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Using of Stopping and Range of Ions in Matter Code to Study of Radiation Damage in Materials

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Abstract: **The aim of this work to investigate the impact of the radiation damage in the materials by the proton energy irradiation. The damage parameter used in the evaluation is displacement per atom (DPA) in material as a function of proton energy. Stopping and Range of Ions in Matter (SRIM) code was used to calculate the total vacancy and the number of atomic displacements based on the Norgett-Robinson-Torrens model by difference energies for proton irradiation damage. The option of this code was calculated by using Ion Distribution and Quick Calculation of Damage (Kinchin-Pease) for Fe and Cu target and also Full damage cascade (F-C) was chosen for only Fe. The result is that, the prediction of the F-C model are higher than the K-P calculation. Comparisons has been made with an international standard definition of DPA.**

Keywords: **Proton Energy Irradiation, Radiation Damage, Displacement per Atom (DPA), Stopping and Range of Ions in Matter (SRIM) Code, Primary Knock-on Atom (PKA)**

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Contents

1. INTRODUCTION

A Monte Carlo simulation code is developed for the study of neutron and proton-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 development of codes for the radiation damage method by neutrons and protons can be highly useful in technology of advanced nuclear systems, for energy and nuclear fusion reactors [1].

There are several codes used that are related to radiation damage [2-6], because radiation damage can be measured as a function of displacement per atom (DPA), which is one of the critical issues for high intensity beams, particularly, for protons. So, for the measurement of the displacement per atom values of the material, there is The Stopping and Range of Ions in Matter Code, in a short, SRIM or TRIM for ion transport in matter which is a one of the types of code for various physical quantities related to ion implantation, energy deposition and other effects of interaction of ions with matter [7-9]. It is also used to calculate radiation damage calculation method exposure unit known as displacement per atom.

Thus, DPA has been used as a standard measure for computing proton induced radiation damage production from different radiation sources [10]. There are two basic types of damage calculation: Quick Calculation of damage (Kinchin-Pease model) (K-P) and Full damage cascade (F-C) [11,12]. Accordingly, this paper is mainly to investigate the effect of radiation damage in materials and demonstrate the displacement per atom in the results of the advanced Monte Carlo transport simulation code.

2. DISPLACEMENT DAMAGE

2.1. Displacements Produced by a PKA

Displacement cascade, in a material can be visualised as a series of elastic collisions initiated with the lattice atoms, where the lattice atom hit by a high energy particle. The initially-bombard a target is named Primary Knock-on Atom (PKA) [13]. Displacement cascade can be created by PKAs, in turn when an energetic incident particle, transferred to the PKA, is high enough, $E >> E_d$, the PKA will be able to continue the PKA process to displace other atoms of the crystal, creating secondary recoil atom displacement. Thus, it can depend on the amount of the energy and mass of the recoil [14]. **Fig. 1** shows collision cascade or displacement cascade by a PKA.

If a lattice atom is hit by a PKA, it must receive energy in the collision in order to be displaced atom from its lattice site. This minimum energy is called the displacement threshold energy. It obviously depends on the initial direction. The lattice atom in collision receives energy that is less than the displacement threshold energy, the atom can be knocked out of its position in the crystal but will not be displaced [13].

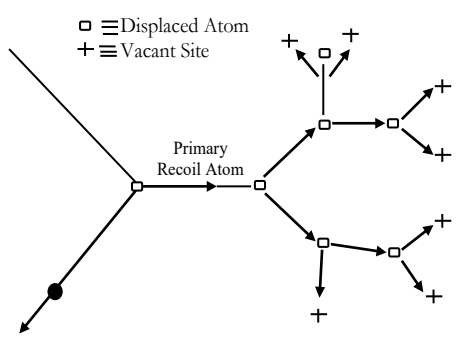

Fig. 1. *Schematic representation of the formation of displacement cascade by a PKA.*

The average number of displacements for a PKA energy E can be estimated by the following derivation given by Kinchin-Pease damage function [15]:

$$N_d(E) = \begin{pmatrix} 0 & if\ E > E_C \\ 1 & if\ E_d < E < 2E_d \\ \dfrac{E}{2E_d} & if\ 2E_d < E < E_C \\ \dfrac{E}{2E_d} & if\ E > E_C \end{pmatrix}, \quad (1)$$

where E_d is the threshold displacement energy and represented the energy required to generate a stable Frankel pair and E_C is the cut-off energy of discrimination of elastic and inelastic.

2.2. Displacement Per Atom (DPA)

The most common measure of the amount of radiation damage for displacement damage in a different type of particles is displacement per atom [16]. E521 ASTM standard particle for neutron radiation damage simulation by charged-particle irradiation recommends the use of the Norgett-Robinson-Torrens secondary displacement model that allows for calculating irradiation damage and it also allows DPA correlations from neutron damage [17].

There are many different ways that have been developed to measure the displacement per atom. One of them is the Kinchin and Pease (K-P) model; they were the first people to come up with a great process. In this model, the actual number of point defects produced by an ion implantation can be derived from the energy, which is transferred from an ion to an atom of the target materials [18].

The majority of the authors in this field have tried to establish a new process for measuring DPA. The Norgett-Robinson-Torrens model was the most successful one. It developed a method in 1975 for calculating DPA [14]. Based on this model, the number of displaced atoms is given by the following equation:

$$N_d(E) = \frac{\beta T_{dam}}{2E_d}, \quad (2)$$

were β = 0.8 factor is the displacement efficiency which was determined from binary collision formulas to account for realistic scattering anisotropy in the screened interaction potential. T_{dam} is the damage

energy and represents the portion of the PKA energy which is lost by elastic collisions with the target atoms.

Stoller et al. [19] have discussed another way for calculating DPA which is based on the number of vacancies produced. Simply summing incoming ion and the target atom from the *vacancy.txt file* provides the average number of vacancies produced.

Unfortunately, the NRT-DPA is not always a good correlation parameter available for all the irradiation correlations since only the actual number of atomic displacement did not control all the radiation effects. Particularly, the NRT-DPA is used merely as an irradiation dose more than an appropriate correlation parameter. The concept of the NRT-DPA is not capable of including spatial fluctuation distribution [20].

3. SRIM/TRIM ANALYSIS

3.1. Vacancies and damage calculation

SRIM-2013 code has used to calculate the total vacancy by difference energies for proton irradiation damage. The option of this code was calculated by using Ion Distribution and Quick Calculation of Damage (Kinchin-Pease model). Calculations were for *H* ion implantation into Fe and Cu for a range of *H* ion energies using 0.5, 1.0 and 9.0 MeV of PKA. The threshold displacement energy used in the calculations was 40 eV for Fe and 30 eV for Cu based on ASTM E521 Standard and the lattice binding energy was set at 0.0 [17,21]. Then, the incident ion was fixed for 5000 ions. At the end, the data has found in the "*vacancy.txt*" output files, which were detailing the number of vacancies created for ions and recoils.

Fig. 2 shows SRIM calculation of vacancy creation cause H into Fe and Cu using 0.5, 1.0 and 9.0 MeV. In the case of 0.5 MeV H into Fe and Cu beams, the prediction of the Cu is greater than the Fe with the total number of vacancies per ion being around 12/Ion for Cu and 8/Ion for Fe. For 1.0 MeV, the total number of vacancies per ion is about 10/Ion for Fe and 16/Ion for Cu. And it is also for 9.0 MeV that the average number of vacancies per ion is 31 for Fe and 48 for Cu. From Fig. 2, the number of target vacancies increase, which is dependent on the ion energy. For example, for 1.0MeV H PKA in Fe is greater damage than the 0.5MeV H PKA in Fe

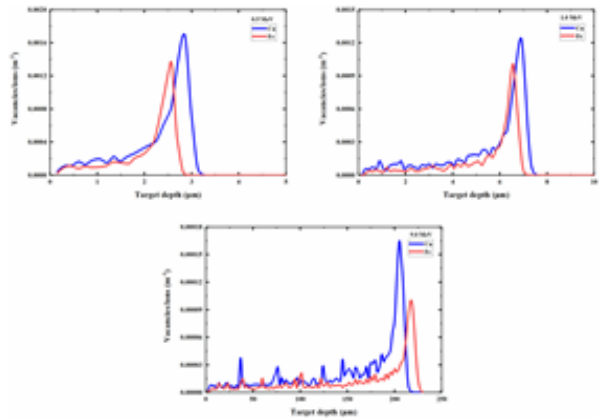

Fig. 2. *Number of vacancies per incident ion versus depth for 0.5, 1.0 and 9.0 MeV H PKA into Fe and Cu.*

because the ion with higher energy can transfer more energy to the recoiling atom.

3.2. Comparison between K-P and F-C

In this section, SRIM-2013 code has used to calculate the total vacancy. The option of this code was selected by using *Full damage cascade* (F-C) and compared with *Quick Calculation of Damage* (Kinchin-Pease model) (K-P). Calculations were carried out for H ion implantation into only Fe for a range of H ion energies using 0.5 and 1.0 MeV of PKA. Then, the incident ion was also fixed for 5000 ions. At the end, the data has found by summing the second column and the third column from the "*vacancy.txt*" output files. The results of the difference between the K-P and F-C models for **Fig. 3** is that, the prediction of the full cascade (F-C) model for 0.5 and 1.0MeV are higher than the Kinchin-Pease (K-P) calculation which is independent of the electronic to nuclear stopping ratio.

3.3. DPA Calculation

Read and de Oliveira [19] has also argued about the damage of radiation energy into SRIM as a result of many different ways, and presented a different mechanism for measuring the amount

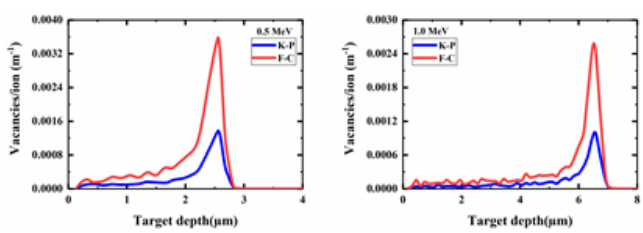

Fig. 3. *SRIM calculation of vacancy creation cause H PKA into Fe and Cu using 0.5 and 1.0 MeV ion.*

of displacement. According to Equation (3), they have illustrated that T_{dam} is able to be calculated by SRIM.

$$T_{dam} = E^{0}_{ions} - E^{I}_{ions} - E^{I}_{target}. \quad (3)$$

In this relation, E^{0}_{ions} can be the incident ion, on the other hand beam energy, E^{I}_{ions} can be the beam energy loss to ionization and E^{I}_{target} is the atom energy target loss to ionization. These values ought to be found in the "*ioniz.txt*" output file.

Furthermore, for determine T_{dam}, the values must be found in the "*phonons.txt*" based on this equation:

$$T_{dam} = E^{p}_{ions} + E^{p}_{target}. \quad (4)$$

where E^{p}_{ions} is the beam energy lost to phonons which is given by the second column (in the TRIM output folder) and E^{p}_{target} is the target atom energy lost to phonons which is given by the third column.

The option of this code was calculated using Ion Distribution and Quick Calculation of Damage. The damage calculated with this option is according to the Kinchin-Pease (K-P) formalism which was used in the NRT standard model. This option is currently used for comparison with proton damage. The ion used was Hydrogen, with ions of energies of 0.5 1.0, 5.0 and 9.0 MeV H PKA into Fe and copper Cu for 5000 incident ion. Then, data has found in the "*phonons.txt*" and obtaining T_{dam} by Eq. (4) and solving in Eq. (2) (NRT equation). The figures show the target depth of the radiation induced damage in the units of displacements per atoms (DPA). **Fig. 4** shows the displacements at Bragg peak can increase,

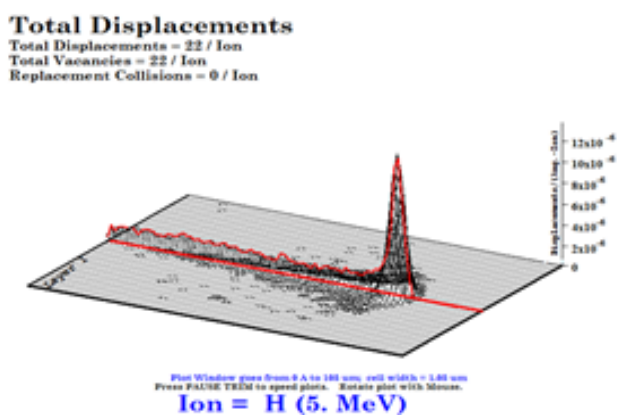

Fig. 4. *Shows the Bragg peak of proton due to H PKA into Fe by using 5.0 Me.*

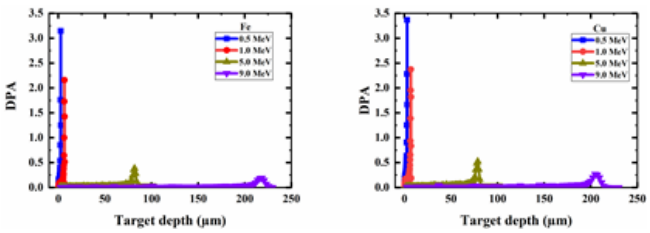

Fig. 5. *Shows TRIM calculation of DPA production due to H PKA into Fe and Cu by using 0.5, 1.0, 5.0 and 9.0MeV.*

therefore protons lose their energy on arriving at Bragg peak.

It can be seen from **Fig. 5** that the target depth change with increase DPA a 0.5, 1.0, 5.0 and 9.0 MeV of PKA energy for Fe and Cu. The results were pretty satisfactory as the DPA behaviour is clear. For lower energy there are taller Bragg peaks which do not distribute their energy through the material easily and so have less DPA an average. For higher energy of 9.0 MeV in Fe have higher displacement damage, which is greater than those for 0.5, 1.0 and 5.0 MeV. The maximum damage level is about 2.85 μm depth, 7.2 μm depth, 87.2 μm depth and 230 μm depth for four energies.

It clearly shows in Fig. 5 hat compared with damage level at 0.5 MeV for copper is lower than those which is at a lower energy around 3.3 μm depth and at higher energy around 2190 μm depth. So, it is clear that the penetration depth varies strongly with its energy. The average displacement per atoms were 0.649 at an ion energy of 0.5 MeV, 0.351 at an ion energy of 1.0 MeV, 0.0639 at an ion energy of 5.0 MeV and 0.035 at an ion energy of 9.0 MeV.

As mentioned before, the factor T_d in Eq. 2 can be called the damage energy as well as can be E_{PKA}. **Fig. 6** shows the plots of damage energy and the

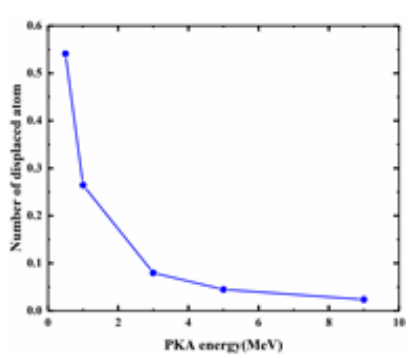

Fig. 6. *Shows the plot of PKA energy with the number of displaced atoms for H into Fe.*

Table 1
DPA of Fe target for two cases

Incident energy (MeV)	DPA - first case	DPA - second case
0.5	2.71E-04	1.46E-03
1	1.38E-04	7.33E-04
5.0	2.50E-05	1.30E-04

average number of displaced atoms (N_d) produced by a PKA of a given energy. It was calculated for iron using a standard method.

3.4. Damage Calculations and Comparison in SRIM

In this section, comparisons has been made with an international standard that the results of DPA, it was calculated for two cases with SRIM model for 5000 incident ions. The first case, the threshold displacement energy used in the calculations was 40 eV for iron and 30 eV for copper based on ASTM E521 Standard and the lattice binding energy was set at zero. The second case, the threshold displacement energy was 25 eV for iron and copper as well as set the lattice binding energy was 3 eV. The data has also found in the "*vacancy.txt*" output files.

Table 1 was compared with DPA by difference in the threshold displacement energy and the lattice binding energy for 0.5, 1.0 and 5.0 MeV H PKA into Fe. The average number of DPA for second case result is greater than DPA for the first case result, which was produced by PKA directly. This is because the Coulomb scattering for the second case is much bigger than that of the first case.

Table 2 shows DPA of Cu target for two cases, the average number of DPA for the second case is also bigger than the number of DPA for the first case.

In addition, when comparing Table 1 and Table 2, the average number of DPA of copper are higher than those of Fe for the both cases. And as is also shown, the number of DPA an decrease with increasing incident ion energy for the both cases.

Table 2
DPA of Cu target for two cases

Incident energy (MeV)	DPA - first case	DPA - second case
0.5	3.75E-04	1.40E-03
1	2.09E-04	7.79E-04
5.0	3.93E-05	8.11E-05

4. CONCLUSION

SRIM-2013 code was used in this work to calculate the total vacancy and the number of displacement based on NRT by difference energies for proton irradiation damage. First, the option K-P model was chosen, and data taken from *vacancy.txt file*. It can be observed that the number of target vacancies increase, which is dependent on the ion energy. Thus, the prediction of the Cu for 0.5, 1.0 and 9.0 MeV were greater than the Fe with the total number of vacancies per ion. Second, using F-C option, and compared with the K-P option. It was found that the results of the F-C model for 0.5 and 1.0 MeV into Fe were greater than the K-P model. So, the F-C option could be more accurate.

Calculations were carried out for SRIM code based on the NRT for determining the number of displacement, which was preferred in the *phonons. txt file* for difference energies into Fe and Cu target when the K-P option was used. It can be noticed that for lower energy there were taller Bragg peaks which did not distribute their energy through the material easily and so had less DPA an average. So, it is clear that the target depth also varies strongly with increasing ion energy. In addition, comparison have been made for SRIM code based on two cases. It was found that the average, the number of DPA of Cu results were bigger than DPA. This is because the Coulomb scattering is much bigger.

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