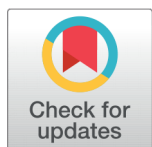


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Simulation of very-low energy alkali ion (≤ 10 KeV) induced effects on Al_2O_3 micro flakes

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Abstract

Objectives: To simulate the Monte-carlo simulation of irradiation of alkali ions (sodium) having very low energy (5 keV and 10 keV) on aluminum oxide micro flakes. **Methods/Statistical analysis:** We have utilized a simulation process namely SRIM (Stopping of ion ranges in matter), which is based on the binary collision approximation technique. We have fixed our target as an aluminum oxide in the layered structure having a thickness about 65 nm. We have incorporated two different types of ion energy as the input parameters which are normally incident on the targets. We have analyzed ion distributions, recoil distributions, and further ionizations. **Findings:** The projected average range for 10 keV is significantly found to be higher, almost double than that of 5 keV. The reason behind this increment is due to the high penetration depth because of higher energy. The straggling of 10 keV is higher than that of 5 keV, which is evident from the recoil distribution where the cascade collision has created a large volume of vacancies, which is very high for higher energy. **Application/Improvements:** This simulation helps us to gather a rich amount of information regarding ion-induced defects, which is highly essential for experiments on aluminum oxide micro flakes. The surface modification after this low ion energy bombardment leads to low detrimental effects which may modify the wetting properties of these flakes

Keywords: Montecarlo simulation; SRIM; Aluminium oxide micro flakes; ion induced defects; BCA

1 Introduction

Aluminum oxide, owing to its various significant chemical, optical and mechanical properties is considered as an effective material⁽¹⁻³⁾ for various industrial applications. Aluminum oxide in nanoscale is often a water remover⁽⁴⁾ and CO_2 ⁽⁵⁾ from gas streams. It is an efficient hydrocarbon remover from air and water purifier⁽⁶⁾ from excessive fluorine content. It is also considered as a potent sorbent of radio nuclides⁽⁷⁾ in power plants. Moreover, the irradiation-induced study

of aluminium oxide nanomaterials can provide rich information regarding the surface modification of alumina.

Here, we have provided a Monte-Carlo based simulation named SRIM^(8,9) that can predict the behaviour of aluminium oxide after collision with an alkali ion. We have also synthesized the aluminium oxide micro flakes using a simple sol-gel method⁽¹⁰⁾. We will complete this low energy irradiation experimentally with sodium ions into the aluminium micro flakes. Before any experimental study, we need to know the datasheets from a simulation study, which we have provided hereafter.

The Stopping and Range of Ions in Matter (SRIM)^(11,12) is an assemblage of software programs that can estimate the irradiation interaction with various target materials. SRIM is widely accepted simulation Programme and widely used in the ion implantation research and semiconductor technology. SRIM⁽¹³⁾ is based on a Monte Carlo simulation technique, namely the binary collision approximation with a random selection of the impact parameter of the next colliding ion. In SRIM calculation, the stopping of ions in target materials has rich data regarding the radiation interaction. After the discovery of various nanomaterials, the importance of irradiation⁽¹⁴⁾ induced effects on these nanostructures was hyped a lot. It has a lot of industrial applications due to its intriguing properties. Hence, it is highly essential to gather a lot of data relating to the ion distribution or recoil distribution. Here, we have tried to simulate the impact of very low energy alkali ions on Al_2O_3 as the target. We have synthesized the aluminium oxide flakes using a simple sol-gel process. The SEM image of the corresponding aluminium oxide is provided below. After getting rich data from the SRIM simulation, the experimentation will be completed in the near future.

2 Simulation Details

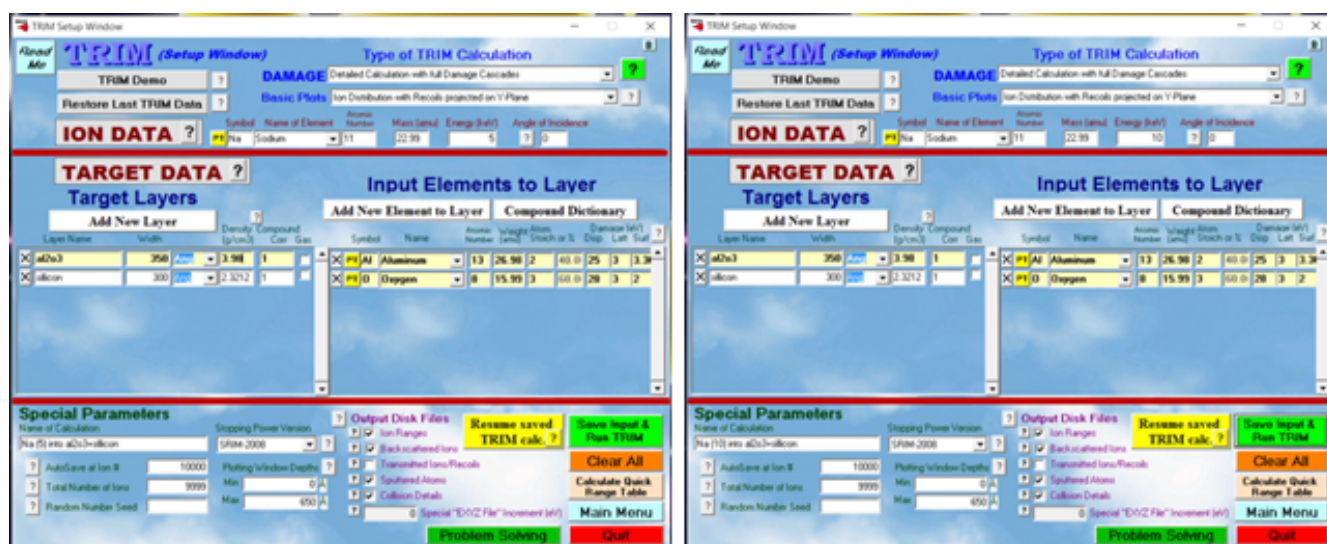


Fig 1. TRIM setup window (a) For 5keV energy, (b) For 10keV energy

Figure 1 shows The TRIM Setup Window which is used to input the data on the ion, target, and type of TRIM calculation. Before doing the irradiation on the micro-flakes experimentally, we have simulated the entire process using the Monte-Carlo simulation package named SRIM. We have utilized the stopping power version of 2008 and simulated over 10000 number of ions. The damage calculated will be based on the detailed calculation with full damage cascades. The ion distribution with recoils is being projected on the XY plane. The angle of incidence is kept at 0 deg. The detailed information obtained from this simulation is provided in this manuscript. Here, we have considered for the target data as aluminum oxide (Al_2O_3) for the first layer, Silicon (Si) for the second layer, and Sodium (Na) as the ion data. Here the energy was taken as very low energies i.e. 5keV or 10keV. Detailed Calculation was completed with Full Damage Cascades. In this method, we simulated by running behind every recoiling atom

and the simulation of every atom eventually stops when the energy decreases than the lowest displacement energy of the target atom.

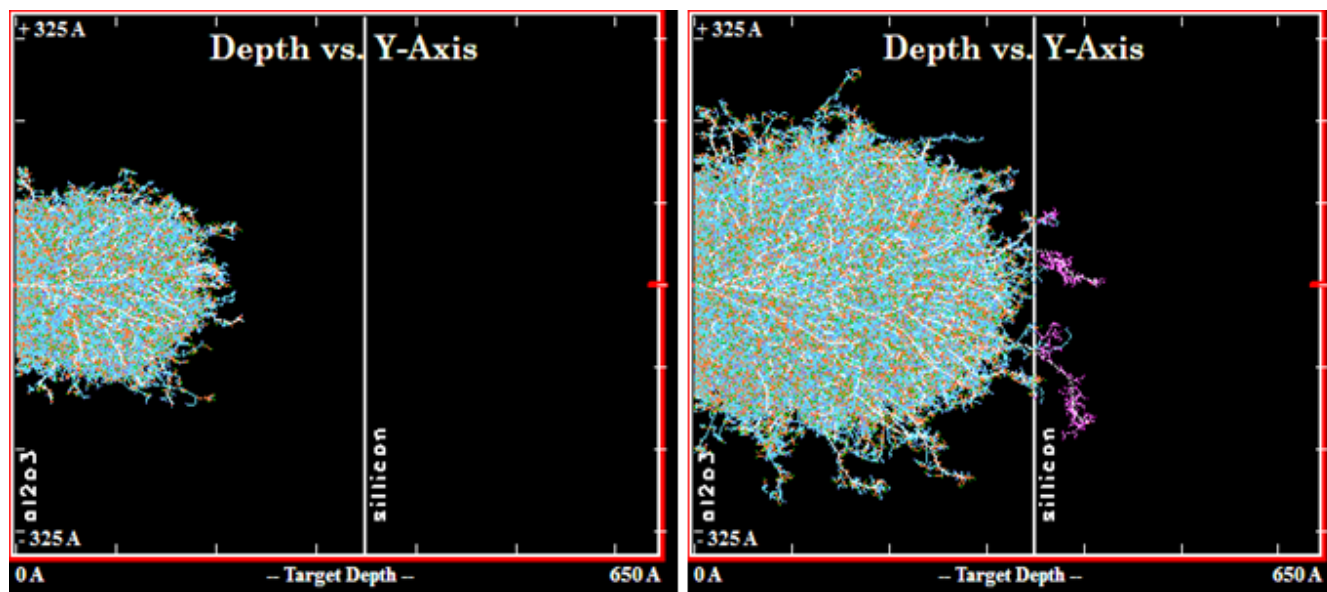


Fig 2. 5keV energy SRIM calculation, (b) 10keV energy SRIM calculation

Figure 2 provides much information about the SRIM⁽¹⁵⁾ calculation when the energy is 5keV and 10 KeV. Here the Ion type is Na and its mass is 22.99 amu, and ions of 5keV and 10keV energies are hitting perpendicular to the target atoms. In the calculation parameters table, we have obtained back-scattered ions 42, transmitted ions 0, vacancies/ion 84.5 for 5keV energy. Similarly, For 10keV energy the back-scattered ions 36, transmitted ions 0, vacancies /ion 156.9 etc. We have also plotted the ion distribution, recoil distribution, energy to recoils graphs in 2D and 3D form for both of these energies (5keV and 10keV).

Figure 2 shows the ion trajectories for 5keV and 10 keV energies respectively. Generally, the first ion track begins to simulate initially. The ion track denoted by a red dot in the Figure 2 shows that one ion hits aluminium oxide atoms from the target and a corresponding vacancy is generated. These generated voids are denoted by the blue dots which is the effect due to recoiling Aluminum Oxide (Al_2O_3) atoms. This process is called a recoil cascade.

When we provided 5keV energy as input incidence energy to SRIM calculation that will only penetrate the primary layer that is Aluminum Oxide layer, but when we increase the energy to 10keV than it will slightly penetrate the second layer that is the Silicon layer. The purple colour ion track shows that much Silicon layer is penetrated by Sodium atom on the Silicon substrate.

After the hard-hitting of Aluminum Oxide (Al_2O_3) atom by the alkali ion, a substantial amount of ion energy is lost. The energy transferred is very low only if the target atom and incident ion masses are very different from each other. After a single binary collision, a blue cascade will be formed. There is a higher probability that the momentum and energy change of the ion happens. Some of the deflections may not be visible in 2D plots, on the contrary, they will be visible in 3D plots. The collision is mainly responsible for bringing out one vacancy. The recoiling of aluminium atom starts immediately which further may create 1000 vacancies. Hence, the cascade collision and the recoiled target atoms are highly responsible for these modifications.

Ion Distribution

Figure 3 (a) and (b) show the 2D distribution of Sodium ions enrichment in the Aluminum Oxide target. We have chosen the thickness of the target as 65 nm so that the maximum number of ions could be visualized easily in the plot. The Y-axis in Figure 3 represents an abstract unit namely “(Atoms/cm³)/ (Atoms/cm²)”. During implantation, the impurity concentration (atoms/vol) vs target depth can be calculated by taking the product of fluence and this

arbitrary unit in the Y-axis. For 5keV energy the Ion Range is 70 Å, Straggle is 33 Å, Skewness is 0.4738 and Kurtosis is 3.0357. But for 10keV the Ion Range is 123 Å, Straggle is 58 Å, Skewness is 0.4059 and Kurtosis is 2.9648.

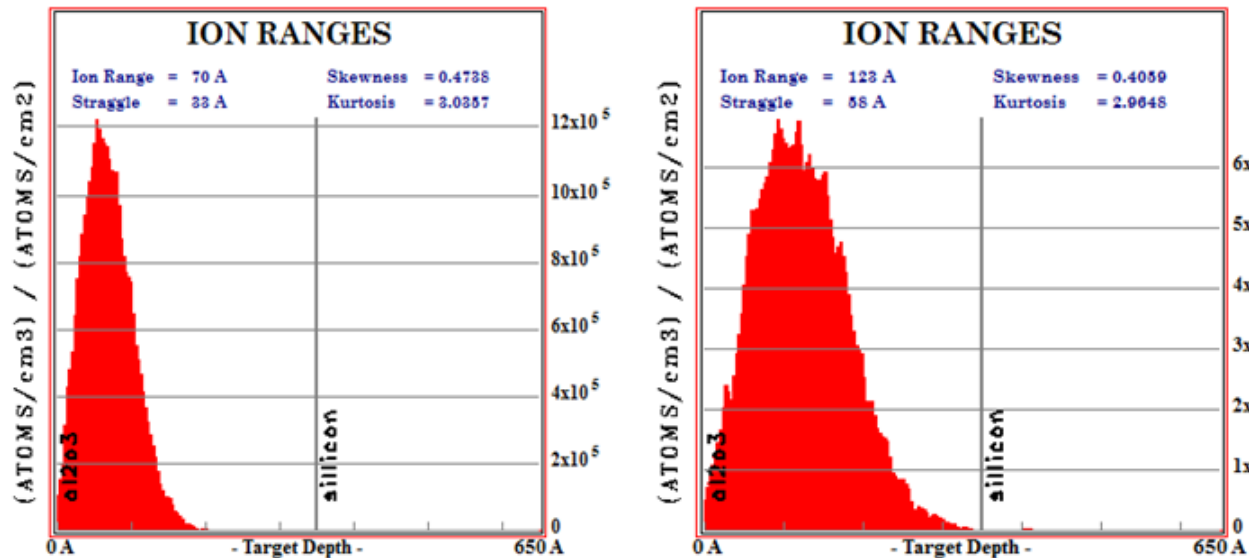


Fig 3. 2D plot of ion distribution (a) for 5keV, (b) for 10keV

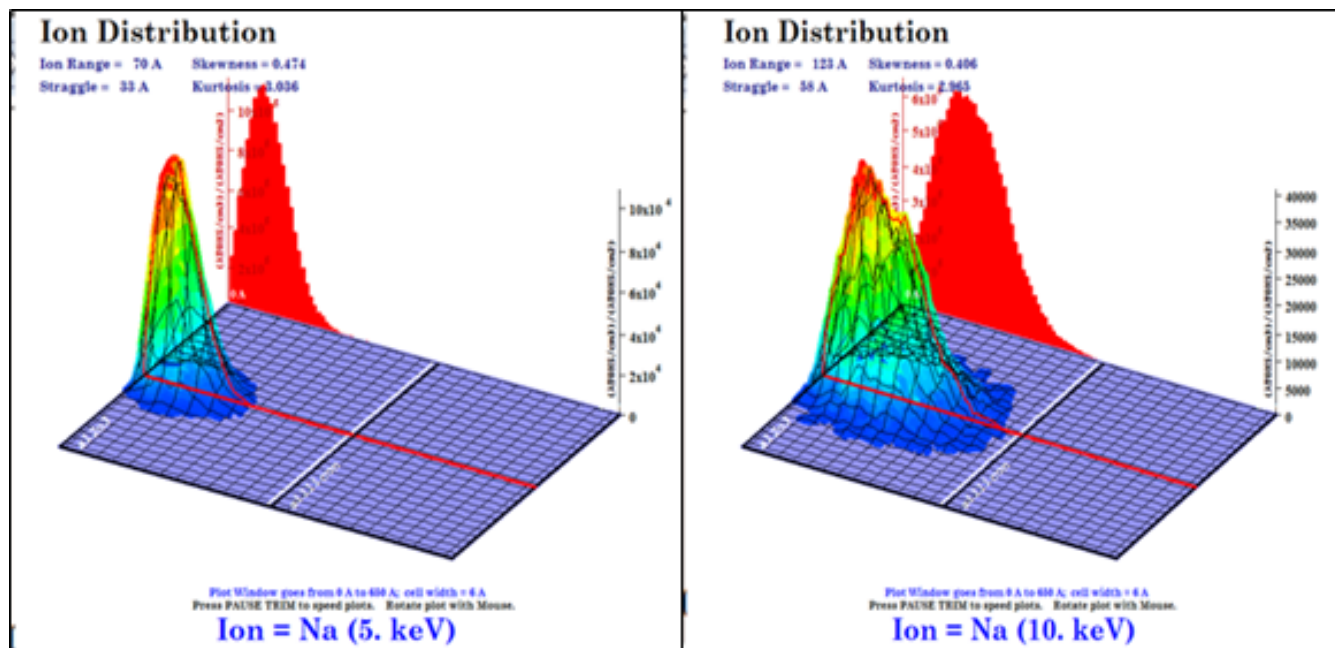


Fig 4. 3D plot of ion distribution (a) for 5keV, (b) for 10keV

The same plot can be also visualized in three dimensions, which is shown in Figure 4. The 3D plot can represent Z-Axis, it will help to show clearly the distribution of Sodium ions building up in the Aluminum Oxide target in the 3D frame. The 3D curves are hereby smoothened for 1st time with widescreen grid lines opted in the curves, in the SRIM 3D workspace. Layer Data-Lines are also visible to differentiate the two layers (i.e. Aluminum Oxide and Silicon). The Z-axis represented the $[\text{number of atoms/vol}]/[\text{atoms/area}]$ which are helpful to calculate the dose

which is required for the irradiation. The 2D red shaded image presented in the 3D images is the projection on the X-Y plane; whereas the 3D images show how the ions are penetrating inside the material and what projected average range of different energetic ions along with skewness and kurtosis.

Recoil Distribution

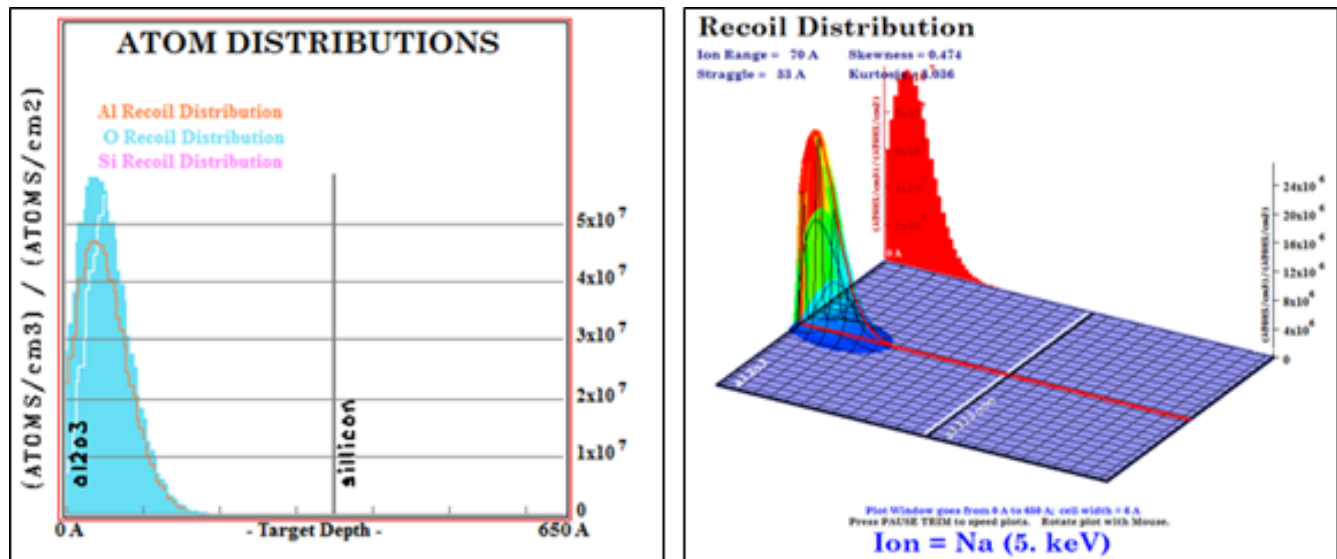


Fig 5. (a) 2D Ion/Recoil Distribution (b) 3D Ion/Recoil Distribution for 5keV energy

Figure 5 (a) shows the plot for the 2D Ion/Recoil Distribution for the Aluminum Oxide. The sky-blue plot shows the Oxygen recoil distribution and the red line shows the Aluminum recoil distribution. Here no Silicon recoil distribution has occurred because the energy is very low (i.e. 5keV). These are all the aluminum oxide atoms hit out from their lattice positions, generating voids. Simultaneously Figure 5(b) reveals the recoil distribution in 3 dimensions. The recoil distribution also provides the same value of ion range as earlier in the ion distribution. Recoil distribution for 10 keV is provided in Figure 6, from which the projected average range obtained as double than that of 5 keV. It is attributable to more penetration for higher energy due to more cascade collisions.

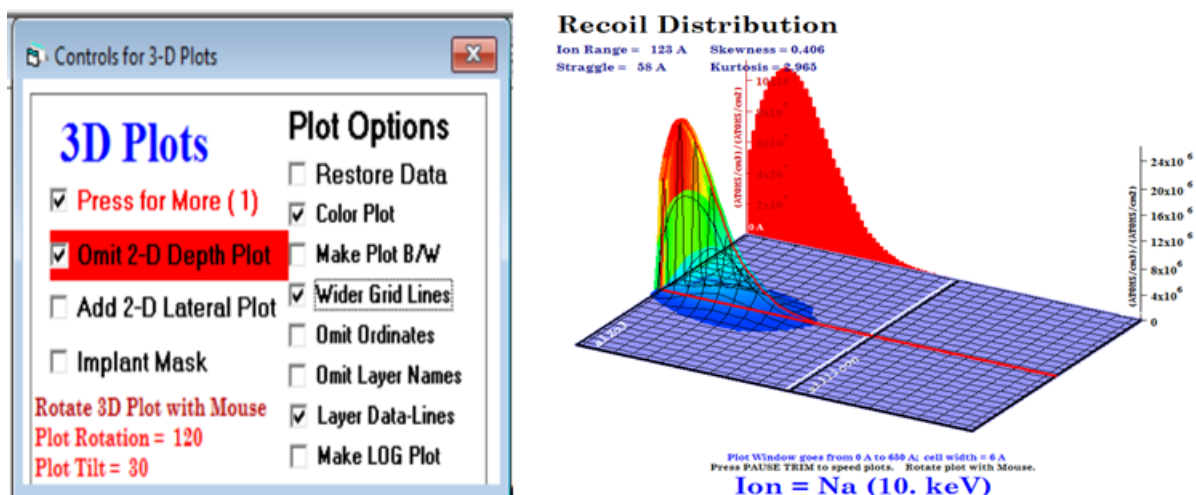


Fig 6. 3D Ion/Recoil Distribution for 10keV energy

Energy to Recoils

This plot shows how the target damage is being created. Energy from ions or Energy absorbed by Aluminum, Oxygen and Silicon atoms will be represented on the left hand side of Figure 7. You can pick all the options from it. But here I only choose three options from it to show the Energy to Recoils, I do not click the Si Energy Absorbed (0 eV/Ion) because there is no penetration occurred in the Silicon substrate due to, I take very low energy (i.e. 5keV).

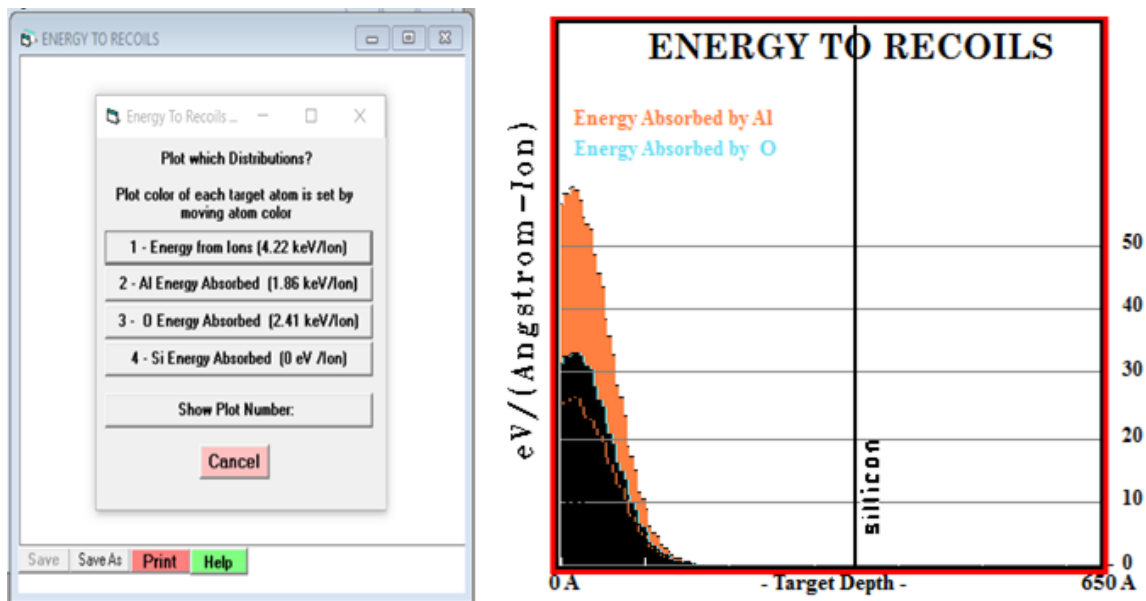


Fig 7. 2D energy to recoils for 5 keV energy

Energy to recoil simulation suggests that the energy received from the ions is 4.22 keV/ion whereas the Al atoms absorbed 1.86 keV/ion (denoted by orange colour pattern) and oxygen atoms absorbed 1.86 keV/ ion (denoted by black colour pattern).

Ionization

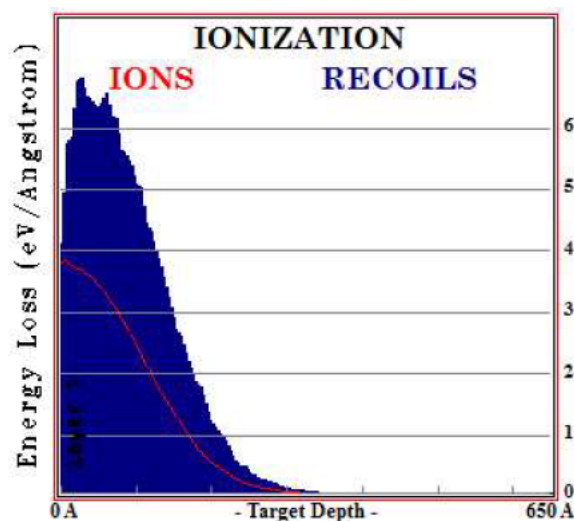


Fig 8. 2D Ionization for 5keV energy

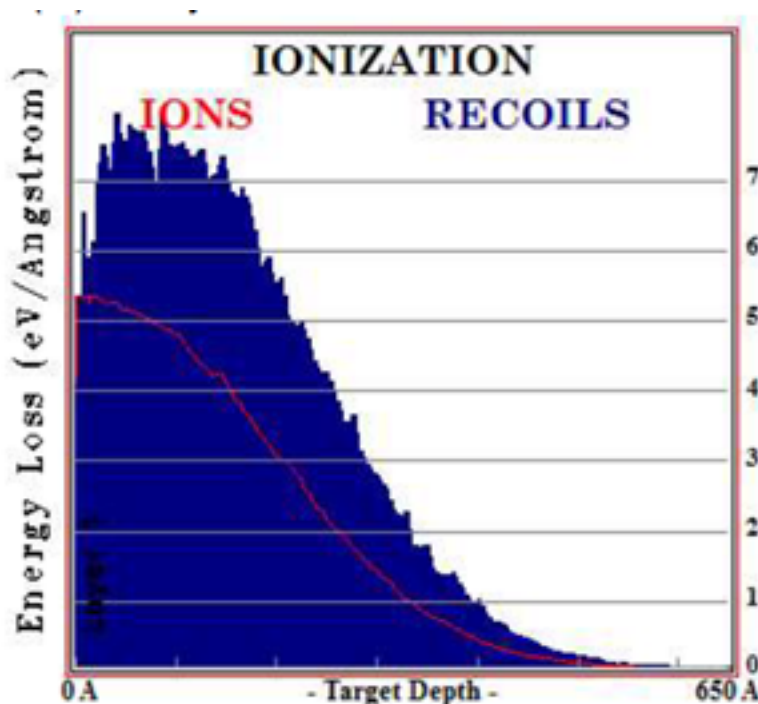


Fig 9. 2D Ionization for 10 keV energy

In Figure 8 and Figure 9, the comparison between 5 keV and 10 keV sodium ions has been shown. The corresponding energy loss in 5 keV ions is comparatively lesser than that of 10 keV ions. The range is smaller as predicted for the low energy case which is expected but the distribution width of energy loss is narrower for low energy case compared to high energy case. Hence, there is a higher possibility to obtain narrow energy distribution in case of low energy sputtering compared to high energy sputtering.

3 Conclusion

Here, we have reported the Monte-carlo simulation for very low energy alkali ion (5 keV and 10 keV) on aluminium oxide before detailed experiments that are to be carried out. We have obtained the ion distribution, recoil distribution, energy to recoils and ionization data, which will help to characterize the experimental data to be obtained after irradiation. The irradiation experiments are not cost-savvy; hence a proper simulation^{16 17} is required to know the irradiation-induced effects which will save time, expenditure to reduce the frequency of the experiments.

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