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Supplementary Information

Enhanced electrochemical capacitance of titanium oxide nanoparticles using low-energy nitrogen ion irradiation

Arpita Patro[1], Manoj K Rajbhar[2], Shitara Radhakrishnan[3], Shyamal Chatterjee[2], Chandrashekhar Rout[3], and Satyanarayan Dhal*[1]

[1]Centurion University of Technology and Management, Odisha, India

[2]School of Basic Sciences, Indian Institute of Technology Bhubaneswar, Jatni, 752050, Odisha, India

[3]Centre for Nano & Material Sciences, Jain University, Bangalore

Corresponding author: Email id: satyanarayan.dhal@cutm.ac.in ;

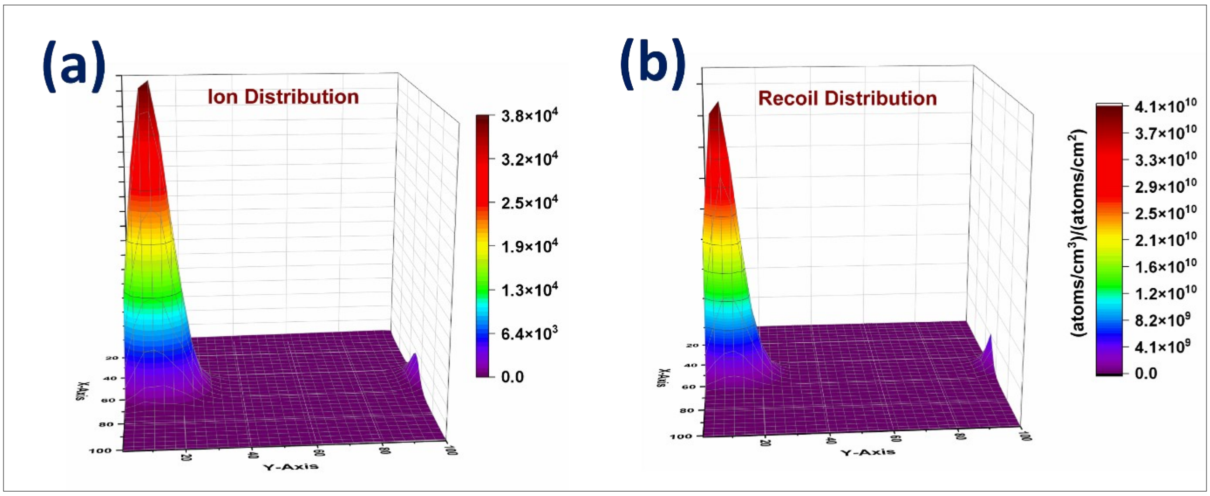

Fig. 1. TRIM simulation of titanium oxide nanoparticles with N^+ ion at 5keV results (a) the ion distribution (b) the recoil distribution.

The trajectory path of the projectile N^+ with 5 keV shows for target TiO_2 nanoparticles which is coated in Si substrate with target depth 1000 A^0 shown in Fig (a). TRIM simulation concludes that the projected range is about 103 A^0 for N^+ ion at 5 keV. The quantity of recoil distribution for both Ti and O in titanium oxide nanoparticles is depicted in Fig. 1(b). Additionally, it was noted that some ions also affected the Si substrate.

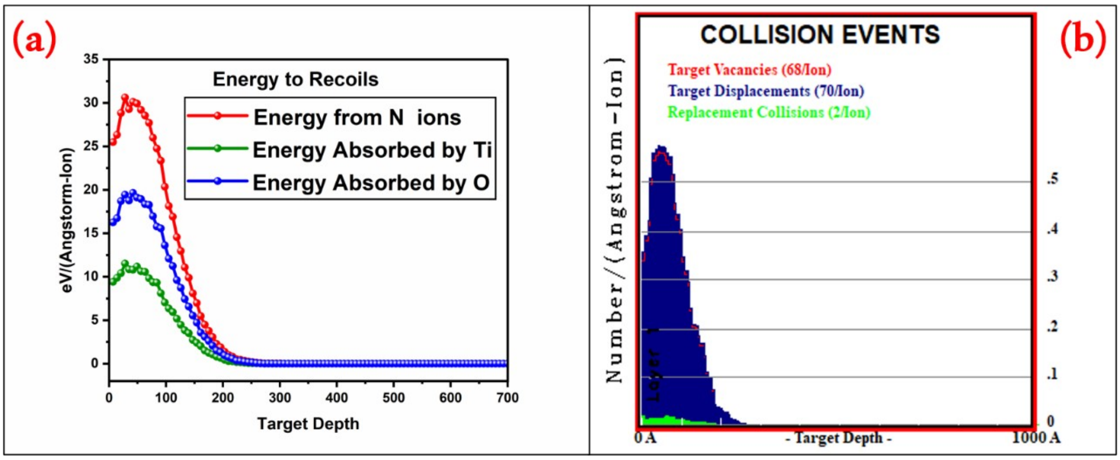

Figure 2. Damage creation in the TiO_2 nanoparticles as a target (a) energy to recoils plot for 5 keV nitrogen ion on TiO_2 as a target (b) Collision Events.

Energy to Recoils plot which deposits about 2.69 keV per ion energy to the target atoms (Fig. 2(a)).

This plot showing the distribution of displacements, vacancies. Titanium and oxygen atoms will both take in all of the energy that the ions have left behind. Up until the ions' mean range, which is around 10 nm, the energy supplied to the target atoms is rather consistent before decreasing as they come to an end (Fig.7(a)). The nitrogen ions give up 70 % of their energy to cascades of recoil and deposit 30 % of it immediately on the target. Each Ti atom absorbs 992 eV / ion whereas each of the oxygen atom absorbs 1.73 keV per ion. The blue curve (Fig. 7(b)) displays the total target displacements i.e., the quantity of atoms that were ejected from their intended lattice location. Target Vacancies are shown in the red curve that indicates that there are fewer vacancies than displacements because it is lower than the Target Displacements curve. Green curve represents the replacement collisions that are displacements when the incident atom loses practically all its energy, is unable to proceed, and falls into the space left by the target atom that is recoiling. In other words, it removes a target atom from the lattice and then replaces it. In this case, almost 3% of the displaced atoms do not leave vacancies, but instead are replaced by another target atom. Having energy 5 keV N^+ reveals that, each ion in the target atoms experiences 69 displacements, 2 replacements, and 67 vacancies. This work clearly demonstrates that the N^+ ions cause a sizable number of defects in the nanoparticles.

When we shoot N^+ ions at titanium oxide nanoparticles with low energy (5 keV), something interesting happens. The ions cause defects like displacements, replacements, and empty spaces called vacancies in the nanoparticles. Both the titanium (Ti) and oxygen (O) atoms in the nanoparticles create these vacancies. Interestingly, the oxygen atoms seem to like absorbing more energy from the ions than the titanium atoms. To make an atom move around because of the ion bumping into it, it usually needs a small kick of energy. This energy requirement is usually between 25 to 28 eV for moving an atom. So, to sum it up, when we shoot ions at these tiny particles, they make defects and vacancies that stick the particles together. Oxygen atoms seem to grab more energy from the ions, and when it comes to pushing atoms away, oxygen atoms are the primary atoms.

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