Monte Carlo Simulation of Atom Displacement Damage in ZnO Crystal Structure by Fast Neutron Radiation Using MCNP Code

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Abstract— An ensemble Monte Carlo simulation has been carried out to study atom displacement damage in ZnO crystal of different sizes and at different distances from a neutron source. The rate of atoms displacement in the crystals has been calculated using a Fortran program that was written based on NRT Model. The damage to crystal is proportional to the energy deposition of neutron directly. Results show that number of atoms displacement in the crystal is related to the neutron radiation damage and increased by enlarging of crystal size.

Keywords: Ensemble Monte Carlo; crystal size; atom displacement; NRT model.

1. INTRODUCTION

In recent years, there has been an increasing interest in using the wide band gap semiconductor ZnO for microwave power amplification and semiconductor detectors. Although, High pure ZnO is very costly and must be kept at low temperature, it is widely used for gamma and x-ray spectroscopy (Hamdani, 1997), (Chen et al. 2001). When this crystal is located in a combined neutron-gamma field, neutron interactions with Ga and nitrogen element induce main crystal damages and distort its energy resolution (Koenenl et al., 1996). Depending on the energy, neutron interactions with matter may undergo a variety of nuclear processes. The main interactions of fast neutrons are elastic scattering and inelastic scattering, but neutron capture is an important interaction for thermal neutrons (Foster and Wright, 1977). Whilst the preferred semiconductor is still silicon, industry is now tooling up for wide band gap semiconductors like ZnO production, which offers high electron mobility and hence the prospect of greater frequency operating rates. Its direct bandgap furthermore allows easier integration with optical devices. For this reason ZnO devices have received much attention in the literature, particularly with respect to their simulation (Kim et al., 1999), (Tsukazaki et al., 2005) in an attempt to understand the basic principles of their operation. Monte Carlo methods have been used to a great extent in this effort because they allow an essentially exact solution of the Boltzmann transport equation and are subject only to statistical errors, unlike drift diffusion models which cannot accurately treat the hot-electron effects that are present to a high degree in other material.

The Monte Carlo method has been widely used to study hot-electron problems (Makino et al. 2001), (Foster and Wright, 1977). The principle of this method is to simulate on a computer the motion of one electron in momentum space through a large number of scattering processes taking note of the time that the electron spends in each element of momentum space during its flight, this time being proportional to the distribution function in the elements. The procedure used for the following the motion of an electron requires random numbers to represent the time which the electron drifts before being scattered, and to represent the final state after the scattering event. The probability distribution for these random numbers can be completely specified in terms of the electric field strength and the transition probabilities due to the various scattering processes. Electrons in bulk material suffer intra valley scattering by polar optical, non-polar optical, acoustic phonons and piezoelectric scattering, inter valley phonons, and ionized impurity scattering. Acoustic and piezoelectric scattering are assumed elastic and the absorption and emission rates are combined under the equipartition approximation, which is valid for lattice temperatures above 77 K. Elastic ionized impurity scattering is described using the screened Coulomb potential of the Brooks-Herring model.

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In this research, we have calculated neutron energy deposition on ZnO crystal using MCNP code. The effect of damage and the atom displacements rate of crystal have been calculated using a computational code based on NRT model. It is well known that the main damages of the crystal are atom displacements and neutron activation that varied for different neutron sources.

2. THEORY OF ATOM DISPLACEMENT

A primary recoil atom is produced when an energetic incident particle such as fast neutron undergoes a collision with a lattice atom. If the energy transferred to the primary knock-on atom (PKA) is large enough, E >> Ed, (where Ed=30eV; the average energy for one displacement) (Mitchell, 1957), the PKA can continue the knock-on atom processes, producing secondary recoil atom displacements, which in turn can displace additional atoms. Such an event will result in many collision and displacement events occurring in near proximity of each other. The multiple displacement sequence of collision events is commonly referred to as a collision or displacement cascade (Kinchin et al., 1955). Transferred energy to a PKA with atomic mass number A, when occurred and that a neutron of energy E recoiled, is given by:

$$T = \frac{1}{2}\left(v_1^2 + v_0^2 + 2v_1 v_0 \cos\theta\right) = \frac{4AE}{(A+1)^2} \qquad (1)$$

where v1 is the velocity of scattering atom after collision, and v0 is the centre of mass velocity. The original model for displacement damage, developed initially for simple metals, is due to Kinchin and Pease (Kinchin et al., 1955), and the standard formulation of it by (Norgett et al., 1975) often referred to as the NRT model, is:

$$v(T) = \begin{cases} 0 & T \le E_d \\ 1 & E_d \le T \le 2E_d \\ 0.8T / 2E_d & T \ge 2E_d \end{cases} \qquad (2)$$

where v (T) is the number of displaced atoms produced by a recoil atom of energy E and damage energy T, and E_d is the average threshold displacement energy for an atom in the crystal lattice.

MCNP is a general-purpose Monte Carlo neutron, photon, and electron transport code. It has continuous-energy physics and is time-dependent. The geometry is any arbitrary configuration of three dimensional surfaces. It is used for radiation shielding, criticality safety, nuclear design, aerospace, medical, nonproliferation, radiation dose and other applications by several thousand users worldwide. This code is used to simulate one neutron at a time and records its history. The neutron energy deposition in the crystal has been calculated by tally F6:n for different neutron sources: mono-energy, Am-Be and 252Cf sources (Briesmeister, 2000).

3. CALCULATION RESULTS

The ZnO crystal is placed at different distances from point neutron sources with constant mono-energy and continuous energy spectrum such as Am-Be and ^{252}Cf source. Then, the amount of deposition energy per gram of crystal was calculated by F6:n tally of MCNP code. The amount of deposition energy per gram for different ZnO crystal for Am-Be source as function of distance, per one neutron of source is illustrated in Fig. 1.

As well as, the amount of deposition energy per gram in 2×2 ZnO crystal due to different mono energy rate in Fig. 3b. Energy deposition and corresponding point sources as A comparison of atom displacements rate due function of distance is illustrated in Fig. 2a, and Fig. 2b shows the atom displacements rate placed on a point 0.5 MeV neutron source as a function of distance. The corresponding result for a ^{252}Cf source is shown Fig. 3a, and the atom displacements atom displacements rate in Fig. 3b. Energy deposition and corresponding atom displacements rate are decreases mostly by $1/r^2$ as we expected.

A comparison of atom displacements rate due to different sources located in 10 cm far from the crystal have been illustrated in Fig. 4. It can be seen that the neutron average energy of the source increases as well as the corresponding damage growing up.

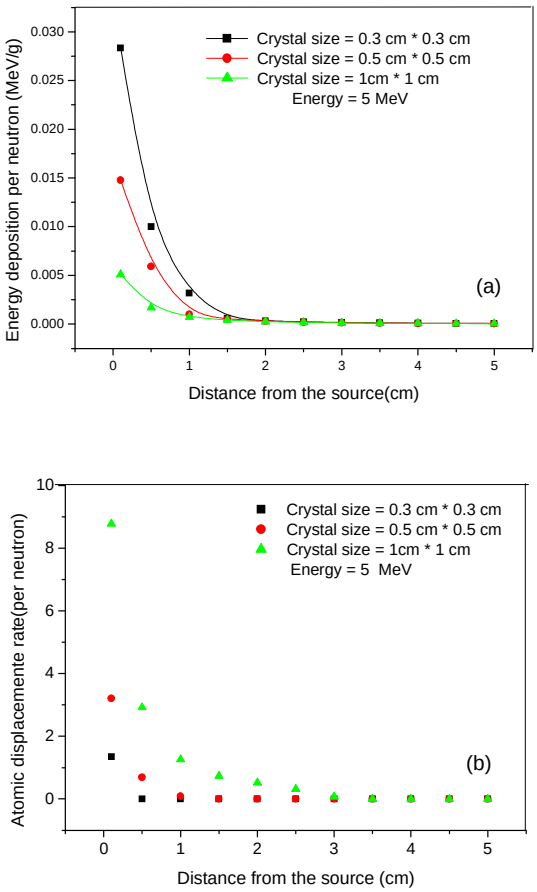
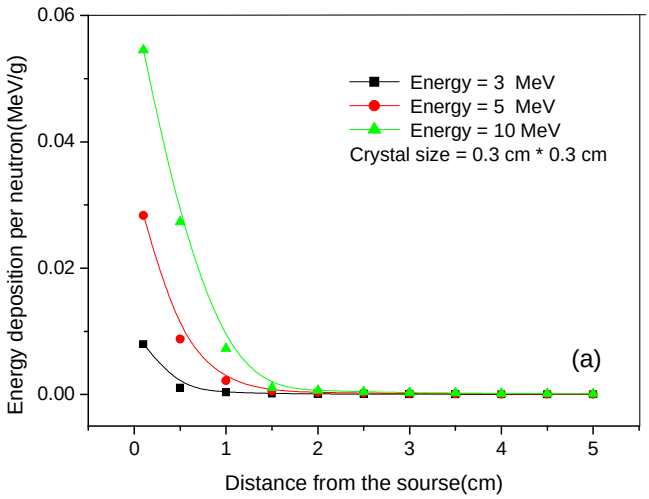


Figure 1: (a) Energy deposition per gram in different ZnO crystal due to an Am-Be source; (b) the atom displacements rate.



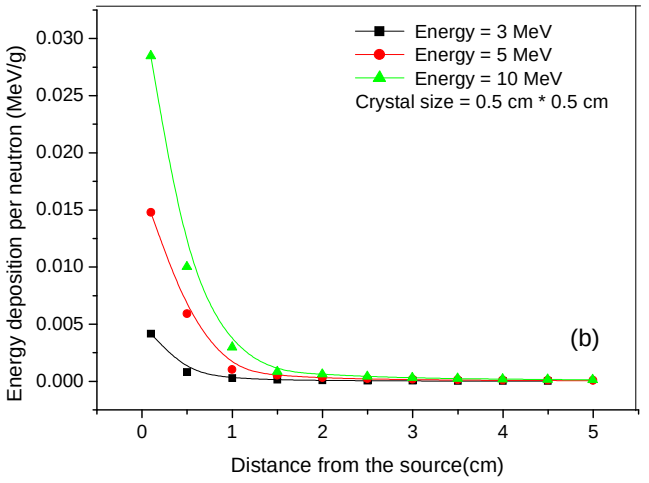
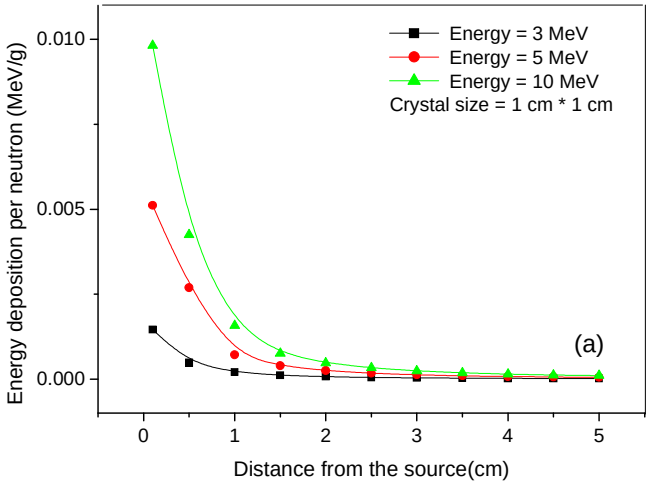


Figure 2: (a) Energy deposition per gram in different ZnO crystal due to different mono-energy point sources; (b) the atom displacements rate.



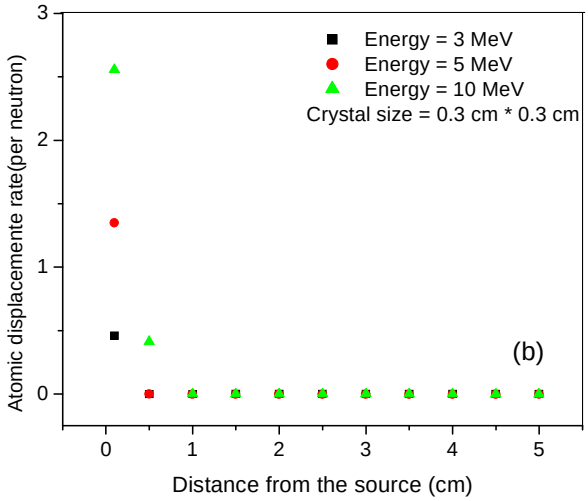


Figure 3: (a) Energy deposition per gram in different ZnO crystal due to a 252Cf source; (b) the atom displacements rate.

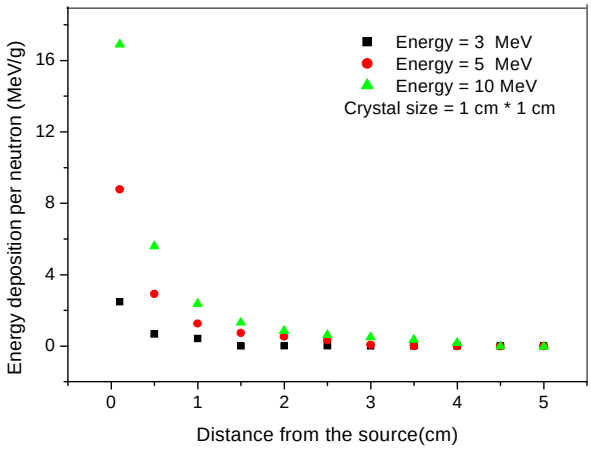


Figure 4: Comparison of atom displacements rate in ZnO crystals that placed on 10 cm of different sources.

4. CONCLUSION

The simulation results show that the amount of deposition energy per gram of ZnO crystals and total number of atom displacements are a function of crystal sizes. Collision and displacement are important events in larger crystal due to a higher neutron diffraction rate. As well as, atom displacements increase when the energy of the source accrues. The amount of deposition energy per gram of crystal decreases if the distance between source and crystal get larger. It is because the reaction surface reduces than reaction volume.

Therefore, by designing of proper shielding for ZnO detectors, we can prevent of radiation damage in this crystal using in mixed neutron- gamma field.

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