# Calculation of Atom Displacement Damage in HPGe Crystal by Fast Neutron

Ali Asghar Mowlavi\* and Sara Mohamadi Physics Department, Sabzevar Tarbiat Moallem University, Sabzevar, Iran

In this research, the amount of neutron energy deposition in HPGe crystal of different sizes and at different distances from a neutron source has been evaluated by using MCNP code. Then, 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.

### 1. Introduction

Semiconductor detectors have high energy resolution and are used commonly for photon and charged particles spectroscopy. High Pure Germanium (HPGe) is one of the best semiconductor detectors, which can be made in large size with a very suitable high energy resolution. Although, High Pure Germanium is very costly and must be kept at low temperature, it is widely used for gamma and x-ray spectroscopy [1-7]. When this crystal is located in a combined neutron-gamma field, neutron interactions with Ge element induce main crystal damages and distort its energy resolution [8]. 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 [9].

We have calculated neutron energy deposition on HPGe crystal using MCNP code. We then evaluated the damage, the atom displacements rate, of HPGe crystal using a FORTRAN 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. Material and method

## 2.1 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,  $E >> E_d$ , (where  $E_d=30eV$ ;

the average energy for one displacement) [10], 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 [11]. Transferred energy to a PKA with atomic mass number A, when occurred and that a neutron of energy E recoiled, is given by:

$$T = \frac{1}{2}A(V_1^2 + v_0^2 + 2V_1v_0\cos\theta) = \frac{4AE}{(A+1)^2}$$
(1)

Where,  $V_1$  is velocity of scattering atom after collision, and  $v_0$  is the center of mass velocity. The original model for displacement damage, developed initially for simple metals, is due to Kinchin and Pease [11], and the standard formulation of it by Norgett et al. [12], often referred to as the 'NRT' model, is:

$$v(T) = \begin{cases} 0 & T \langle E_d \\ 1 & E_d \langle T \langle 2E_d \\ 0.8T / 2E_d & T \rangle 2E_d \end{cases}$$
(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.

<sup>\*</sup>amowlavi@sttu.ac.ir

# 2.2 Calculation of neutron energy deposition using MCNP code

MCNP4C 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 <sup>252</sup>Cf sources [13].

### 3. Result and discussion

The Ge crystal is placed at different distances from point neutron sources with constant mono-energy and continuous energy spectrum such as Am-Be and <sup>252</sup>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 Ge crystal for Am-Be source as function of distance, per one neutron of source is illustrated in Fig. 1a. By using this data in FORTRAN code [14] that we wrote based on NRT model, the atom displacements rate for Ge crystals have been evaluated. These results are shown in Fig. 1b. As well as, the amount of deposition energy per gram in  $2'' \times 2''$  Ge crystal due to different mono-energy point sources as 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 <sup>252</sup>Cf source is shown Fig. 3a, and the atom displacements rate in Fig. 3b. Energy deposition and corresponding atom displacements rate are decreases mostly by  $\frac{1}{2}$  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.



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



Fig. 2: (a) Energy deposition per gram in  $2'' \times 2''$  Ge crystal due to different mono-energy point sources; (b) the atom displacements rate.



Fig. 3: (a) Energy deposition per gram in different Ge crystal due to a <sup>252</sup>Cf source; (b) the atom displacements rate.



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

## 4. Conclusion

These results show that the amount of deposition energy per gram of Ge crystals and total number of atom displacements are a function of crystal sizes. Collision and displacement events occur more in larger crystal, because a neutron leaves crystal, after more collision. 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 Ge detectors, we can prevent of radiation damage in this crystal using in mixed neutron- gamma field.

### References

- J. Ljungvall and J. Nyberg, Nucl. Instr. Meth. Phys. Res. A 546, 553 (2005).
- [2] T. Siiskonen and H. Toivonen, Nucl. Instr. Meth. Phys. Res. A 504, 403 (2005).
- [3] H. W. Kraner, C. Chasman and K. W. Jones, Nucl. Instr. Meth. Phys. Res. 62, 173 (1968).
- [4] N. Fourches, A. Huck and G. Walter, IEEE Trans. Nucl. Sci. 38, No. 3, 1728 (1991).
- [5] L. S. Darken, Nucl. Instr. Meth. Phys. Res. B 74, 523 (1993).
- [6] J. Llacer and H. W. Kraner, Nucl. Instr. Meth. Phys. Res. 98, 467 (1972).
- [7] L. S. Darken, R. C. Trammell, T. W. Raudorf, R. H. Pehl and J. H. Elliott, Nucl. Instr. Meth. Phys. Res. 171, 49 (1980).
- [8] M. Koenenl, J. Brucknerl, U. Fabian, H. Krusel, H. Wankel, A. N. F. Schroeder, R. Star, L. G. Evans, J. I. Trombka, D. M. Drake, P. A. J. Englert and J. Dempsey, IEEE Trans. Nucl. Sci. 43, No. 3, (1996).
- [9] A. R. Foster and R. L. Wright, *Basic Nuclear Engineering*, 3rd Edition (Allyn and Bacon, 1977).
- [10] Mitchell EWJ. British J. Appl. Phys. 8, 89 (1957).
- [11] G. H. Kinchin and R. S. Pease, Rept. Prog. Phys. 18, 1 (1955).
- [12] M. J. Norgett, M. T. Robinson and I. M. Torrens, Nucl. Eng. Des. 33, 50 (1975).
- [13] J. F. Briesmeister, MCNP: A general Monte Carlo N-particle transport code, Version 4C, Los Alamos National Laboratory, LA-13709-M (2000).
- [14] Microsoft FORTRAN PowerStation 4.0 software, Microsoft Company (1994).

Received: 22 October, 2008 Accepted: 26 June, 2009