Simulation of neutron and electron damage in Al_2O_3 and MgO using the FLUKA code

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Abstract. We report on the simulation work performed using the FLUKA particle transport code to estimate the damage induced by 1 MeV neutron and 1 MeV electron irradiations in Al_2O_3 and MgO. The simulation results reveal that both electrons and neutrons can induce damage in our target samples, however at differing rates. The neutron damage rate is higher than that of the electrons in both materials and is constant throughout the materials whilst that of electrons is pronounced at shallow depths and decreases with an increase in depth of the materials. The response of both Al_2O_3 and MgO to radiation is revealed to be comparable.

1. Introduction

One of the key interest pertaining to radiation interaction with matter is on the effect radiation has on materials. Materials operating in high radiation environments get affected by radiation. Empirical evidence obtained from nuclear reactor operation [1] and from experimental campaigns conducted to assess the impact of radiation on materials reveals radiation to have a negative impact on materials [2]. These materials endure undesirable physical and mechanical property changes. When in this state the materials are said to be radiation damaged and are therefore not suitable for optimal and safe running of operations.

The energy transfers that occur from the impinging particle to the target material are the onset of material damage by radiation. The energy transfers, however, have to be above a critical energy threshold value known as the Threshold Displacement Energy (TDE) for the process of material damage to be set in motion [3]. The TDE is the minimum energy required to removing atoms from their sites by radiation [2] and energy transfers below the TDE do not result in materials damage.

The aim of this work was to perform Monte Carlo based simulations to assess the radiation response of metallic oxides Al_2O_3 and MgO to neutrons and electrons. These investigations are carried out because Al_2O_3 and MgO are materials considered for use as electron multipliers (dynodes) in photomultiplier tubes (PMT) due to their high secondary electron emission [4, 5]. They are required, however, to be radiation resistant as their exposure to radiation makes them susceptible to radiation damage. MgO has a simple cubic crystal structure while Al_2O_3 has a hexagonal closely packed structure [6] and their structural makeup maybe key to how each material respond to neutron and electron irradiations.

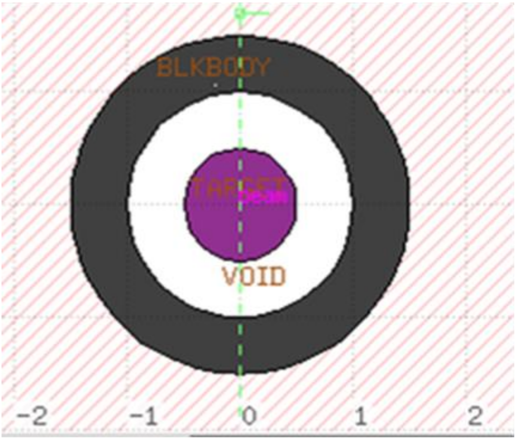
To achieve our aim, the FLUKA code was used to simulate neutron and electron displacements per atom (dpa) in Al_2O_3 and MgO. The dpa is an entity used to measure the radiation damage extent in materials and it relates the number of atoms removed in a material over the number of atoms present in that given material. This simulations offer a primary approach in understanding the effects of radiation in materials.

2. Materials and Method

We used FLUKA, a multi-particle transport code developed and managed jointly by the Italian National Institute for Nuclear Physics (INFN) and European Organization for Nuclear Research CERN [7] to perform simulation work to assess the damage effect of 1 MeV neutrons and 1 MeV electrons in Al_2O_3 and MgO. FLUKA Version 2020.0.4 and FLAIR Version 2.3-0 were used for this simulation work. FLUKA uses a card based input system implemented through the advanced graphic interface FLAIR [8] to create the simulation input file. In addition to creating an input file, FLAIR is used for running the simulation, and for visualization of the geometry model and plotting the simulation results. FLAIR uses the gnuplot plotting program to visualize the simulation results.

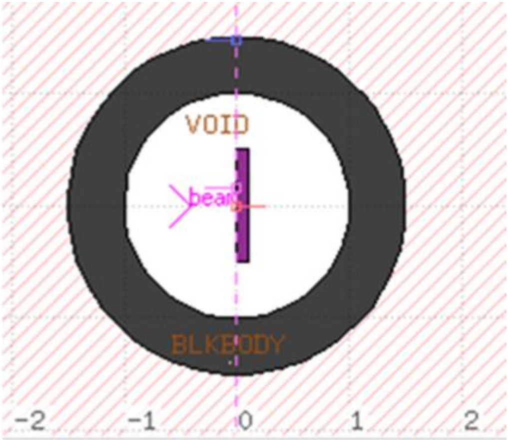
With regards to the input file, the BEAM card is used to define the source term being the particle type, size and energy with the BEAMPOS card used to define beam positioning and direction of propagation relative to the target. The material type and its composition are defined using the MATERIAL and COMPOUND cards, with allocation of the material type to geometry regions achieved using the ASSIGNMA card. Combinations of cards are used to describe the physics settings and the combination is depended on the problem being simulated. For radiation damage estimation, we used the PHYSICS, MAT-PROP, and IONTRANS cards. The PHYSICS card implements the intra-nuclear cascade model that governs hadrons to nuclear interactions while the MAT-PROP card was used to define the material TDE, with the IONTRANS used for defining the ions transportation. Particle transport thresholds are implemented using the PART-THR and EMFCUT cards for hadrons and electromagnetic radiation respectively. These cards are used to define the energy cut-off values of particles being transported. The USRBIN card was used to score the dpa. USRBIN makes use of a mesh grid that is independent of the geometry to estimate the spatial distribution of the scored quantity.

Figure 1 shows the geometry model of the simulation created with FLAIR. The target is modelled as a 10 mm diameter disc of 1 mm thickness. A 4 mm diameter beam was directed perpendicularly to the target depth in the z-direction as seen in the frontview and sideview of the geometry model in Figure 1(a) and Figure 1(b) respectively.



(a)

Figure 1(a). The frontview of the geometry model showing the beam interacting with the target.



(b)

Figure 1(b). The sideview of the geometry model showing the beam interacting with the target.

The interaction of the particles with the target occurs in vacuum (VOID) and particles escaping beyond the vacuum into the background (BLKBODY) are not tallied. Simulations were performed separately for both Al_2O_3 and MgO materials with $1x10^6$ neutron particles and $1x10^6$ electron particles simulated respectively. FLUKA calculates the dpa by implementing the Norgett, Robinson, and Torrens (NRT) model [9].This model is an update on the earliest damage model introduced by Kinchin and Pease, and is now the standard used to calculate the defect density introduced in materials by radiation. Table 1 lists the key parameters used in the simulation to calculate the dpa. FLUKA calculates the dpa per bin, with the dpa value for a given bin being the average dpa in that bin. We divided the depth of our target materials into 50 bins of 0.002 cm bin width. The material dpa was calculated as the aggregate of the dpa per bins.

Table 1. Material and beam parameters used in the simulation

Parameter	Value
Beam Energy (MeV)	1
Irradiation Fluence (n/cm^2)	$1x10^{15}$, $1x10^{17}$, $1x10^{20}$
Irradiation Time (hrs)	8
TDE (eV)	69 for both Al_2O_3 and MgO

3. Results

Figure 2(a) and Figure 2(b) show the dpa/primary result of neutrons and electrons in Al_2O_3 respectively. The dpa/primary relates the damage rate per particle interacting with the material. The dpa/primary in Al_2O_3 by neutrons is $1.17x10^{-21}$ while for electrons is $3.59x10^{-24}$. The dpa/primary profile of neutrons in Al_2O_3 observed in Figure 2 (a) shows the damage caused by 1 MeV neutrons is uniform throughout the material. On the other hand, the dpa/primary profile of electrons in Al_2O_3 observed in Figure 2 (b) shows the damage caused by 1 MeV electrons is non uniform in the material.

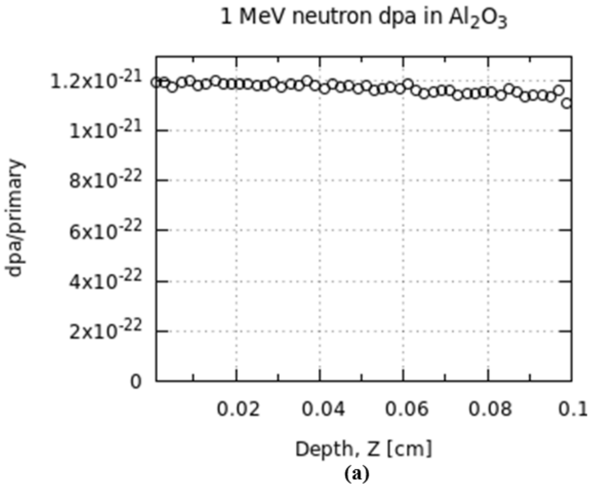


Figure 2(a). The dpa/primary profile of 1 MeV neutrons in Al_2O_3.

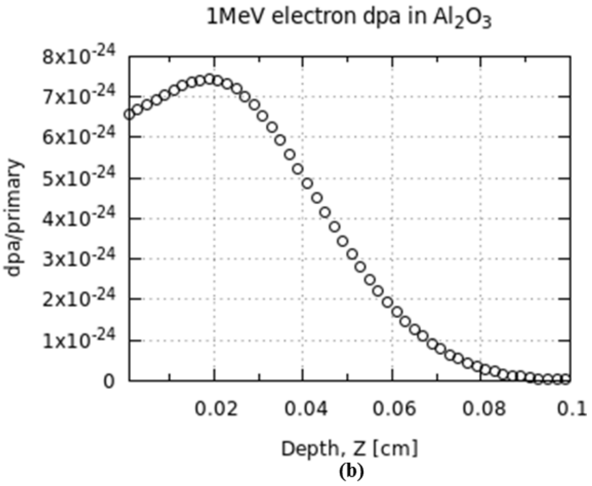
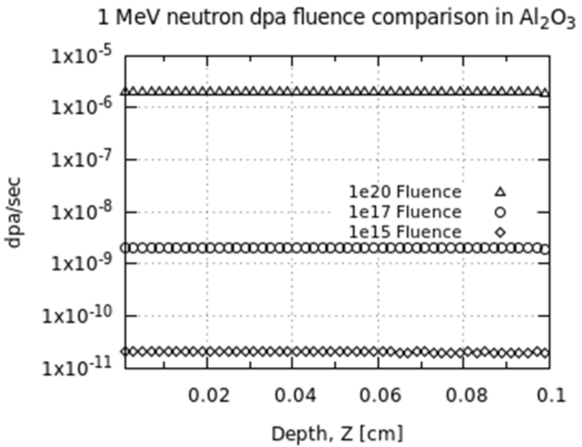


Figure 2(b). The dpa/primary profile of 1 MeV electrons in Al_2O_3.

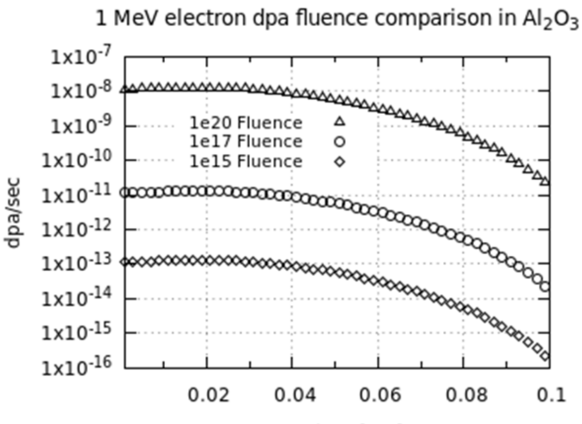
The results observed are consistent with the interaction nature of neutrons and electrons with materials. Neutrons being neutral particles interact directly with the materials nuclei and therefore travel throughout the material. Electrons on the other hand are charged particles that interact through the Coulomb force with the atomic electrons of materials. They get scattered in all directions depositing most of their energy at shallow depths in the material. Less energy is therefore available to effect any meaningful damage deeper into the material, hence we observe the damage profile shown in Figure 2(b).

Figure 3(a) and Figure 3(b) show respectively the neutron and electron dpa rates in Al_2O_3 when bombarded at fluences reported in Table 1. It is observed in both Figure 3(a) and Figure 3(b) that an increase in the particle fluence results in an increase in the dpa rate. This is because over the eight hour irradiation period, more particles interact with the material for particles at higher fluences that result in higher energy transfers from the impinging particles. This then translates to a pronounced displacement of atoms for higher particle fluence as compared to lower particle fluence.



(a)

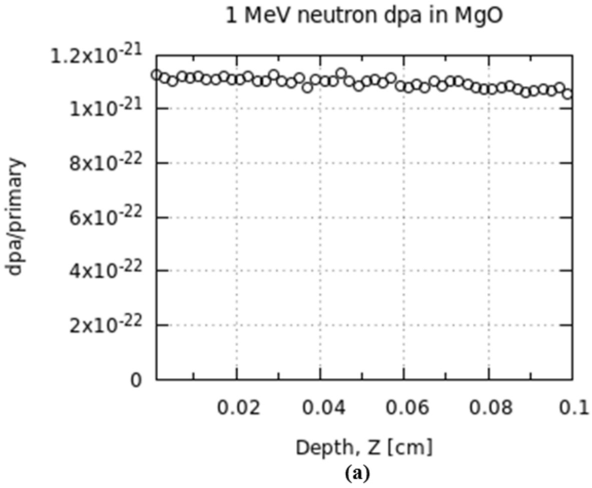
Figure 3(a). The dpa rate profiles of 1 MeV neutrons in Al_2O_3 at different neutron fluence.



(b)

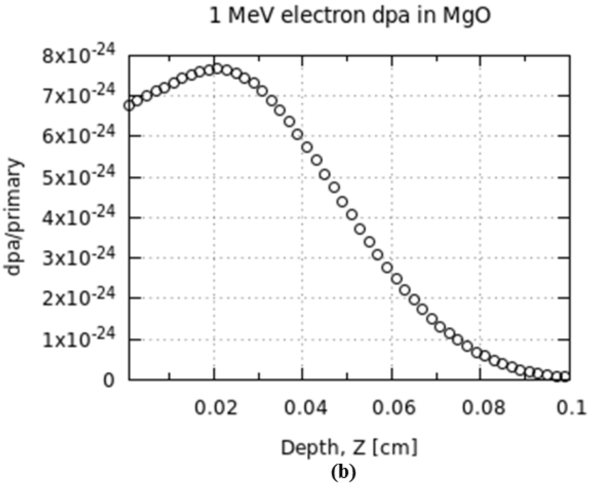
Figure 3(b). The dpa rate profiles of 1 MeV electrons in Al_2O_3 at different electron fluence.

Figure 4 shows the dpa/primary result of neutrons and electrons in MgO. The dpa/primary in MgO by neutrons is $1.1x10^{-21}$ while for electrons is $4.06x10^{-24}$. It is observed with MgO, as was observed with Al_2O_3 that neutron irradiation of MgO result in uniform damage throughout the material, whilst the electron damage is not uniform and maximum damage is limited to shallow depths in the material.



(a)

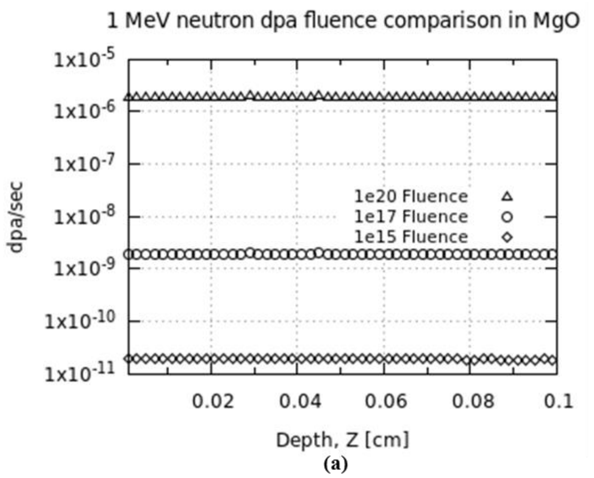
Figure 4(a). The dpa/primary profile of 1 MeV neutrons in MgO.



(b)

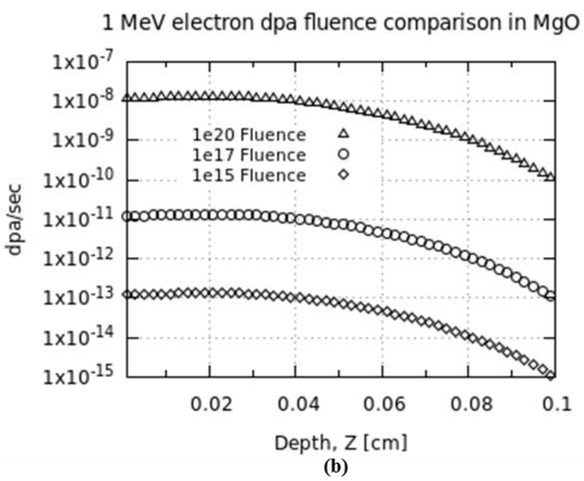
Figure 4(b). The dpa/primary profile of 1 MeV electrons in MgO.

Figure 5 shows the dpa rate results of MgO when bombarded at neutron and electron fluences reported in Table 1. Both Figure 5(a) and Figure 5(b) show that as the particle fluence increases, the dpa rate in both materials increases as was the case with Al_2O_3.



(a)

Figure 5(a). The dpa rate profiles of 1 MeV neutrons in MgO at different neutron fluence.



(b)

Figure 5(b). The dpa rate profiles of 1 MeV electrons in MgO at different electron fluence.

4. Conclusion

In this work, we performed FLUKA simulation of 1 MeV neutron and 1 MeV electron irradiations in Al_2O_3 and MgO to estimate the dpa. We observed that neutron irradiation leads to a high dpa as compared to electron irradiation in both Al_2O_3 and MgO. It was further observed that neutron damage occurs uniformly throughout the materials whilst electron damage is maximized at shallow depths in the materials and is not constant throughout the materials. In terms of their response to electron and to neutron irradiations, Al_2O_3 and MgO dpa rates are comparable. This shows that these materials are most likely to endure similar damage when exposed to radiation. Future work will involve performing experiments of neutron and electron irradiation of Al_2O_3 and MgO to verify the simulation results.

References

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