




## The Use of the Stopping and Range of Ions in Matter Code for Calculation of Damage in Three Different Types of Steel

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### ABSTRACT

In recent years, nuclear power plants have been built worldwide. This amount large of power is better than other energy sources for the environment, it does not have a greenhouse gas. A pressurized water reactor (PWR) is a type of light water reactor to generate electricity and it needed enriched Uranium and large cost. The purpose of this work was to investigate three different types of steel for PWR reactor vessels such as SA30400, SA302B and SA355B-1 steel. The result shows that SA355B-1 performs better than the other. On the other hand, phonons, ionization and collision events show very little damage to all materials.

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### 1. Introduction

A reactor pressure vessel (RPV) in a pressurized water reactor (PWR) is a primary circuit component. It provides a pressure boundary in which the core is contained and performs as an essential safety barrier between fission products from the core and the surroundings. It also supports the core and all its components and directs coolant flow [1-3]. It is generally formed from tempered and quenched ferritic/bainitic steel that has good toughness. A common standard is A533B Class 1 plate or A508 Class 3 (forging) specification. Reactor pressure vessels undergo typically about 0.015 dpa from neutron irradiation. This damage can be emulated using proton irradiation damage. This idea is explored further since although neutron damage could be assessed through the testing of samples from spent components of an RPV, via the implantation of in situ test pieces into the primary circuit or with materials test reactors, all of these methods are time consuming and expensive. Using protons, simulations of neutron damage processes that could take years which can be performed in a matter of

hours. The capability of accelerated protons to emulate neutron damage in a short term way would be very useful as a means of testing material viability quickly during the design of a plant and would also offer the ability to test numerous variables (dose, dose rate, hardness, irradiation temperature, etc.) [4-10].

In terms of nuclear plant safety, RPV is the most important primary pressure boundary component in a PWR. Materials used in shields are SA302B, SA302B modified, SA533B-1, SA533B-1 low cu/p, SA508-2 and SA508-3 in RPV, the Earliest RPVs used SA302B steel. Most vessels are made from SA533B Latest RPV's used low Cu/P contents inside RPV is lined with stainless steel (types 304(early), 308 & 309) to reduce corrosion [11]. Table 1 shows PWR vessel materials [12].

Accordingly, this paper is mainly to investigate ion distribution and calculation of damage for PWR steel materials in the results of the advanced Monte Carlo transport simulation code.

Table 1. PWR vessel materials

UNS designation (steel)	Cr	Ni	C	Mn	Si	P	S	N	Cu
SA302B						0.013	0.020		0.16
SA302B modified		0.49				0.014	0.021		0.23
SA533B-1		0.52				0.011	0.014		0.12
SA533B-1 low Cu/P		0.60				0.007	0.014		0.07
SA508-2		0.79				0.013	0.014		0.15
SA508-3		0.72				0.008	0.007		0.04
S30400	0.18	0.8	0.008	0.2	0.075	0.0045	0.003	0.01	
S30800	0.19	0.10	0.008	0.2	0.1	0.0045	0.003		
S30900	0.22	0.12	0.02	0.2	0.1	0.0045	0.003		
S30800	0.19	0.10	0.008	0.2	0.1	0.0045	0.003		

## 2. Monte Carlo simulation

SRIM (The Stopping and Range of Ions in Matter) is a group of software code which calculate the stopping and range of ions into matter using a quantum mechanical treatment of ion-atom collisions (assuming a moving atom as an "ion", and all target atoms as "atoms") [13, 14]. The Transport of Ions in Matter, in short, (TRIM) is the most comprehensive program included. Moreover, it is a significant program that can be used to gain information regarding the penetration depth of the ions inside the surface of materials. TRIM is possible to simulate complex targets with various aspects of an irradiated material and several target layers. It can measure the final 3D distribution of the ions and all kinetic phenomena for this ion's energy loss. Based on Kinchin-Pease formalism which can calculate the type of TRIM using

(Ion Distribution and Quick Calculation of Damage) [15-17]. The main purpose of the code is to simulate the elastic collision and inelastic collision between the target atom as well as energetic ions, so it can measure for recoil angle ( $\phi$ ) the scattering angle ( $\theta$ ) and also the energy of transfer (T). Figure 1 shows TRIM setup windows, in the upper part can select the ion type and the energy, in the middle part there is a list of layers on the right where an areal density of the target material is entered. In the bottom part can select the number of ions and the type of data must be generated in the output file. So, this work has calculated the ion damage for the same steels which used in the PVR such as (SA302B steel, SA533B steel and S30400 steel) and we have to calculate the ion damage on the Fe shield for comparing the steels and the Fe shield.

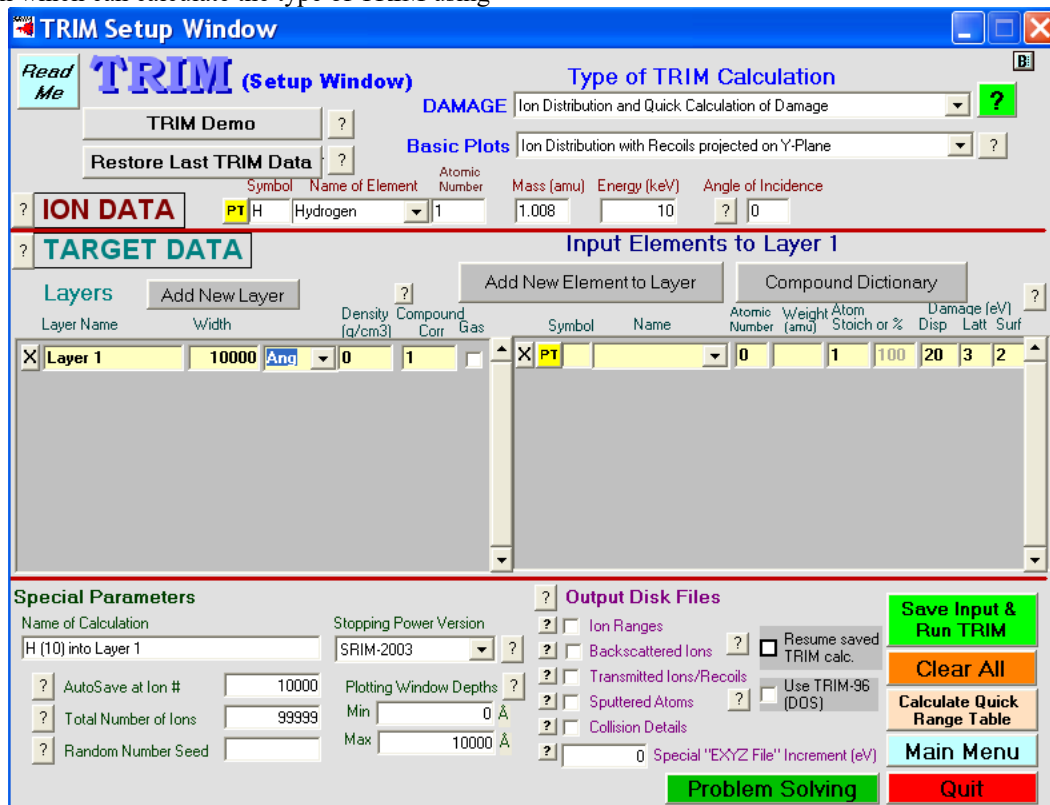


Figure 1. TRIM setup window

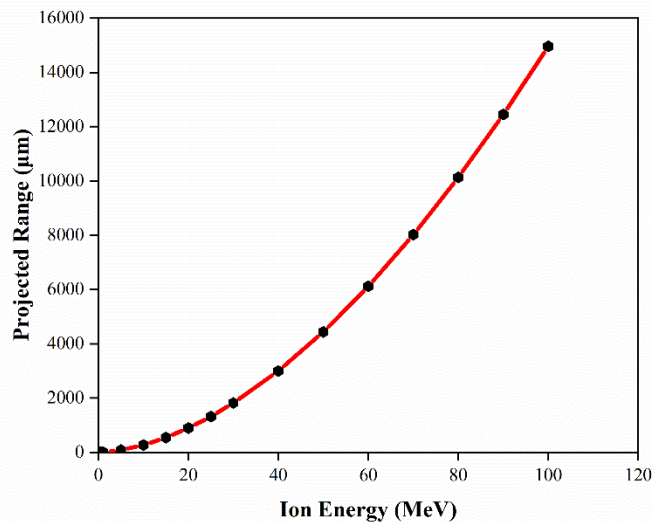
### 3. Results and calculations

TRIM software code has been used to calculate the damage by different energies. The option of this code was calculated by using Ion Distribution and Quick Calculation of Damage (Kinchin-Pease model) for three types of reactor vessel steel such as SA302B, SA355B-1 and SA30400 steels. Calculations were carried out using ion energies 0.025 to 100 MeV. Table 2 and figure 2 show ion energy and

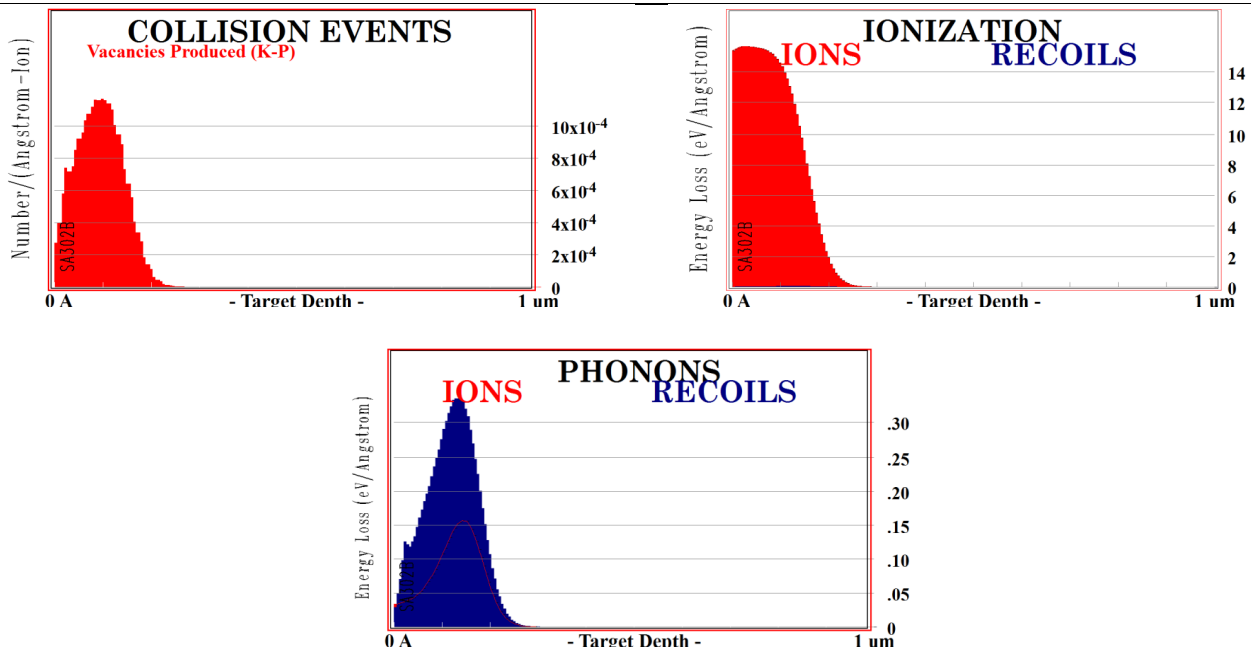
projected range for SA302B steel which contains P, S and Cu. As can see that an ion with an energy of 100 MeV can make a depth of 14960  $\mu\text{m}$  in the SA302B layer. An increase in ion energy can increase the projected range. Figure 3 shows collision events, ionization and photons for SA302B steel using 25 keV ion energy. In this result can be seen that there is small damage for SA302B steel if they are used in the PWR reactor vessel because the moderator high-speed neutrons became thermal neutrons with 25 KeV.

**Table 2.** Ion energy and projected range for SA302B steel

Ion Energy (MeV)	Projected Range ( $\mu\text{m}$ )
0.025	0.1485
0.1	0.5114
0.5	2.91
1	7.3
5	86.26
10	273.27
15	545.66
20	896.4
25	1320
30	1820
40	3000
50	4440
60	6120
70	8020
80	10130
90	12450
100	14960



**Figure 2.** Ion energy against range of depth in SA302B steel



**Figure 3.** Collision events, ionization and photons for SA302B steel using 25 keV ion energy

Table 3 and figure 4 show ion energy and projected range for SA533B-1 steel which contains Ni, P, S and Cu. An ion with an energy of 100 MeV can make a depth of 13060 μm in the

SA355B-1 layer which was smaller than SA302B steel because the depth of ion for SA355B-1 material came from accelerated ions.

**Table 3.** Ion energy and projected range for SA533B-1 steel

Ion Energy (MeV)	Projected Range (μm)
0.025	0.1445
0.05	0.2651
0.1	0.4827
0.5	2.58
1	6.48
5	75.66
10	239.15
15	477.09
20	783.38
25	1150
30	1590
40	2620
50	3880
60	5340
65	6150
70	7000
80	8850
90	10870
100	13060

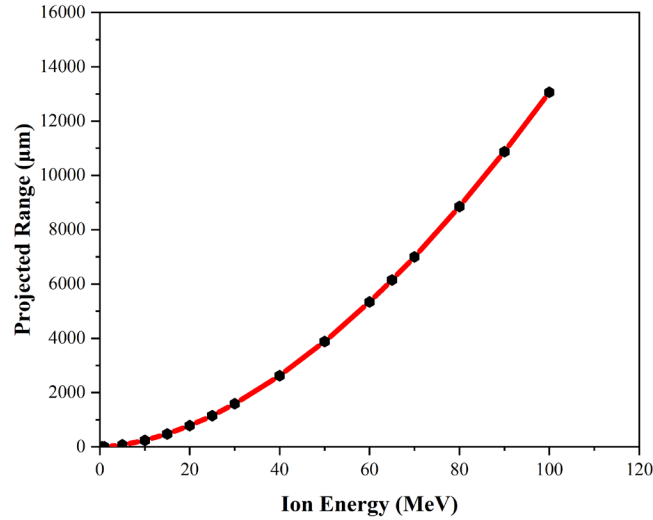


Figure 4. Ion energy against range of depth in SA533B-1 steel

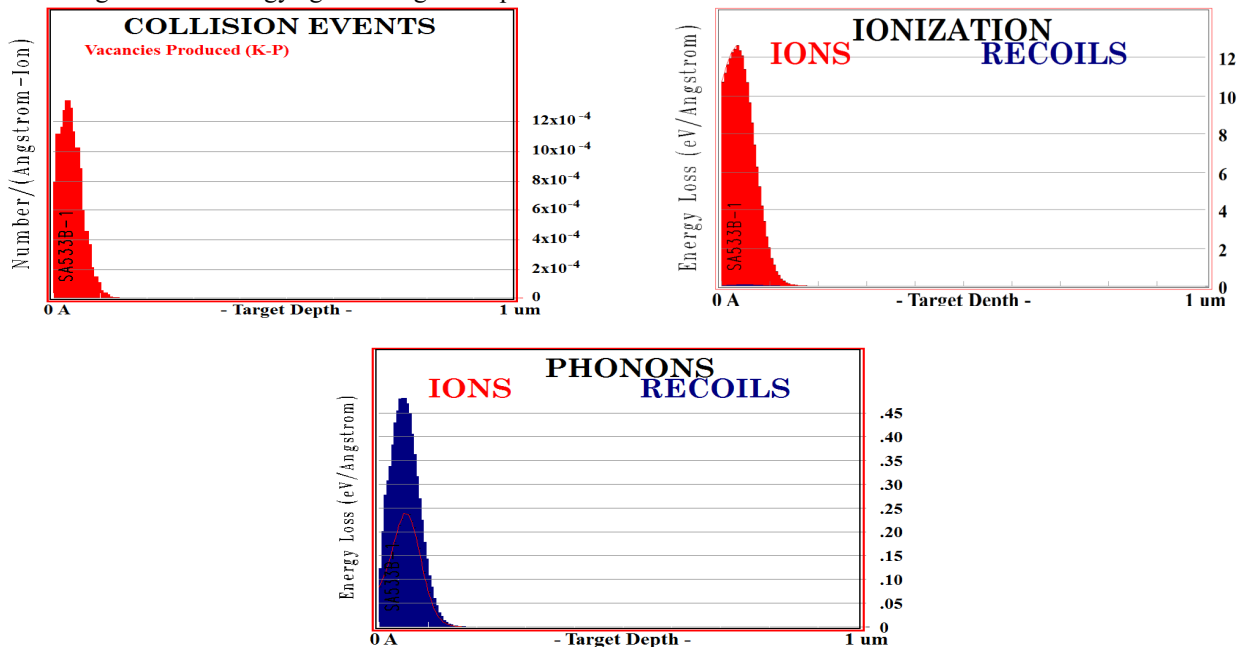


Figure 5. Collision events, ionization and photons for SA355B-1 steel using 25 keV ion energy

Table 4 and figure 6 show ion energy and projected range for SA30400 steel which contains Cr, Ni, C, Mn, Si P, S and N. An ion with an energy of 100 MeV can make a depth of 14140 µm in the SA30400 steel layer. Notice that, a combination of Cu precipitation hardening and grain

refinement might be expected. It mains that those steels contained with Cu are better than another, and Ni is used in steels because of its resistance to corrosion and its small cost.

Table 4. Ion energy and projected range for SA30400 steel

Ion Energy (MeV)	Projected Range (µm)
0.025	0.1517
0.05	0.2729
0.1	0.4878
0.5	2.62
1	6.71

5	80.53
10	256.21
15	512.57
20	843.04
25	1240
30	1710
40	2830
50	4190
60	5780
70	7570
80	9570
90	11760
100	14140

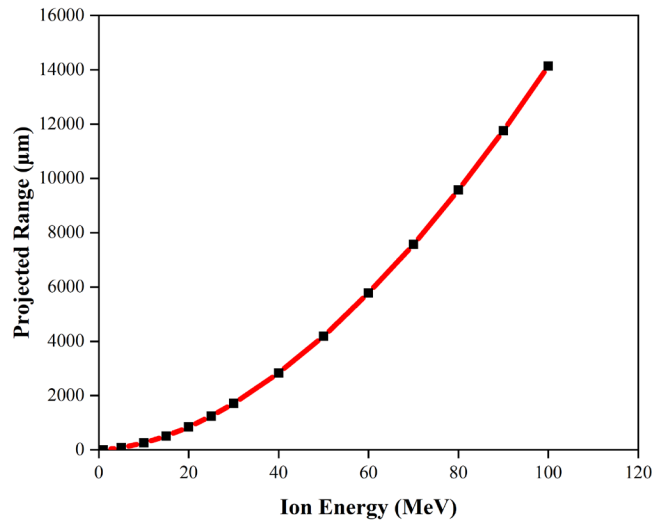


Figure 6. Ion energy against range of depth in SA30400 steel

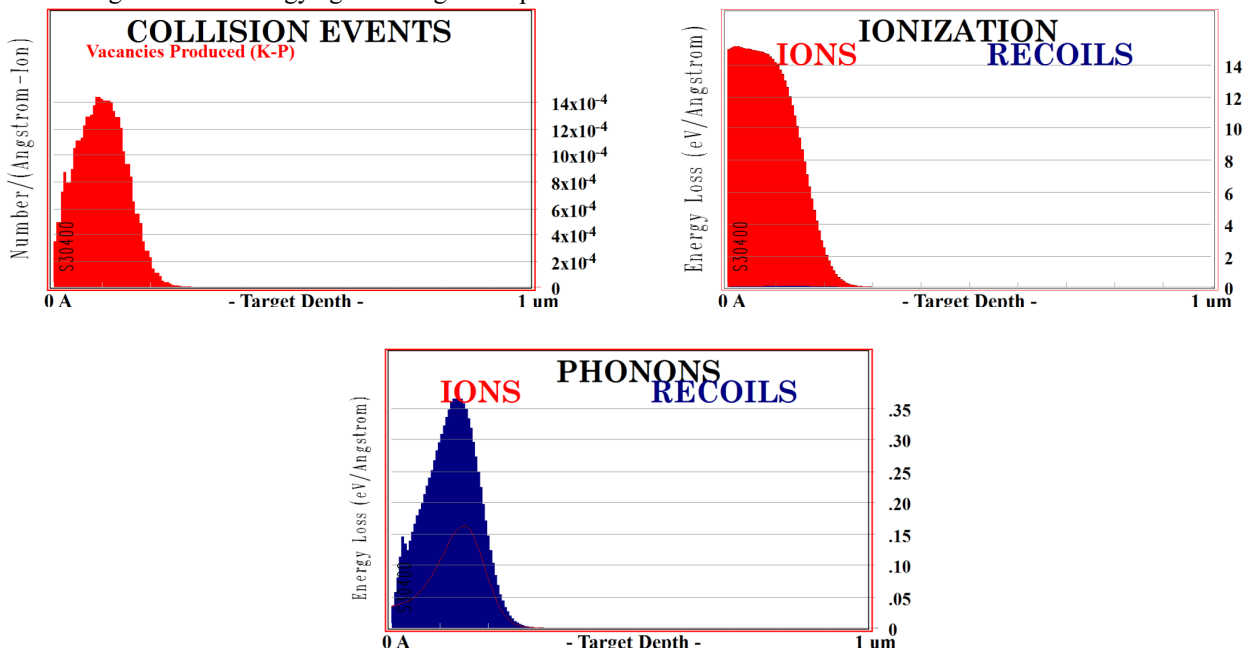


Figure 7. Collision events, ionization and photons for SA30400 steel using 25 keV ion energy

#### 4. Conclusion

This work investigates ion damage in three types of material. These materials are SA30400, SA302B and SA355B-1 steel used in different types of PWR reactor vessels, they are different in components and that makes them special. SA355B-1 is better than the other two types because the depth of ion for SA355B-1 material came from accelerated ions, which was smaller than another. An ion with an energy of 100 MeV can make a depth of 13060  $\mu\text{m}$  in the SA355B-1 layer but the same ion can reach a depth of 14960  $\mu\text{m}$  in the SA302B and 14140  $\mu\text{m}$  in the SA30400.

On the other hand, phonons, ionization and collision events can be shown that there is small damage for all three types of material if they are used in the PWR reactor vessel because the moderator high speed neutrons became thermal neutrons (neutrons with 0.025 eV), and shield must be longanimity for many years. In this study, we use accelerated protons to emulate neutrons, the results indicate that there is small damage for all 99999 ions volleyed the steels and the type of SA533B-1 steel is better than others.

#### References

[1] Hiwa MQ, Ari MH. Investigation of long and short term irradiation hardening of P91 and P92 ferritic/martensitic

steels *Вопросы атомной науки и техники. Серия: Термоядерный синтез*. 2019; **42** (2): P. 81-88.

[2] Zinkle SJ, Was GS. Materials challenges in nuclear energy *Acta Materialia*. 2013; **61** (3): P. 735-758.

[3] Zinkle SJ, Busby JT. Structural materials for fission & fusion energy *Materials today*. 2009; **12** (11): P. 12-19.

[4] Qadr HM. Effect of ion irradiation on the hardness properties of Zirconium alloy *Annals of the University of Craiova, Physics*. 2019; **29**: P. 68-76.

[5] Qadr HM. Effect of ion irradiation on the mechanical properties of high and low copper *Atom Indonesia*. 2020; **46** (1): P. 47-51.

[6] Qadr HM. A molecular dynamics calculation to cascade damage processes *The Annals of "Dunarea de Jos" University of Galati. Fascicle IX, Metallurgy and Materials Science*. 2020; **43** (4): P. 13-16.

[7] Qadr HM. Comparison of energy resolution and efficiency of NaI (TI) and HPGe detector using gamma-ray spectroscopy *Journal of Physical Chemistry and Functional Materials*. 2020; **3** (1): P. 24-27.

[8] Qadr HM. Pressure Effects on Stopping Power of Alpha Particles in Argon Gas *Physics of Particles and Nuclei Letters*. 2021; **18** (2): P. 185-189.

[9] Qadr HM, Hamad AM. MECHANICAL PROPERTIES OF FERRITIC MARTENSTIC STEELS: A REVIEW *Scientific Bulletin of Valahia'University. Materials & Mechanics*. 2019; **17** (16): P.

[10] Qadr HM. Proportional Counter in X-Ray Fluorescence *Aksaray University Journal of Science and Engineering*. 2021; **5** (1): P. 1-7.

[11] Shah VN, MacDonald PE. Aging and life extension of major light water reactor components 1993: P.

[12] Tanaka Y, Reactor pressure vessel (RPV) components: processing and properties, Irradiation embrittlement of reactor pressure vessels (RPVs) in nuclear power plants, Elsevier 2015, pp. 26-43.

[13] Biersack JP, Ziegler MD, SRIM, the stopping and range of ions in matter, SRIM Company 2008.

[14] Qadr HM. Experimental Study of the Pressure Effects on Stopping Power for Alpha Particles in Air *Gazi University Journal of Science*. 2022: P. 272-279.

[15] Ziegler JF, Ziegler MD, Biersack JP. SRIM—The stopping and range of ions in matter (2010) *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*. 2010; **268** (11-12): P. 1818-1823.

[16] Qadr HM, Mamand D. A Review on DPA for computing radiation damage simulation *Journal of Physical Chemistry and Functional Materials*. 2022; **5** (1): P. 30-36.

[17] Mohammad QH, Maghdid HA. Using of stopping and range of ions in Matter code to study of radiation damage in materials *Rensit*. 2020; **12** (4): P. 451-456.