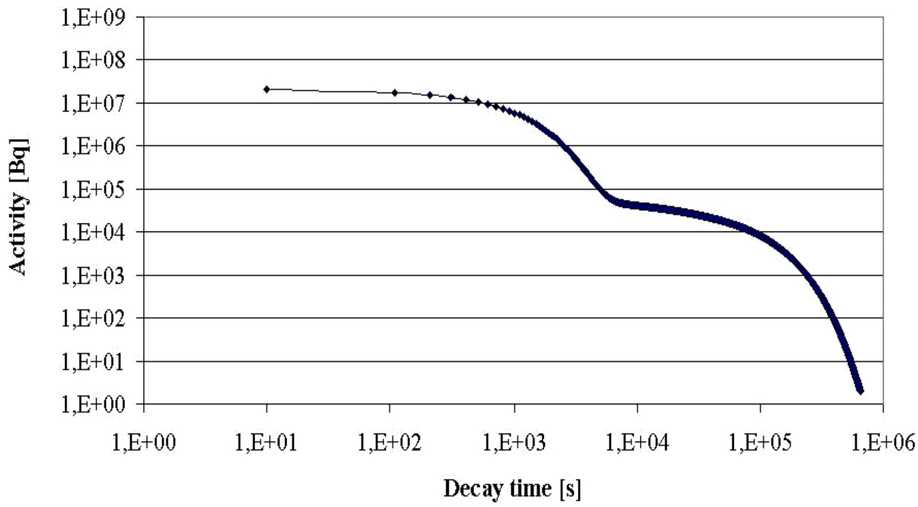


*FIG. 5. The decreasing of the specimen activity in the time dependence.*

Induced activity of the investigated specimen is of about 20.5 MBq. The drop of the activity to practically non-active level (< 10 Bq) is observed at decay time of about 1E06 sec (about 12 days). There are two plateaus caused by two important radionuclides $^{62}$Cu and $^{64}$Cu.

TABLE III: NUCLEAR REACTION IN THE SPECIMEN.

| Target isotope | Reaction | Product | Number of reactions [1/(source neutron·cm$^3$)] |
|---|---|---|---|
| $^{63}$Cu | (n,2n) | $^{62}$Cu → $^{62}$Ni stable (st.) | 1.82378E-02 |
| | (n,n´p) | $^{62}$Ni st. | 1.06331E-02 |
| | (n,n´α) | $^{59}$Co st. | 5.10850E-04 |
| | (n,p) | $^{63}$Ni → $^{63}$Cu st. | 1.86386E-03 |
| | (n,d) | $^{62}$Ni st. | 3.84324E-04 |
| | (n,$^3$He) | $^{61}$Co → $^{61}$Ni st. | 1.55531E-07 |
| | (n, α) | $^{60}$Co → $^{60}$Ni st. | 1.70658E-03 |
| | (n,γ) | $^{64}$Cu → $^{64}$Ni st. (61%) → $^{64}$Zn st. (39%) | 1.28033E-04 |
| $^{65}$Cu | (n,2n) | $^{64}$Cu → $^{64}$Ni st. (61%) → $^{64}$Zn st. (39%) | 1.62292E-02 |
| | (n,n´p) | $^{64}$Ni st. | 3.02890E-04 |
| | (n,n´α) | $^{61}$Co → $^{61}$Ni st. | 1.39880E-05 |
| | (n,p) | $^{65}$Ni → $^{65}$Cu st. | 4.37881E-04 |
| | (n,d) | $^{64}$Ni st. | 1.73503E-04 |
| | (n,$^3$He) | $^{63}$Co→ $^{63}$Ni → $^{63}$Cu st. | 4.66784E-08 |
| | (n, α) | $^{62}$Co → $^{62}$Ni st. | 1.82165E-04 |
| | (n,γ) | $^{66}$Cu → $^{66}$Zn st. | 1.47605E-05 |

**5. Simulation of defects creation in the copper by TRIM 98.01 code**

The model has been constructed to find out the protons concentration in the defined sample depth. The hydrogen ions (protons) have been implanted at the energy of 95 keV into pure copper. The depth distribution of protons was estimated by summation of 10 particular implantations with the doses of $10^{18}$ ions/cm$^2$ to get the total dose of $10^{19}$ ions/cm$^2$. There have been created defects in the form of voids. The high implantation dose of about $10^{19}$ ions/cm$^2$ caused destroying of the structure, the lattice atoms have been displaced and the hydrogen atoms cumulated in the voids. According to the simulation results the accumulation of the voids is in the depth from 400 nm to 800 nm (Fig. 6).

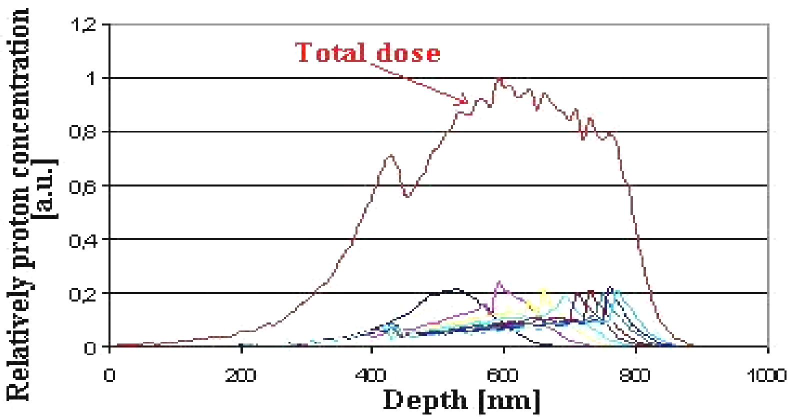


*FIG. 6. The plot of TRIM 98.01 code proton $H^+$ implanted profile in Cu substrate.*

## 6. Summary and conclusion

Calculations have been performed by Monte Carlo method using the continuous energy MCNP-4C2 transport code to determine the nuclear parameters in the Cu specimen. The parameters include high energy neutron fluence distribution, the defect production in form of primary knock-out atoms, H, D and He atoms, photon production, nuclear heating, yield of the nuclear reactions on the $^{63}Cu$, $^{65}Cu$ isotopes of the copper and induced activity of the specimen. The average neutron fluence is 7.139E-01 neutrons/(source neutron·$cm^2$), the number of PKA is 8.76E-02 atoms/(source neutron·$cm^3$). The helium production in the specimen is 2.413E-03 atoms/(source neutron·$cm^3$), and the hydrogen production is 1.324E-02 atoms/(source neutron·$cm^3$). The calculated activity of the specimen is of about 20.5 MBq. The creation of the voids filled by hydrogen, observed by TRIM 98.01 code have been identified in the region of about 400-800 nm. The results of the Monte Carlo calculations will be used at the understanding and the verification of PAS experimental values [1, 2]. Neutron irradiated specimen are currently prepared for evaluation by PAS measurement.

## 7. References


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