Journal of Physical Chemistry and Functional Materials

Home Page of Journal: https://dergipark.org.tr/jphcfum

A Review on DPA for Computing Radiation Damage Simulation

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ABSTRACT

A Monte Carlo code is developed for the radiation damage in the metals which results from nuclear collisions that create energetic recoil atoms of the host material. The development of the simulation codes for the radiation damage method by neutrons and protons can be highly useful in technology of advanced nuclear systems and nuclear fusion reactors. The aim of this review is to investigate the impact of the radiation damage in the materials by the neutron and proton energy irradiation. The damage parameter used in the evaluation is displacement per atom (DPA) in material as a function of neutron and proton energy. For this purpose, there are some software codes used which are related to radiation damage because radiation damage can be measured as a function of DPA, which is one of the critical issues for high intensity beams, particularly, for protons and neutrons.

ARTICLE INFO

Keywords:
MCNP
DPA
FULKA
SRIM
PHTIS

Received: 2021-11-24
Accepted: 2022-02-18
ISSN: 2651-3080
DOI: 10.54565/jphcfum.1027393

1. Introduction

Radiation damage has always been an interesting subject to study and the standard damage parameter is displacement per atom (DPA) [1-3]. So, for the measurement of the displacement per atom values of the material component of a nuclear power, there are a large number of Monte Carlo codes such as MCNPX, SRIM, FLUKA, PHITS and MARS15. The SRIM (formerly TRIM) is one of the types of code for measuring radiation damage calculation method exposure unit known as displacement per atom [4-6]. Thus, DPA has been used as a standard measure for computing neutron and proton induced radiation damage production from different radiation sources [6, 7]. MCNPX is a general-purpose Monte Carlo N- particle Computer code which can be widely used in a number of different transport modes such as neutron and proton. MCNPX was developed by the Monte Carlo staff at Los Alamos National Laboratory (LANL) [8, 9]. A general-purpose Monte Carlo simulation code used for transport of particle physics and interaction with matter is called FLUKA. It can be widely applied in many fields such as dosimetry, radioprotection, calorimetry, activation, cosmic ray physics, accelerator design, shielding design, detector design, neutrino physics, medical physics, hadron therapy and etc [10, 11].

PHITS can handle the transport of almost all particles, including Protons, neutrons, photons, heavy ions an electron, over wide energy ranges, by utilizing nuclear data libraries as well as some nuclear reaction models. PHITS is a Monte Carlo transport simulation code which is used in various research fields such as radiotherapy, space radiation, accelerator, medical application and in many other applications which are related to particle and heavy ion transport Monte Carlo code system [12-14].

The MARS code system is a Monte Carlo program for inclusive and exclusive simulation of hadronic and electromagnetic cascades in a three-dimensional geometry of accelerator, detector, spacecraft and shielding components with particle energy range from a fraction of an electron volt up to 100 TeV. The code was developed in 1974, with three studies done at IHEP, SSCL, and Fermilab. The major developments and new features of the MARS15 version combines the theoretical models for strong, weak, modelling of elementary particle, heavy ion and lepton with their interaction cross-section; a module for modelling particle electromagnetic interaction [15-17]

Several authors have argued about evaluating the displacement cross section and displacement per atom in some difference ways using several software codes, such as PHITS, SRIM, NJOY, MCNPX, MARS15 and FLUKA. The purpose of this review is to calculate displacement cross sections and displacement per atom values by different software codes and compares radiation damage by different radiation source for neutron and proton.

2. DPA and DPA Cross Section Calculation

In review, displacement cross section can be archived by the following equation: -

$$\sigma_d(E) = \int_{T_d}^{T_{max}} \frac{d\sigma(E,T)}{dT} V(T) dT \qquad (1)$$

Where T_d is the displacement threshold energy, T_{max} is the highest recoil energy based on kinematics, E is the kinetic energy of the projectile and T is the primary knock-on atom (PKA) energy. In summary, for computing DPA in TRIM model from ion irradiation to the result of proton with the international standard values (ASTME521) [18, 19]. The recommendation by Stoller et al [20], the following recommendations must be complied with:

a) Run SRIM code by using the Quick Kinchin and Pease formula damage option to calculate the number of Frankel Pairs (FP) produced by a primary Knock-on of kinetic energy.
b) Select the displacement threshold energy (E_d) as an example from ASTM E521 Standard particle for neutron radiation damage simulation which is 40 eV for iron [18].
c) Set the lattice binding energy which is equal to 0.0
d) Compute the damage energy (T_{dam}) by equation $T_{dam} = E^p_{ions} + E^p_{Target}$
e) By using damage energy (T_{dam}) to measure the number of displacements.

Many different ways were developed in order to calculate DPA. Kinchin and Pease [20] were the first ones to come up with a great technique. There was a linear relationship between the number of Frenkel pair produced and the initial energy of a PKA. This paper is still the most cited for radiation damage related topics. After Kinchin and Pease, many authors tried to establish a new and better technique for calculating DPA. The most successful ones were Norgett, Robinson and Torrens (NRT) [21, 22]. They developed a method for calculating DPA for a PKA with a given energy. This type of calculation is very interesting because it makes the comparison of different types of radiation easier. The NRT model gives the number of stable Frenkel pairs produced by a PKA with energy [23-25]:

$$\text{Number of displacements } (N_d) = \frac{K T_d}{2E_d} \qquad (2)$$

Where K is the displacement efficiency which is equal to =0.8 factor, T_d is the total energy which is entering the material lattice and E_d is the displacement energy required to produce a stable Frenkel Pair.

Sato, Tatsuhiko, et al. [26] have considered the radiation damage model in PHITS and also presented a different mechanism for measuring the amount of displacement damage. Briefly, according to Iwamoto et al. [27] there are three parts of calculations which improved damage in PHITS; an energy transport calculations including nuclear collision, Coulombs scattering as well as a cascade damage approximation. Figure 1 shows damage calculations in PHITS which can create secondary particles from nuclear reaction and Coulomb scattering.

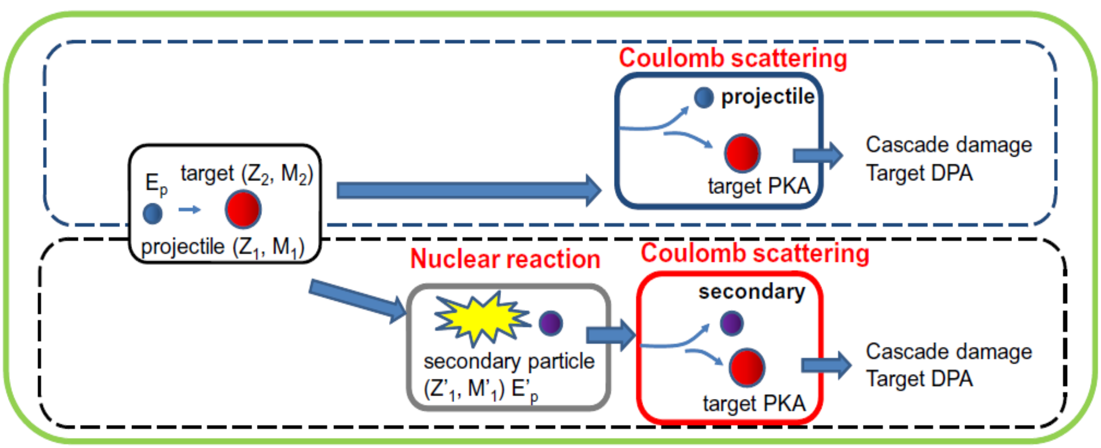

Figure 1: Damage calculations in PHITS [27]

Iwamoto et al [28] have calculated displacement cross section for 20 MeV/u and 200 MeV/u into thick copper and tungsten targets by using two software codes which are SRIM and PHITS as shown in figure 2. Figure 2 shows the case of 20 MeV/u ion into thick copper and tungsten targets for the calculations of the displacement cross section using 5 cm-radius and 0.1 cm. Based on a comparison with ion rang in materials of Proton, Helium-3 and Calcium-48 are less than the mean free path for nuclear collisions, because the majority of the ions can stop without undergoing collisions. So, the displacement cross section for the 20 MeV/u ion beams also exhibits a so-called Bragg-peak. And also showing increasing effect secondary ions with increasing energies. The result of SRIM and PHITS gave good agreement, and therefore the production rate of the secondary particles is very small.

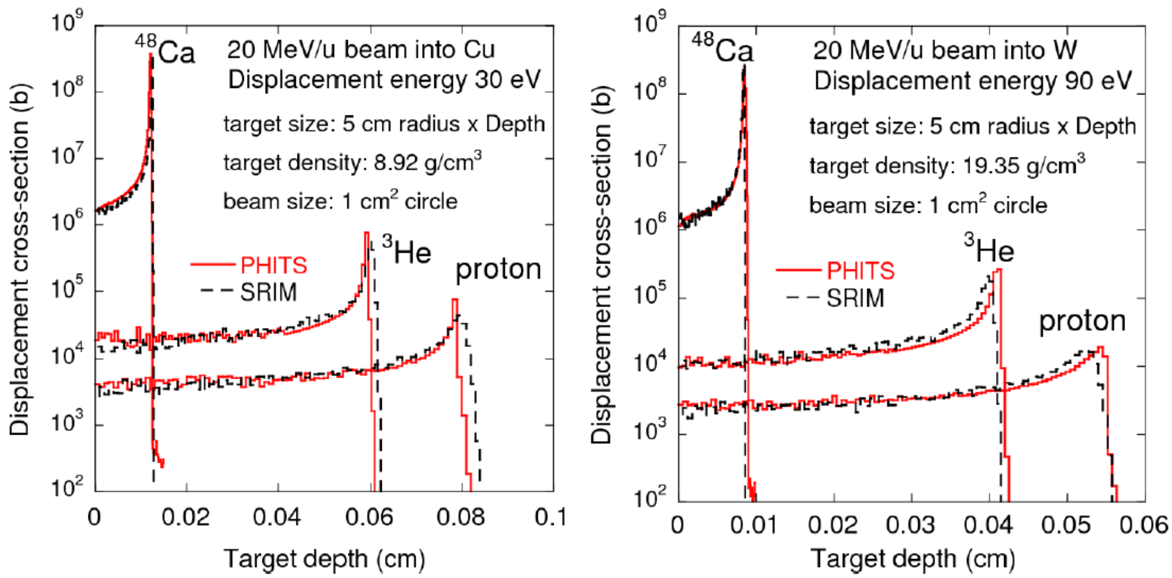

Figure 2: The depth dependence of the displacement cross section values for 5 cm radius and 0.1 cm thick copper target in the left hand, and 5 cm and 0.06 cm thick tungsten in the right hand, both irradiated by 20 MeV/u proton, ^{3}He and ^{48}Ca beam [28]

For 200 MeV/u Proton and Helium-3 ions show the target depth with a displacement cross section in figure 3 from experimental data of Iwamoto et al [28]. In this case, nuclear collisions happen before the stopping range is reached and damage cross sections only created primary knock-on atoms dramatically produced by the secondary particles which are increased for Proton and Helium-3 incidences. There is a difference between PHITS and SRIM. PHITS results are much larger than SRIM ones in tail part.

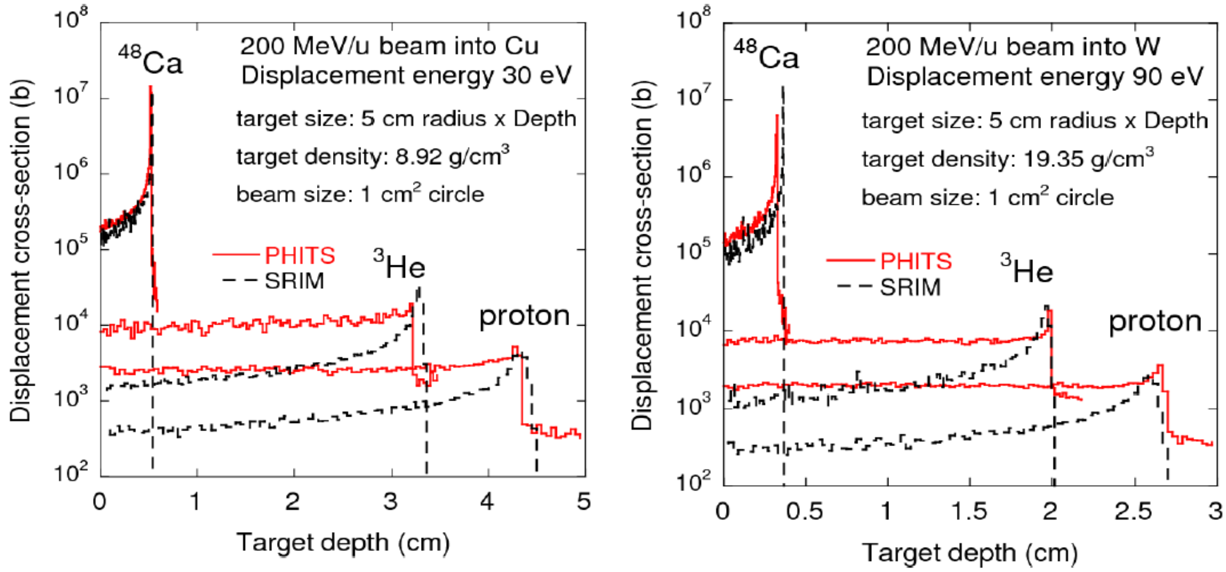

Figure 3: The depth dependence of the displacement cross section values for 5 cm radius and 5 cm thick copper target in the left hand, and 5 cm and 3 cm thick tungsten in the right hand, both irradiated by 200MeV/u proton for proton, ^{3}He and ^{48}Ca beam [28]

Harada et al. [29] have discussed neutron displacement cross section calculated by PHITS, NJOY and LAHET using the threshold displacement energy for Iron-56 is 40 eV based on ASTM E521 Standard. In an energy range from 20 MeV to 150 MeV, the displacement cross section values for PHITS and LAHET codes are lower than NJOY code with LA-150 as shown in figure 4. Notice that at lower energies (<150MeV), the nuclear collision model used in PHITS code did not give good agreement with experimental data. Therefore, it adopted the displacement cross section values for neutrons below 150 MeV obtained by NJOY with LA150.

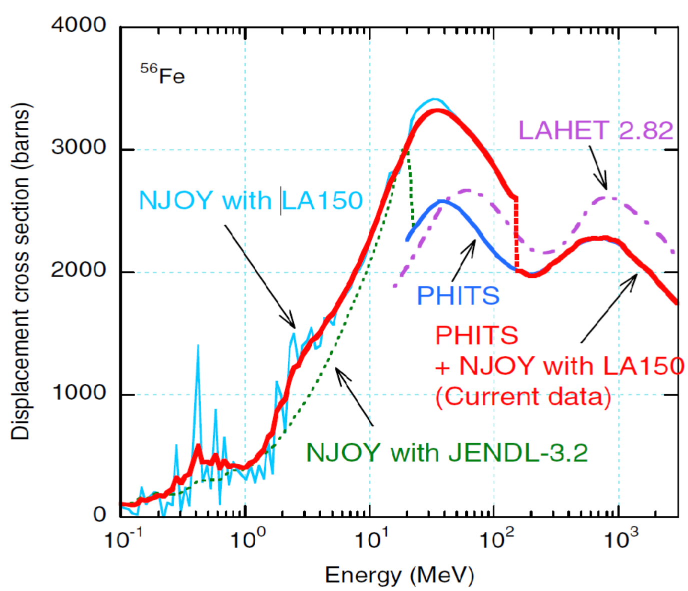

Figure 4: Displacement cross section values of ^{56}Fe for neutrons [29]

Harada et al [29] have also discussed the displacement cross section of Iron-56 and Aluminum-27 for neutron and proton calculated by an only PHITS code which is the code combined with the LA150. As can be seen from figure 5, displacement cross section of Iron-56 for neutrons is much higher than those for protons. Also, displacement cross section of Aluminum-27 for neutrons is higher than those for protons which is up to approximately 150 MeV and 300

MeV. This is because the Coulomb scattering cross section for neutrons is much bigger than that for protons [27].In addition, displacement cross section of Iron-56 is higher than those of Alumium-27 at E>20 MeV for protons. Also, displacement cross section of Iron-56 is higher than those of Almnium-27 at E>8 MeV for neutrons.

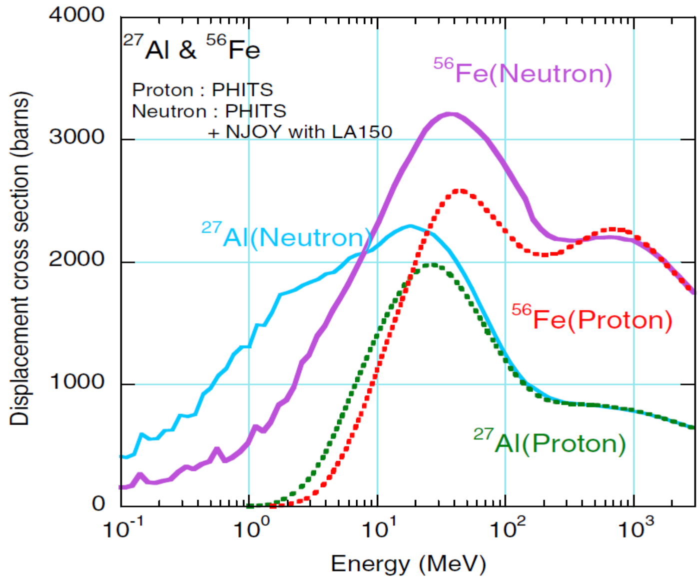

Figure 5: Displacement cross section values of ^{56}Fe and ^{27}Al for protons and neutrons [29]

Mokhov et al., [30] have made a comparison SRIM code with the prediction of other simulation codes such as PHITS MCNPX, MARS15 and FLUKA as a result of DPA calculation. The comparison of the DPA calculated with other codes includes 1000 MeV protons on 3 mm thick iron target with a beam area of 1 cm^2. The results from SRIM, PHITS, and MCNPX are courtesy of Susana Reyes as shown in table 1. Calculated by SRIM code is much smaller value than other codes result [30].

Table 1: DPA calculation comparison [30]

Material	SRIM	PHITS	MCNPX	MARS15	FLUKA
Fe	1.18E-22	2.96E-22	3.35E-21	8.73E-21	2.80E-21
Be	2.97E-20	5.02E-22		2.13E-20	1.68E-20
W	8.04E-16	1.25E-17		1.43E-16	

Table 1 shows 320 MeV/u uranium beam onto 1 mm thick beryllium (Be) target with a beam area of 9 cm^2. In addition, SRIM and PHITS results are a courtesy of Susana Reyes of N. Mokhov. Based on the result, calculated by SRIM code is a much closer value than MARS15.Table 1 also shows 130 MeV/u Germanium beam onto 1.2 mm thick tungsten (W) target with a beam area of 0.035 cm.

Figure 6 can be shown that the results of SRIM code were compared with PHITS and MARS15. Displacement threshold energy used in the calculations was 25 eV for SRIM and 90 eV for MARS15 and PHITS. There is a quite substantial difference between the codes, with a lower DPA value compared with SRIM and MARS15 results, but higher than those from PHITS results, courtesy of Yosuke Iwamoto.

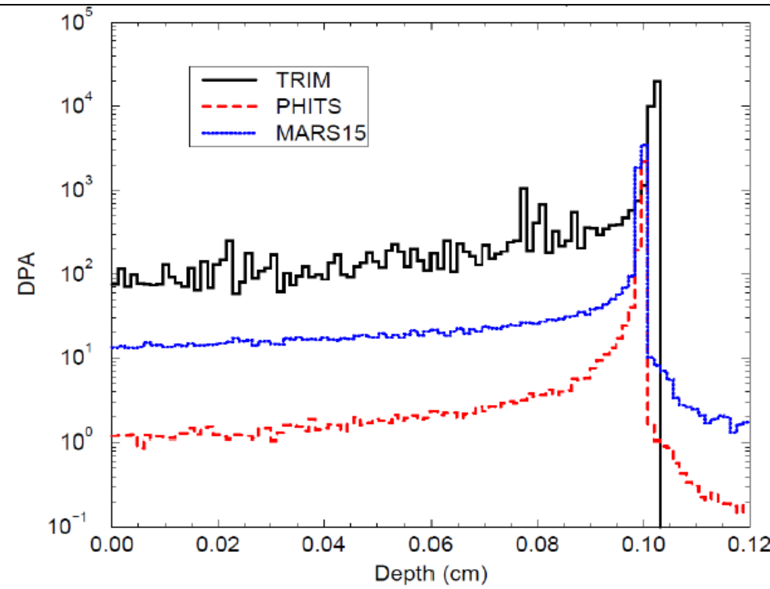

Figure 6: DPA calculation comparison by using SRIM, PHITS and MARS15 cod for 130MeV/u Germanium ion into a tungsten target [30]

Mokhov et al. [30] have also showed that Coulomb scattering produced by the Germanium projectiles is more dominant than that produced by the secondary particle from nuclear reactions. However, SRIM code cannot create secondary particles from nuclear reaction and only can treat Coulomb scattering for the projectile

3. Conclusions

In summary, displacement per atom and displacement cross section calculated for proton, neutron and heavy ion irradiated of various targets at various energies. In addition, comparison have been made in experimental data. DPA cross section calculated for Cu and W target using PHITS and SRIM for protons. It was found that for 20 MeV proton, ^{3}He and ^{48}Ca, the result of SRIM and PHITS gave a good agreement with the experimental data. But, for 200 MeV proton and ^{3}He, PHITS results were much larger than SRIM ones in tail parts. It is also DPA cross section calculated for neutron and proton using only PHITS code. The prediction is that DPA cross section of ^{56}Fe and ^{27}Al for neutrons were much higher than those for protons.

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