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Evaluation of neutron-GaN displacement damage cross-section

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Abstract (max. 35 words):

The displacement damage cross-section of the neutron - GaN interaction is calculated. The differences with the neutron - Silicon interactions are presented and the impacts on the estimation of TNID levels are evaluated.

Index terms: Displacement damage, cross-section, GaN, Si, neutron, NIEL, Geant4, Monte-Carlo simulations.

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I. INTRODUCTION

RADIATIONS can induce two types of cumulative effects in electronics: ionizing dose and non-ionizing dose. While total ionizing dose effects (TID) mainly degrade dielectrics, nonionizing dose effects (TNID), so-called displacement damage dose (DDD), are mainly induced in the semiconductor constituting the conduction channel of electronic carriers. Displacement dose effects in microelectronics have been known and studied extensively for a long time [1]. These effects can be induced by different types of particles such as heavy ions, protons, neutrons or electrons and vary according to the channel material. The most studied material is naturally silicon while the second is GaAs [2][6][8]. In addition, the panel of produced defect types can be very different depending on the incident particle, its energy and material compounds. Usually [13], in order to limit the number of experimental characterizations for the qualification of electronics in a radiation environment, the measured degradations are reduced to a single type of particle, at a given energy and a given fluence. This is done using an "equivalent damage factor" that we will call F. These so-called F factors are based on displacement damage cross-section ("D") ratios. For silicon components, it is usual to use a Si neutron equivalence at 1 MeV in a neutron environment and a Si proton equivalence at 10 MeV in a proton environment [10].

GaN components seem to have good predispositions for operation under irradiation [10][11]. Nevertheless, it is necessary to assess specific effects induced in this material [12]. To our knowledge, there is no available data of displacement damage cross-sections induced by neutrons in GaN components. Thus, this study aims at providing the community with displacement cross section of the neutron-GaN interaction.

Without this data, users in the frame of space qualification procedure may be tempted to use the silicon damage cross section in place of GaN. It would not be very relevant according to the fact that neutron nuclear interaction cross sections can exhibit large differences from a material to another. At energies around few MeV and below, identifying the magnitude and location of the resonance peak is an important point. The first goal of this study is to estimate the possible error induced by this potential misuse of Si data. The second objective is to determine some energy characteristics of primary knock-on atoms (PKA) from n-GaN interactions. The definition of the PKA characteristics being the first step of a displacement damage defect study, the data provided here will be used following the scientific approach described in [14].

II. DISPLACEMENT DAMAGE CROSS-SECTION: A TWO STEP PROCESS

As done in previous studies [2][6], the displacement damage cross-section is calculated with the following formula:

$$D(E_n) = \sum_R \int_0^\infty E_r \cdot n(R, E_r) \cdot \frac{d\sigma_R(E_n, E_r)}{dE_r} dE_r \quad \text{(Eq. 1)}$$

Where:

- *D* is the displacement damage cross section expressed in [MeV.mb]
- E_n is the incident neutron energy
- *R* the secondary particle type: PKA type
- *E_r* is the energy of the recoil particle expressed in [MeV]
- σ_R is the production cross section of the R particle expressed in [mb]
- *n*(*R*, *E_r*) is the energy partition function of the R particle as a function of the *E_r* energy

The two main parameters are:

- the production cross-section, which can be estimated with the study of secondary particles from the neutron-atom interaction.
- the energy partition function, which defines the part of the energy which will be transferred into displacement damages.

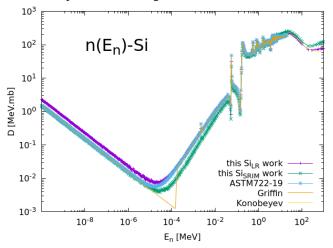


Fig. 1 Displacement damage cross-section in silicon material: ASTM722-19 norm, Griffin work, Konobeyev work and this silicon work with two options (LR and SRIM) [8][9]

Fig. 1 shows a comparison between the displacement damage cross-section D of neutron in silicon calculated in Geant4 with data from the literature. As can be seen, our calculations are in good agreement with the literature. ASTM722-19 is based on the NJOY database (~ENDF format). Geant4 also uses the ENDF database. The small differences come from the different database versions. Details of our calculation are given in the two following sub-sections.

A. Interaction of the neutron with the target atoms

The estimation of the cross-sections can be carried out using Monte Carlo tools (MCNP, Geant4, etc.) or databases (NJOY, JANIS). In this work, Geant4 has been used [15][17]. The energy spectrum from 0.1 meV to 1 GeV has been split into a large number (~700) of smaller energy bins (a few percent of mean neutron energy as in [8]) in order to take the neutron resonances into account. The dimensions of the target volume are large (> m) in order to record all cascades of events. Each simulation takes into account a large number of interaction histories to have a good statistical response. A full description of the process used will be added in the final paper.

B. The energy partition function

The energy distribution function is the second key parameter to estimate the displacement cross-section. There are different formulas and methods to calculate it, in this work we focus on three methods.

The first one is based on the Lindhard-Robinson ("LR") formula [3]. This formula depends on the atomic number Z and mass number A of the target material and PKA. As presented by Jun [4] and Fig. 1, this formula gives good results for silicon D calculations.

The second method is based on the SRIM database [5]. The displacement energy is estimated by integrating the nuclear stopping power for each ion (Z) type in a target (Si or GaN).

The third method is based on a function based on Lindhard formula with a displacement threshold energy (" LT_d ") as used in [2] and [6]. The silicon results are also very good even if improvements are still in progress for electron irradiations [18].

Today, we do not know precisely the physical processes involved in the displacements in GaN. As for silicon [19], an exhaustive study with atomistic modeling (molecular dynamics, *ab initio...*) will probably be necessary after this first step consisting in determining the PKAs of interest. For this summary, these first evaluations were conducted using the first method. In the final presentation, a study with the second method and different threshold energies will be presented.

III. DATABASE VALIDATION OF THE NEUTRON-NITROGEN AND NEUTRON-GA INTERACTION MODELING

The first step is to validate the neutron interaction cross section estimation of the N and Ga targets.

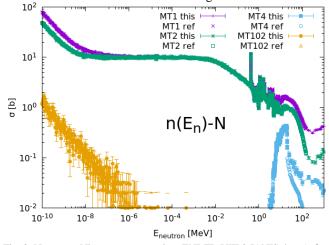


Fig. 2 Neutron – Nitrogen cross-section: ENDFB-VIII.0 JANIS data (ref) and this work (this).

Fig. 2 and Fig. 3 present a comparison between the crosssections of n-N and n-Ga. The calculated cross-sections are compared with ENDFB-VIII.0 JANIS data base [20]. MT1 is the total cross-section, MT2 the elastic cross-section, MT4 is the non elastic cross-section and MT102 is the capture crosssection.

For n-N interaction, the calculated data are in good agreement with the JANIS data. For the n-Ga interaction, the calculated data are between the data of the two isotope interactions: n 69 Ga (60.1%) and n- 71 Ga (39.9%). Thus, we consider that the calculated and the JANIS data cross-sections are in agreement. For n-N interactions, the elastic interaction is the main contributor to the total cross-section.

For n-Ga interactions, it is more complex: the cross-section is mainly driven by:

- capture at low energies (< ~10 meV),
- · elastic interaction, at medium energies
- and inelastic reaction at high energies (> a few MeV).

Only a few data are available in the literature for energies above 100 MeV. Thus, the validation by comparison is not accurate for the 100 MeV - 1 GeV energy range.

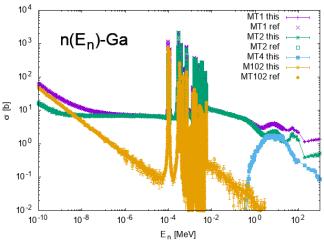


Fig. 3 Neutron – Gallium cross-section: ENDFB-VIII.0 JANIS data and this work.

IV. N-GAN RESULTS

A. Contributions to the cross-section

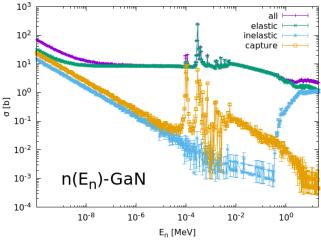


Fig. 4 Neutron - GaN cross-sections: this work

Fig. 4 presents the n-GaN cross-sections as a function of neutron energy. The n-GaN cross-sections are the average of the n-Ga and n-N ones, so it is a mix of the n-N and n-Ga interactions:

- the main contributors are:
 - the elastic reaction (such as n-N) below ~20 MeV
 and the inelastic reaction at high energy,
- the order of magnitude of the cross-section is close to the n-Ga one.

The resonance phenomena are smoothed by the assembly of the two interactions. The amplitudes of the n-Ga resonances are smaller, and those of the n-N have almost disappeared.

B. Displacement damage cross-section

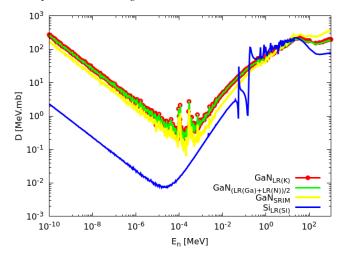


Fig. 5 Neutron Displacement damage cross-sections in Si and GaN

Fig. 5 presents the results of the Displacement damage crosssection in Si and GaN calculated according to method 1 and based on the cross sections estimated previously with Geant4. As mentioned in §II.B, for this summary, we used the Lindhard – Robinson formula and SRIM for the energy partition function. We investigated three assumptions:

- GaN_{LR(K)}: where the function uses the average Z and A of the two target atoms, i.e. the K atom
- $GaN_{(LR(Ga)+LR(N))/2}$: where the GaN function is the average of the N function and the Ga function.
- GaN_{SRIM}: where nuclear stopping power from SRIM database is used.

As we can see, the first two assumptions have little influence on the result. Although the two LR formulas used are not identical, the obtained results are close ($<\sim$ 1 %) The results with the SRIM function are slightly different: below for energies below MeV and above for energies above. The differences can go up to a ratio of 2. In the final presentation, other formulas (e.g. LTd) will be used to estimate their influence. When comparing the cross sections of the two materials, it can be noticed that:

- at low and high energies: D is larger for GaN than for Si.
- at energies close to MeV: D is slightly higher for Si than for GaN.
- there are more resonances for Si.

C. Relative damage factors

The relative damage factor is a parameter used to estimate the equivalent 1 MeV fluence of a given neutron spectrum [13]. This factor makes it possible to carry out experimental characterizations on neutron facilities whose energy is close to one MeV and where the dosimetry for displacement damage is expressed in 1 MeV equivalent neutron fluence in Si or GaN.

Fig. 6, showing this relative damage factor in GaN and Si, clearly illustrates that the GaN function is larger than the Si function. The differences can be up to an order of magnitude.

The historical exponential formula $(E_n(1-exp(-2.8/E_n))[1]$ also underestimates the level. In order not to underestimate the TNID level, it is essential not to use the Silicon equivalence function for GaN components.

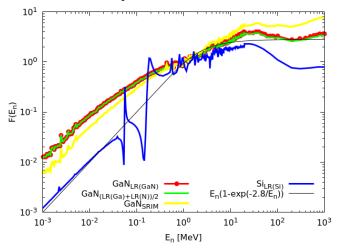


Fig. 6 Relative damage factor $F(E_n)$ in GaN, Si and [1] Si formula.

D.PKA contributions to the displacement damage

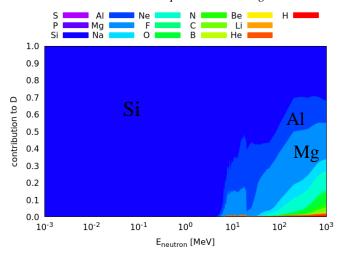


Fig. 7 PKA contributions to the n-Si displacement damage cross-section

Fig. 7 and Fig. 8 illustrate the contributions of the different PKA species to the displacement cross-section for Si and GaN respectively. For silicon, the silicon PKA is the first contributor for energies below a few tens of MeV. Mg and Al ions are also important contributors for energies above ~10 MeV. Above 100 MeV, the contributions of Na, Ne, F and O ions increase with increasing neutron energy. At energies close to 1GeV, almost all ions with an atomic number lower than silicon participate in the displacement effects.

For GaN, the distribution is different depending on the energy range:

- below 100 keV, the N ion is the first contributor at more than 70% and Ga the second;
- around 1 MeV, the contributions of N and Ga ions are almost equal;
- around 10 MeV, the Ga ion is the first contributor at more than 70% and the N the second;

 near 1 GeV, the heavy ions (Ga, Zn, Cu, Ni, Co, Fe, Mn, Cr, V, Ti, Sc, Ca, K, etc.) share the main contribution while the lightest ions (Z<7) have only a small contribution.

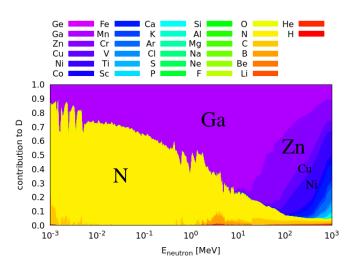


Fig. 8 PKA contributions to the n-GaN displacement damage cross-section

V.SUMMARY

In this abstract, we have presented and used a numerical method to evaluate the effective damage displacement cross section for GaN components under neutron irradiation between 1 meV and 1 GeV.

After a quick presentation of the method models, we have chosen some of them for evaluations of the effective displacement cross section of the n-Si and n-GaN interactions presented in this abstract. With these assumptions, we observed that these two displacement damage cross-sections are different. The results show that using Si data for GaN components leads to underestimate the TNID levels. In some spectrum cases, the underestimation can reach a ratio of 10. Thus, a more in-depth study seems interesting to better understand the reasons for these differences.

We can already say that the PKA distributions are different according to the energy ranges. For Si, the main PKA is almost always the Si ion. For GaN, the main PKA at low energy is the N ion while it will be an heavier ion at high energy. In the final paper, we will develop in more details the presentation of the models used and study the variations they induce on the obtained estimations.

These first results confirm the intuition of the two first PKA of interest: N (low energy) and Ga (medium energy). This work will be used in a later work for an exhaustive study with atomistic modeling to understand the reliability of GaN components.

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