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RADIATION DAMAGE AND DPA IN IRON USING MCNP5

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Abstract

A Monte Carlo simulation code is developed for the study of neutron induced radiation damage in the materials which results from nuclear collision as well as reactions that create energetic recoil atoms of the host material or reaction creates. The aim of this work is to investigate the impact of the radiation damage in the iron by the neutron energy irradiation. The damage parameter used in the evaluation is displacement per atom DPA in material as a function of neutron energy. For this purpose, the simulations were carried out using the Monte Carlo transport code MCNP to calculate the DPA cross section for iron. It was determined that the maximum number of displaced atoms was approximately 1.73E-03 DPA.

Keywords: *MCNP, Radiation damage, Neutron cross section, DPA, Iron.*

Introduction

MCNP is general-purpose Monte Carlo N-particle Computer code which can be widely used in a number of different transport modes: neutron, proton and electron or coupled Monte Carlo transport Code : neutron/ photon/ electron transport [1, 2]. MCNP is usually a software package code that used for analysing nuclear techniques (the transport of gamma rays and neutron). It was first understood in 1970 as a proton and neutron transport. It was developed by the Monte Carlo staff at Los Alamos National Laboratory (LANL) [3-5]. It has been widely used as tool in many fields such as accelerator application, proton and neutron therapy, radiation shielding, radiation protection and dosimetry, fission and fusion reactor design, and other applications by several thousand users worldwide [6, 7].

The MCNP can deal with neutrons, gamma ray transport as well as coupled transport, such as secondary gamma rays as a result of the collision and also electron transport, both primary and secondary electron sources created resulting from gamma ray collision. The MCNP can provide geometry-independent mesh tallies for visualisation of does, flux and energy deposition over continuous space volume with no complicating particle transport over the geometry [8, 9]. The MCNP can use a surface card, cell card and data card or other physical property card that they are able to show the definition of the geometry. Furthermore, they are able to simulate the particle distribution [10].

The most common measure of the amount of radiation damage for displacement damage in a different type of particles is displacement per atom [11-15]. E521 ASTM standard particle for neutron radiation damage simulation by charged particle irradiation recommends the utilise of the NRT secondary displacement model that allows for calculating irradiation damage. Also it

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allows DPA correlations from neutron damage [16]. The purpose of this paper is to investigate the effect of radiation damage in iron and demonstrate the DPA calculation model using MCNP.

Calculation of displacement cross-section

The Norgett-Robinson-Torrens was proposed NRT model as a mean of predicting the total number of displacements N_d produced by a primary knock-on atom (PKA) with potential energy E_{PKA} [17]. Based on the Athermal Recombination-Corrected (ARC-DPA) model, the number of stable defects produced under irradiation is given by the following equation.

$$N_d(T) = \begin{pmatrix} 0 & T_d < E_d \\ 1 & E_d \leq T_{dam} < \dfrac{2E_d}{\beta} \\ \dfrac{\beta T_{dam}(\xi_{ARC-DPA})}{2E_d} & \dfrac{2E_d}{\beta} \leq T_{dam} < \infty \end{pmatrix} \tag{1}$$

Where E_d is the threshold displacement energy and represented the minimum energy required to generate a stable Frankel pair. The damage energy denoted T_{dam} and represents the portion of the PKA energy which is lost by elastic collisions with the target atoms. Also, β is equal to 0.8 factor which was determined from binary collision formula.
Where the defect generation efficiency $\xi_{ARC-DPA}$ is equal to the following equation [18].

$$\xi_{ARC-DPA} = \frac{1 - c_{ARC-DPA}}{\left(\frac{2E_d}{\beta}\right)^{b_{ARC-DPA}}} T_{dam}^{b_{ARC-DPA}} + c_{ARC-DPA} \tag{2}$$

Where $c_{ARC-DPA}$ and $b_{ARC-DPA}$ are parameters. Figure 1 shows an example of displacement cross-section for iron calculated using the ARC-DPA and NRT model. Values of displacement cross-section were calculated using nuclear data libraries from JEFF-3.3 [19]. In this figure, energy can depend on DPA-neutron cross section, which is multiplied with neutron incident energy spectrum to calculate displacement cross section.

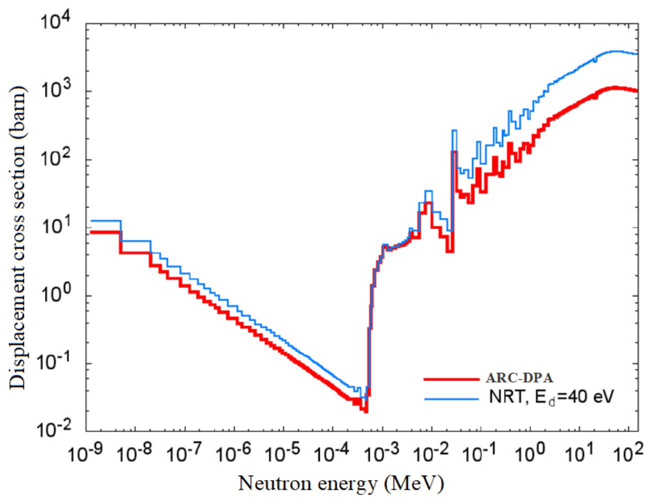

Fig. 1. Displacement cross section against neutron energy for iron

MCNP5 Method

The Monte Carlo transport simulation code (MCNP5) has been used to model the interaction of neutrons within iron. The geometry modelled in MCNP5 consists of a 2 cm of length, 1 cm of high and 1 cm of thickness for slab target iron. The target iron slab was based on 5.9% Fe-54, 9.1% Fe-56, 2.1 Fe-57 and 0.28% Fe-58 which are surrounded by air as shown in figure 2. For the slab geometry, the model described a mono-directional source of 2 MeV neutrons which interact with the iron slab. Mono-directional source neutrons were emitted from a 1.5 cm x 1.5 cm square surface source, placed 1.5 cm far from the iron slab.

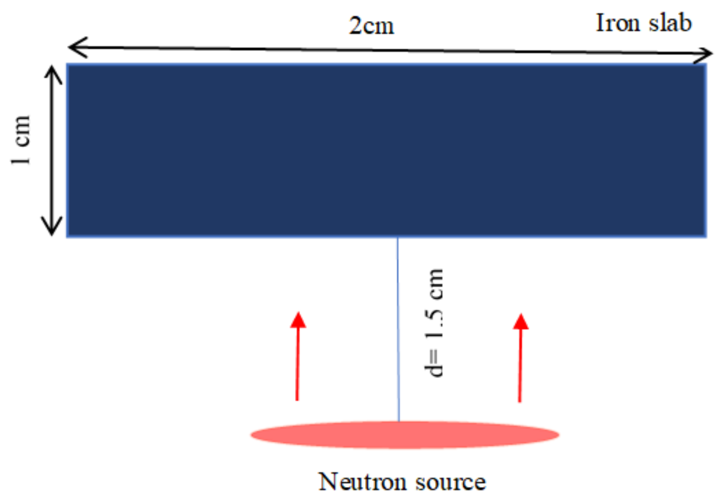

Fig. 2. Schematic diagram showing the slab geometry by a monodirectional neutron source.

The first simulation was started by running 2000000 histories for 2 MeV neutron source. And the graph was plotted between the number of histories and the statistical tests, which were found them from the output file. Once important thing is the reliability of the result of the test which can be determined either by passing all the ten statistical testes particularly the relative error. Also, it can be determined by considering on the figure of merit (fom).

Figure 3. shows that the figure of merit tends to be fluctuating at the end of the way. However, the statistical tests were not passed, the value of that tally. Moreover, the total number of neutron flux was passed through the slab surface which was about 1.53891E-01 neutrons per cm^2, with 0.0003 of error.

MCNP5 calculation of DPA

For the calculation of the DPA within iron, MCNPX was used. There are two kinds of methods which can calculate the DPA with model of specific geometry. The first method calculates flux and fold with DPA cross section. The second method calculates DPA directly with the MCNPX (HISTP/ HTAPE). Both methods produces radiation damage energy cross section

[20, 21]. The DPA was calculated using the radiation damage cross sections that are not able to a part of the MCNPX cross section libraries. Cross section is developed by using Norgett-Robinson-Torrens (NRT) model or new methods such as advanced models Molecular Dynamics (MD) simulation coupled with the binary collision approximation (BCA) or other simulation methods [22, 23]. The flux in MCNPX as a function of energy was tallied by using the F4 tally (F4 is necessary to carry out the calculations) which multiplied by the neutron displacement per atom cross section for iron material. Therefore, the displacement per atom (DPA) was calculated in MCNPX which is given by.

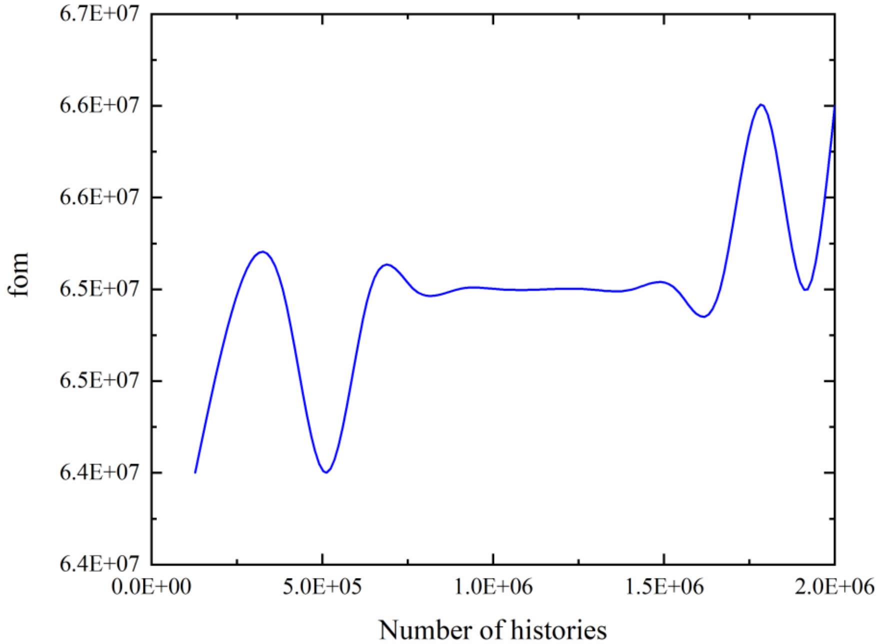

Fig. 3. Number of histories against figure of merit

$$DPA = \int \sigma_{disp}(E)\frac{d\emptyset(E)}{dE}\,dE \quad (3)$$

Where $\emptyset(E)$ is the flux-spectrum (particles/cm^2), and $\sigma_{disp}(E)$ is the displacement cross section (barns).

Figure 4. illustrates the absorption cross section for neutron by using iron slab in different layers of the shield. It is clear that the DPA cross-section decreases with increasing neutron energy until a minimum is reached, after that it stays constant as well as then fluctuating dramatically towards the end of the plot. MCNPX was calculated using the number of the displacement per atom by using tally. So, the maximum number of atomic displacement was about 1.73E-01 DPA.

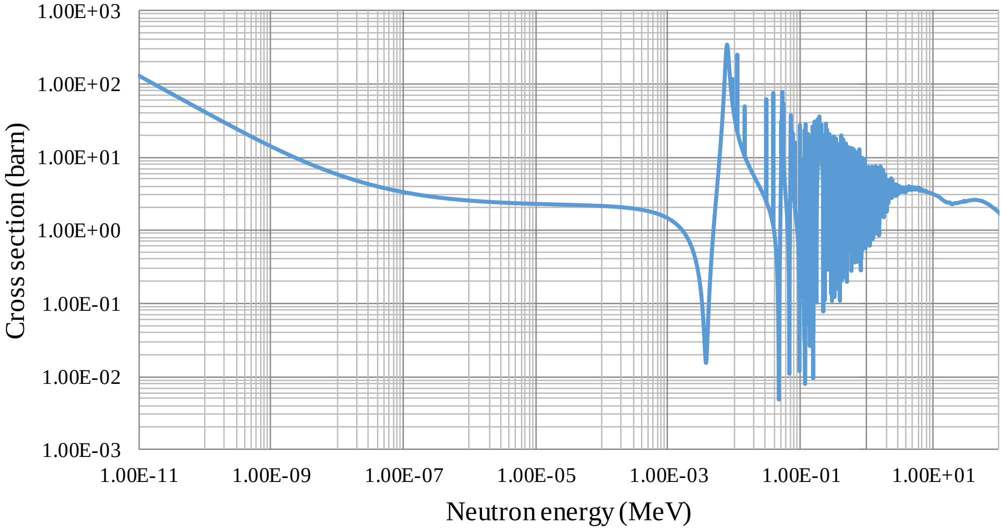

Fig. 4. Neutrons incident energy against displacement damage cross section using iron

Conclusion

MCNP method could be used to determine the total number of neutron cross section on a surface as well as how using MCNP geometry problem solving. Calculations have been performed by Monte Carlo method using MCNP5 transport code to model the interaction of neutrons within iron. Then, MCNP5 was calculated using the F4 tally for determining the number of DPA cross section. The results demonstrated in figure 4 that the DPA cross section reduces with increasing neutron energy; after that it stays constant and then fluctuating dramatically towards the end plot. The average number of the DPA was 5.6E-03.

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