NIEL calculations for estimating the displacement damage introduced in GaAs irradiated with charged particles

E El Allam, C Inguimbert, S Addarkaoui, A Meulenberg, A Jorio and I Zorkani

1 Solid State Physics Laboratory, Faculty of Sciences Dhar el Mahraz, University Sidi Mohamed Ben Abdellah, P.B 1796 Atlas-Fez, Morocco
2 ONERA-DESP, 2 avenue E. Belin, 31055 Toulouse, France
3 Science for Humanity Trust, Inc. Tucker, GA, USA

E-mail: elmehdi.elallam@usmba.ac.ma

Abstract. The application of Non-Ionizing Energy Loss (NIEL) in estimating the impact of electron, proton, and heavy ion irradiations on Gallium Arsenide is presented in this paper. The NIEL for deuteron, alpha particle, lithium ion and oxygen ion is computed using the SR-NIEL and NEMO codes. The NIEL calculations are compared with the introduction rate of displacement damage measured in n-type GaAs. Very good agreement is found between the NIEL and experimental results for protons (< 20 MeV), electrons, and a variety of ions. However, a discrepancy can be observed for high-energy protons.

1. Introduction

The space radiation environment includes high energy particles such as electrons, protons, and heavy ions. These charged particles may degrade the electrical performance of many devices used in space applications. Estimation of degradation introduced by the radiation in these devices is not always reliable and needs to be improved.

A variety of experimental techniques has been used to study the effect of radiation in gallium arsenide (GaAs). The type and density of the produced defects, can be investigated by means of photoluminescence spectroscopy (PL) and deep level transient spectroscopy (DLTS) [1, 2]. It has been shown that various defects can be produced in silicon doped GaAs [1]. Some simple defects such as gallium vacancies ($V_{Ga}$), silicon impurity at the arsenic site ($Si_{As}$), and more complex defects can be introduced when charged particles pass through n-type GaAs doped with silicon. These microscopic defects are the so called displacement damage responsible for the degradation of electrical and optical properties of semiconductor materials that leads to a degradation of semiconductor device performance (e.g., LED’s, laser diode, solar cells etc.). It has been reported that the introduction rate of these displacement damages in GaAs is inversely proportional to the energy of heavy charged particles, such as protons and heavy ions, and proportional to the energy of incident electrons [3]. That is to say that the number of defects is proportional to the amount of atomic displacements produced by the incident radiation field and thus to the Non-Ionizing Energy Loss (NIEL). The amount of atomic displacements produced can be estimated from the Non-Ionizing Energy Loss which gives the amount of energy deposited by an incident particle that can lead to displacement damage [4]. NIEL has been calculated for many incident particles on different materials by different authors [e.g., 4, 5, 6, 7]. In many cases, NIEL is demonstrated to correlate with experimental degradation measurements. But in...
some cases, the NIEL fails to give good degradation predictions, for example, in GaAs irradiated with protons having energies greater than 10 MeV [8, 9, 10].

This paper proposes a comparison between experimental data of displacement damage effects due to electron, proton and heavy ion irradiations in n-type GaAs and NIEL calculations for these incident particles in order to investigate the limit of the NIEL scaling approach for GaAs semiconductor.

Calculation of NIEL
Non-Ionizing Energy Loss (NIEL) is defined as the part of the incident particle energy consumed through Coulombic, nuclear elastic, and nuclear inelastic interactions that can occur between the incident particle and the lattice atoms, to produce vacancy-interstitial pairs (i.e., displacement damage). NIEL Can be calculated as [6]

\[
NIEL(E) = \frac{N_A}{A} \int_{T_d}^{T_{max}} Q(T) \left( \frac{d\sigma}{dT} \right)_E dT
\]

Where \( N_A \) is Avogadro’s number, \( A \) is the atomic mass of the lattice atom, \( E \) is the incident particle kinetic energy, \( T \) is the kinetic energy transferred to the target atom, \( Q(T) \) is Lindhard partition function, \( (d\sigma/dT) \) is the differential cross section (Coulombic and nuclear elastic/inelastic) for atomic displacements. The integral is calculated from the threshold energy for displacement \( T_d \), i.e., the energy needed to displace the target atom from its lattice position, to the maximum energy \( T_{max} \), which can be transferred by the incident particle to target atoms. The unit of NIEL is MeV.cm\(^2\)/g.

In this paper, two tools are used to calculate the NIEL for heavy ions in GaAs. The first is the NEMO code developed by the French Aerospace Lab (ONERA) [4] and the second is the SR-NIEL code developed by National Institute for Nuclear Physics (INFN) [7, 11].

![Figure 1. NIEL for charged particles in GaAs. For, protons and electrons, the data were taken from C.Baur et al [11]. For deuterons, alpha particles, lithium ions, and oxygen ions, the NIELs were calculated in this study by SR-NIEL [7] and NEMO code [4].](image)

The two methods of calculation (and the results) are similar. Both methods use the \( Q(T) \) Lindhard-Robinson partition function [12], with a threshold displacement energy \( T_d = 10 \) eV for both Ga and As. In the case of electrons, the SR-NIEL code [7], employs the Mott differential cross section [13]. In
the case of protons, the NIEL is the sum of the contribution from the Coulomb scattering and the nuclear interactions. NIEL (Coulomb) is calculated [14] by using the elastic Coulomb cross section discussed by Boschini, and NIEL (nuclear) [15] was evaluated by Jun. Concerning the NEMO code; electron NIEL is computed [4] using McKinley and Fesbash scattering cross section. For protons, the calculation is based on cross-section calculations, which combine both Coulombic and nuclear elastic scattering, and by solving the Schroedinger equation for a given optical potential [4]. The nuclear inelastic contribution is estimated [4] by using the GEANT4 toolkit. For heavy ions, in both methods only the Coulombic contribution is taken into account. It is estimated according to the ZBL screened Coulomb potential discussed by Messenger [16]. The inelastic contribution remains negligible in comparison to the Coulombic process in the energy domain of interest (< 30 MeV) of our study. The results of NIEL for GaAs as a function of particle energy are shown in Figure 1. It can be seen that the NIEL curves obtained from SR-NIEL and NEMO code are quite similar.

2. Experimental data and comparison
A lot of work has been done on the effect of irradiation with charged particles in semiconductors such as GaAs. The authors of [1, 3], by using the technique of photoluminescence (PL), concluded that radiation introduces two type of defects in n-type GaAs doped with silicon. The first is the gallium vacancy defect (V\textsubscript{Ga}) and the second is silicon at the arsenic site (Si\textsubscript{As}). The latter is an acceptor impurity (i.e., the silicon dopant atom is transferred from the gallium site (Si\textsubscript{Ga}), where it is a donor, to the arsenic site (Si\textsubscript{As}) under the effects of radiation).

![Figure 2. Introduction rate of displacement damage (Si\textsubscript{As}) measured in GaAs as a function of energy for different particles.](image)

In irradiated n-type GaAs, the degradation of Hall mobility is demonstrated to be correlated to the introduction of two types of microscopic defects V\textsubscript{Ga} and Si\textsubscript{As} [17]. This degradation depends on the type and the energy of incident particles and is related with the defect introduction rate associated with each type of particle and therefore to their respective NIELs. Figure 2 shows the defect introduction rate (e.g., Si\textsubscript{As}) in n-type GaAs irradiated with 7 MeV electrons, protons with energies ranging from 0.6 MeV up to 200 MeV, alpha particles with energies in the range [2.5 MeV, 10 MeV], lithium ions with energies going from 5 MeV up to 20 MeV, and oxygen ions from 10 MeV up to 30 MeV. These
measurements, performed by Jorio et al [3], are in good agreement with the defect introduction rate measured by Carlone et al [9] for protons in the range [200 MeV to 500 MeV]. These experimental data can be compared to the NIEL values (Figure 3).

The NIEL values shown in figure 1 have been compared to the measured defects introduction rate \( (\Delta \lambda_{\text{dis}}) \) for the various particles presented in Figure 2. To make this comparison, the NIEL values have been normalized to the experimental defect introduction rate of 10 MeV protons. Good agreement is found between the NIEL and the defect introduction rate in most cases except for protons of energies greater than 20 MeV. The relative damage rates of 7 MeV electrons and heavy ions are quite well estimated. But, for proton energies above 20 MeV, the NIEL seems to overestimate the damage level introduced by the incident radiation.

3. Discussion
Most studies of radiation effects on semiconductor materials and devices, typically compare NIEL with some change in device characteristics (e.g., changes in carrier lifetime of GaAs-LEDs [8], degradation of the maximum power of GaAs solar cells [11], etc.). As shown in the previous section, the microscopic defects are responsible for these changes. The overall good agreement between experimental data and NIEL values presented in the literature and in this work validates the NIEL scaling approach except for high energy protons for which a systematic discrepancy is observed (GaAs).

By looking at Figure 3, one observes that for 7 MeV electrons, the measured values of the introduction rate (7 MeV) agree well with the corresponding NIEL calculation. Similarly, a good correlation can be observed for protons of energies up to 20 MeV. The displacement damage produced by 10 MeV protons is approximately 2 orders of magnitude larger than for 7 MeV electrons. However,
for protons, at high-energy the NIEL seems to overestimate the real damage produced. This
discrepancy could be attributed to the production of clusters of defects by high energy PKAs (Primary
Knock on Atoms) in which annealing processes can reduce the amount of stable defects [18].

**Table 1.** Introduction rate of displacement damage (Si_{AD}). Comparison with the predicted
values of NIEL for both SR-NIEL code [7] and NEMO code [4]. The NIEL values are
normalized to 1 for proton NIEL.

| Particles | 5 MeV | 10 MeV | 5 MeV | 10 MeV | 5 MeV | 10 MeV |
|-----------|-------|--------|-------|--------|-------|--------|
| Proton    | 1     | 1      | 1     | 1      | 1     | 1      |
| Deuteron  | 1.4   | 1.9    | 2     | 1.7    | ***   | ***    |
| Alpha     | 17    | 16     | 15,5  | 13     | 16,4  | 15     |
| Lithium   | 70    | 40     | 50    | 42     | 65    | 58     |
| Oxygen    | ***   | 1132   | 764   | 654    | 854   | 806    |

It is assumed that the particle energies are those corresponding to the energy of the particle in the
sensitive region of the test devices. The strong dependence of damage with particle path length in a
test sample, makes miscalculation of the actual energy values in the sensitive region a possible source
of systematic error in the model. The good representation of most defect introduction rates by the
NIEL calculations indicates the validity of this portion of the general radiation-damage approach. The
non-random variations can lead to a search for specific deviations from the model. The greatest source
of error would now appear to be that of accurately determining the energy profile(s) of the radiation
environment within the sensitive regions of both the test devices and the devices being studied.

However, the possibility of radiation annealing or other moderating effects in the high damage regions
of PKAs would need to be explored. As a practical matter, few environments and spacecraft
component locations would provide a significant component of radiation damage from this portion of the
spectrum and the NIEL calculation appears to err on the safe side. For heavy ions, even if there is a
limited set of data, the results presented here indicate that there is a proportionality between NIEL and
experimental results at the energies considered in this study. In Table 1, a comparison of the relative
damage rate of protons and heavy ions is presented for two energies (5MeV, and 10 MeV). The case
of protons is taken as reference, and both the experimental defect introduction rate and theoretical
NIEL values are arbitrarily equated to 1. As can be seen in this table, in the case of 10 MeV incident
energy, the relative experimental damage rate for the oxygen ions, lithium ions, alpha particles and
deuterons are respectively 1132, 40, 16 and 1,9 times greater than the one measured for the protons.
These values are close to those predicted by NIEL. This validates the NIEL scaling approach for these
particles in this domain of energy.

**4. Conclusions**

This paper presents a comparison of the NIEL with some measured defect introduction rate in GaAs.
Two different toolkits have been tested (NEMO [4] and SR-NIEL [7]). They provide NIEL values
very close to each other. Good agreement is found between experimental data and theoretical NIEL
calculations for various types of particles and energies. Protons with energies in the range [0.6 MeV,
200 MeV], 7 MeV electrons and a variety of ions with energies going from some MeV up to 30 MeV
have been compared with the corresponding NIEL values. The introduction rate of displacement
damage for high-energy protons (>20 MeV) is lower than the predicted values of NIEL. Even if there
are some discrepancies for high-energy protons, the NIEL factor is demonstrated to be a relevant
parameter for predicting degradation of GaAs-semiconductor devices in a complex space radiation
environment.
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