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Modified structural, surface morphological and optical studies of Li^{3+} SHI irradiation on zinc oxide nanoparticles†

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Nanoparticles of ZnO samples were irradiated using Li^{3+} of 50 MeV energetic swift heavy ions at fluences 5×10^{11} and 1×10^{13} ions/cm^2 at constant current 1 particle nano ampere (PNA). The energy loss, atom distribution phonon recoil and collision event were investigated by using TRIM software. Ion collision was calculated by depth verses Y axis for each ion per target atom collision. The moving ions are shown in red color and when they are stopped is indicated by green color. It is evidently showed that the ions are rapidly moved in the ZnO samples. The Ions recoil distributions with full damage cascade to create target atom recoils, it reveals that the zinc was higher recoils as compared to oxygen it is due to creation of cascade. The energy loss to target phonon consists of the direct creation of phonon by the ion and the additional energy loss by target recoil atoms to phonons. It is evidently shows that the samples are almost recoiling as compared to ions. The ion collision, ion recoil distribution, energy loss of target phonon and energy loss of vacancy production plots are shown in figure 1.

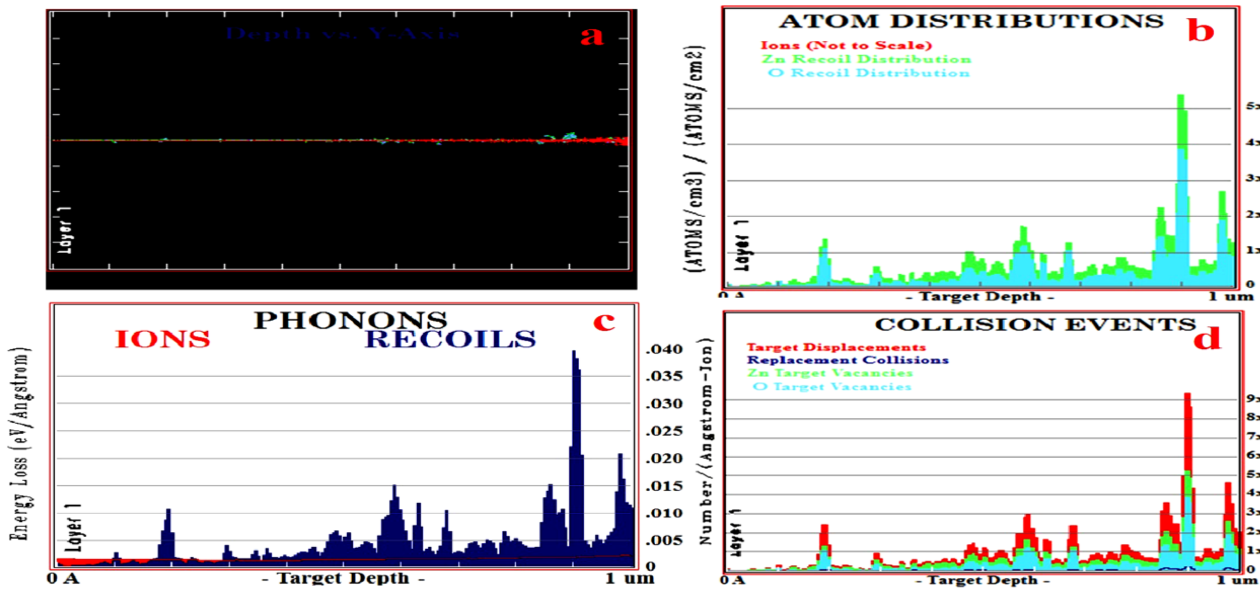

Fig. 1 Li^{3+} SHI irradiation on ZnO samples with 50 MeV energy plots of (a) Ion collision (b) Ion recoil distribution (c) Energy loss to target phonon (d) Energy loss to vacancy production.

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Energy loss to vacancy production shows that the number of vacancies depend on the displacement energy assigned to each target atom element is shown separately. These are a special type of collision in which the moving atom collides with an identical target atom, it transfers an amount of energy greater than that atom displacement energy, and does not have enough energy to move out of the lattice site. Lattice binding energy is the energy that every recoiling target atoms loses when it leaves its lattice site and recoils in the target. Typically it is about 1 - 3 eV, therefore in ZnO nanoparticle samples, it is 3 eV for zinc and 3 eV for oxygen. Changing the binding energy from 1 to 3 eV may lower the sputtering yield up to 2. Surface binding energy of 50 MeV for zinc it was 1.35 eV and for oxygen 2 eV. This energy that target atoms must overcome to leave the surface of the target, this is not the traditional chemical binding energy for surface atoms, it includes all surface non-linearities such as those produced by radiation damage, surface relaxation, surface roughness, etc. Displacement energy is the energy that recoil needs to overcome the lattice forces and to move more than one atomic spacing away from its original site. If the recoiling atom does not move more than one lattice spacing, it is assumed that it will hop back into its original site and give up its recoil energy into phonons. In ZnO nanoparticles of 50 MeV energy, it was obtained 25 eV for zinc and 28 eV for oxygen. The lattice binding energy, surface binding energy and displacement energy are tabulated in table 1.

Table 1. Lattice binding energy, surface binding energy and displacement energy of ZnO nanoparticles are calculated by TRIM software.

TARGET DATA

? Li (10) into Layer 1 (1 layers, 2 atoms)

		Moving atom colors ->					
		Stopped atom colors ->					
	Layer Name	Width (A)	Density	Zn (65.39)	O (15.999)	Solid/Gas	Stop Corr.
1	Layer 1	10000	4.780	0.50000	0.50000	Solid	1
	Lattice Binding Energy			3	3		
	Surface Binding Energy			1.35	2		
	Displacement Energy			25	28		