RSC Adavances

Electronic Supplementary Information (ESI)

A study of 160 MeV Ni^{7+} swift heavy ions irradiation effect of defect creation and stiffening of phonons mode on Mn$_x$Zn$_{1-x}$O thin films†
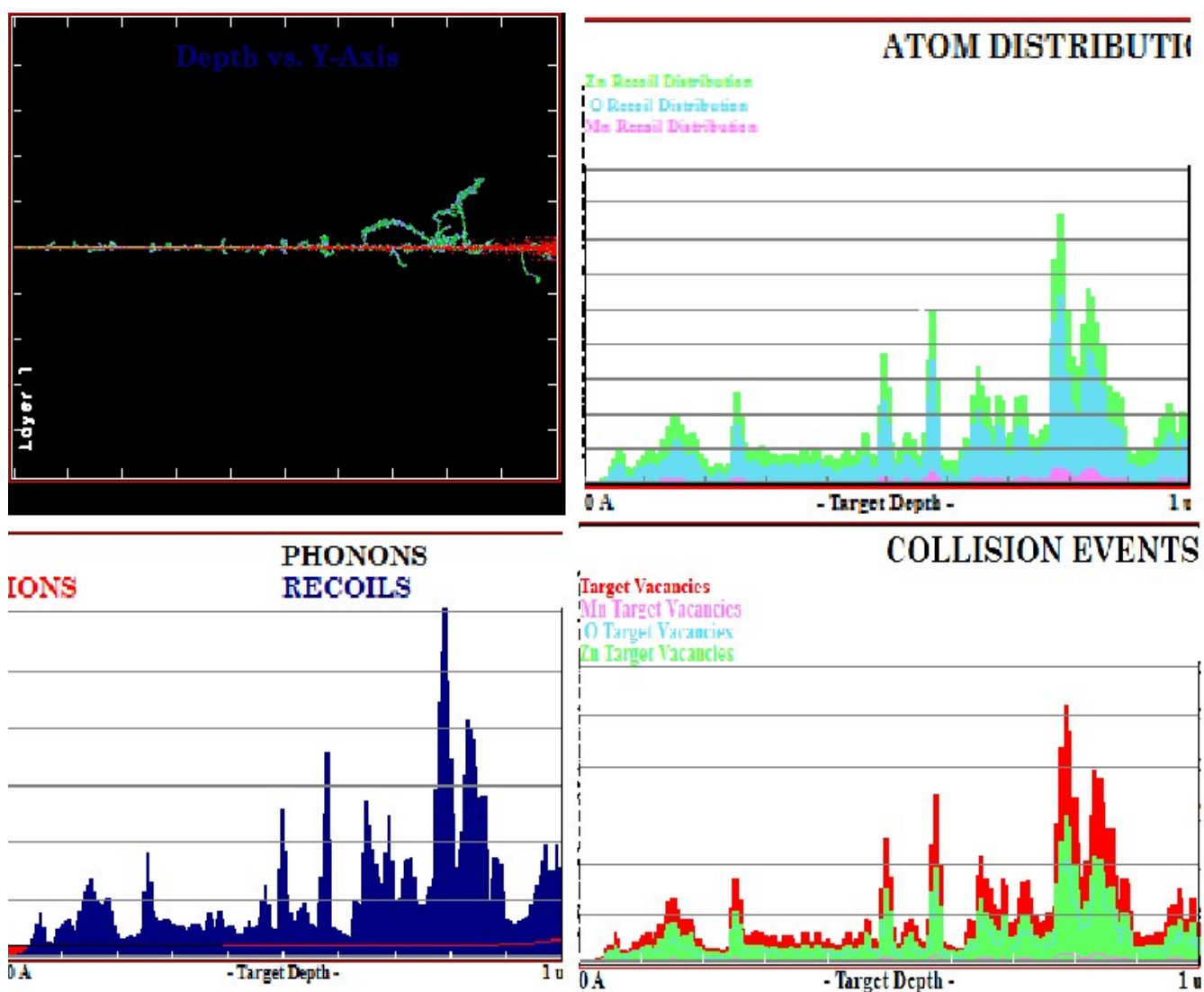
H. A. Khawal and B. N. Dole[a]*

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.

RSC Adavances

Electronic Supplementary Information (ESI)

Nanoparticles of Mn doped ZnO samples were irradiated using Ni^{3+} of 160 MeV high energetic swift heavy ions at fluence 1×10^{13} ions/cm² at constant current 1 particle nano ampere (PNA). The energy loss, atom distribution phonons recoil and collision event were investigated by using SRIM and 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 colour and when they are stopped is indicated by green color. It is evidently showed that the ions are rapidly moved in the Mn doped 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.

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 Mn doped ZnO nanoparticle samples, it is 3 eV for zinc, 3 eV for oxygen and 3 for manganese. Changing the binding energy from 1 to 3 eV may lower the sputtering yield up to 2. Surface binding energy of 160 MeV for zinc it was 1.35 eV for oxygen 2 eV and for manganese it is 2.98 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 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 Mn doped ZnO nanoparticles of 160 MeV energy of Ni^{7+} ions, it was obtained 25 eV for zinc, 28 eV for oxygen and for Mn it was 25. 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							
?	N (160000) into Layer 1 (1 layers, 3 atoms)							
	Moving atom colors ->							
	Stopped atom colors ->							
	Layer Name	Width (A)	Density	Zn (65.39)	O (15.999)	Mn (54.93)	Solid/Gas	Stop Corr.
1	Layer 1	10000	5.610	0.48781	0.48781	0.02439	Solid	1
	Lattice Binding Energy			3	3	3		
	Surface Binding Energy			1.35	2	2.98		
	Displacement Energy			25	28	25		
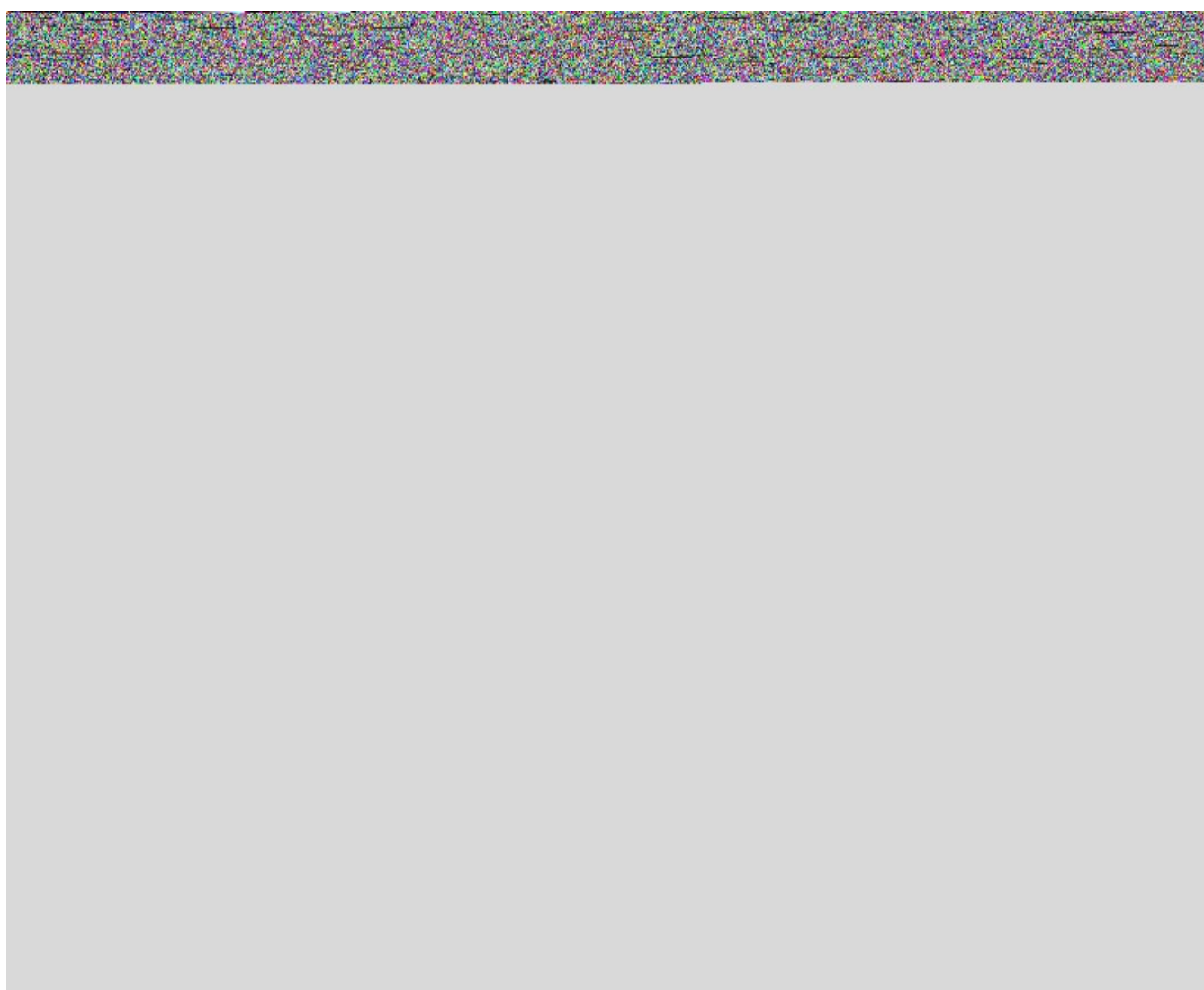
Fig. 1 Li^{3+} SHI irradiation on ZnO samples with 50 MeV energy plots of (a) Ion collision (b) Ion recoil distribution (c) Energy loss to target phonon (d) Energy loss to vacancy production.

RSC Adavances

Calculation Parameters

Backscattered Ions		0
Transmitted Ions		9999
Vacancies/Ion		5.1

ION STATS	Range	Straggle
Longitudinal	n/a	n/a
Lateral Proj.	n/a	n/a
Radial	n/a	n/a

Type of Damage Calculation

? | Full Cascades

Stopping Power Version

? | SRIM-2008

% ENERGY LOSS	Ions	Recoils
Ionization	99.95	0.01
Vacancies	0.00	0.00
Phonons	0.01	0.03

SPUTTERING YIELD

	Atoms/Ion	eV/Atom
TOTAL		
Zn	0.000200	8.12
O	0.000100	5.94
Mn	0.000000	0.00

? | ☑ Save every | 10000 | ions

Random Number Counter | 3887112

HELP