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Neutron displacement damage cross-section in GaN: numerical evaluations and differences with Si

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Abstract— The displacement damage cross-section of the neutron - GaN interaction is calculated in the energy range from meV to GeV. Different calculation methods are used and discussed to estimate the modeling uncertainty. The Non-Ionizing energy loss (NIEL) and the relative damage factors are also deduced. Differences with the neutron - Silicon interactions are presented and the impacts on the estimation of Total Non-Ionizing Dose (TNID) levels are evaluated as a function of neutron energy.

Index Terms—Displacement Damage, neutron, GaN, NIEL, TNID, cross-section, Geant4, Monte Carlo

I. INTRODUCTION

IRRADIATIONS can induce two types of cumulative effects in electronics via ionizing and non-ionizing mechanisms. While total ionizing dose effects (TID) mainly degrade dielectrics, non-ionizing dose effects (TNID), so-called displacement damage dose (DDD) effects, are mainly induced in the semiconductor constituting the conduction channel of electronic carriers. DDD effects in microelectronics have been studied extensively for a long time [1][2][3]. They result from the creation of defects within semiconductors and can be induced by different types of particles such as heavy ions, protons, neutrons or electrons. The panel of produced defect types can be very different depending on the incident particle, its energy and the target material compounds. The most studied material is naturally silicon, another one being GaAs [4][5][6]. Some GaN devices show the potential to be extremely radiation-tolerant for dose radiation in space [7]. GaN components seem to have good Single Event Effect predispositions for operation under space radiation environment [8][9], but less under terrestrial neutrons [10]. It is thus necessary to assess specific dose effects induced by neutrons in this material [11]-[16]. Usually [17], in order to limit the number of experimental TNID 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 ("DD") ratios. For silicon components, it is usual to use a Si neutron equivalence at 1 MeV in a neutron environment [18][19] and a Si proton equivalence at 10 MeV in a proton environment [8]. Today, there are only a few studies to know about neutron NIEL in GaN and no reference standard validated by a standards organization like in Si and GaAs. Until very recently, to our knowledge, there were no available data of displacement damage cross-sections induced by neutrons in GaN components. This study aims at providing the community with displacement damage cross section, NIEL and relative damage factor of the neutron-GaN interaction from low to high energy with different calculation methods to estimate a modeling uncertainty. Since a few months (July 2022), the SR-NIEL team [3] proposed model-based calculations for the NIEL of n-GaN interactions at energies below 20 MeV. In this study, these new data are used as a reference for comparison.

Experimenters use NIEL curves of different materials and particles in order to test the effects of damage displacement on different available irradiation machines. This is to validate or invalidate equivalence between particle effects [20]. Without any data consistent with GaN device technology, experimenters may, by mistake, by habit or for lack of anything better, use the widely used Silicon data [21][22]. It would not be very relevant according to the fact that neutron nuclear interaction cross sections can exhibit large differences from one material to another. The main goal of this study is to perform an initial characterization of displacement damage cross sections in GaN along with their sensitivity to model variations, as compared against corresponding Si data. The secondary objective is to determine some of the energy characteristics of primary knock-on atoms (PKA) from n-GaN interactions. The definition of the PKA characteristics being the first step of a more complete displacement damage defect study, the data provided here will be used in future work, following the scientific approach described in [23].

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

As done in previous studies [4][5][24], the displacement damage cross-section is calculated with the following formula:

$$D(E_n) = \sum_r \int_0^{\infty} E_r \cdot n(R, E_r) \cdot \frac{d\sigma_R(E_n,E_r)}{dE_r} dE_r$$

(1)
where:

- $D$ is the displacement damage cross section expressed in [MeV.mb]. This term is also called microscopic displacement kerma.
- $E_r$ is the incident neutron energy
- $R$ is the secondary particle type: PKA type
- $E_s$ is the energy of the recoil particle expressed in [MeV]
- $n(R, E_r)$ is the energy partition function of the Recoil particle as a function of the $E_r$ energy which can be calculated by different formula and numerical methods exist to evaluate it as discussed further,
- $\sigma_d(E, E_r)$ is the production cross section of the R recoil particle expressed in [mb]

The two main parameters are:

- the production cross-sections, which can be estimated with the study of secondary particles from the neutron-atom interaction; and
- either, the energy partition function, which defines the part of the energy which will be transferred into displacement damage, or equivalently the displacement energy, which is the product of the energy partition function with the PKA energy:

$$E_{\text{displacement}} = E_r \times n(R, E_r)$$  \hspace{1cm} (2)

Fig. 1 shows a comparison between the displacement damage cross-section D of neutrons in silicon calculated with 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 tool, which uses the B-VII version of the evaluated nuclear data files (ENDF) database. Geant4 uses another ENDF database version (the ENDF/B-VIII.0 for Geant4-10-05). The small differences come from the different database versions and energy partition functions. Details of our calculations are given in the following two sub-sections.

### A. Neutron interaction with the target atoms

The estimation of the damage cross-sections can be carried out in either of two ways: a) by using Monte Carlo tools (such as MCNP or Geant4) which use the nuclear data files to generate recoil particles that are then followed via charged particle transport modeling to yield the damage assessment; or b) by using processing codes (such as NJOY, FRENDY, or GRUCON) which use the characteristics from the nuclear data files in conjunction with kinematic constraints and apply damage partition functions to the recoil particle energy spectra.

In this work, Geant4 has been used [25][26][27]. 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 done in [4]) in order to take the neutron resonances into account. The dimensions of the target volume are large (greater than 1 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 (~10^5). The Geant4 master version (10.5) with capture, fission, elastic (high precision) and Bertini (high precision) INC (intraneutron cascade) models has been used. The results are stored into a database with one file for each energy.

### B. The energy partition function

The energy partition function is the second key parameter to estimate the displacement cross-section. Different formulas and methods exist to calculate it, and we have chosen to focus on four methods.

The first one is based on the Robinson (“LR”) formula [28] based on [29][30]. This formula (3) depends on the atomic number Z and mass number A of the target material (ZL and AL) and of the PKA (ZR and AR). As presented by Jun [31] and Fig. 1, this formula gives good results for silicon D calculations.

$$LR(E_r) = \frac{1}{1+F_L(3.4008Z_{\text{en}}^{1/6}+0.4024A_{\text{en}}^{3/4}+\varepsilon)}$$  \hspace{1cm} (3)

where:

- $E_r$ is the recoil energy
- $\varepsilon = \frac{E_r}{E_L}$
- $E_L = 30.724Z_RZ_L\sqrt{Z_R^{2/3} + Z_L^{2/3} \frac{A_R + A_L}{A_L}}$
- $F_L = \frac{0.0793Z_R^{2/3}Z_L^{1/2}(A_R + A_L)^{3/2}}{(Z_R^{2/3} + Z_L^{2/3})^{3/4} A_R^{3/2} A_L^{1/2}}$

The Lindhard model is limited to ion energies less than about (24.8 x Z^{4/3} x A [keV]), which means ~4.6 MeV for N and ~170 MeV for Ga. As noticed in [28], this formula applies only to monatomic systems.

The second formula type, that we call “LTea”, is the previous Robinson formula, but with the additional application of the Kinchin-Pease [32] treatment of the threshold for lattice displacement using a displacement threshold energy ($E_d$), as used in [3] and [4].
The first step is to do a verification of the results of our interaction database by comparison with the literature. Fig. 2 and Fig. 3 present a comparison between the interaction cross-sections (elastic, inelastic, capture and total) of n-N and n-Ga with the ENDF/B-VIII.0 database from JANIS [43]. The results are very close because the Geant4 modeling uses the same underlying ENDF/B-VII nuclear data file to describe the reaction probabilities. Other databases available on JANIS have been used for comparison but they are not displayed in order to leave a readable figure.

For n-N interactions, the Geant4-produced cross sections for natural N are in good agreement with those displayed in the JANIS data viewer. For the n-Ga interaction, the calculated data of natural Ga are a data mix of the two isotope interactions: n-65Ga (60.1%) and n-69Ga (39.9%). Thus, we consider that the calculated and the JANIS data cross-sections are in good agreement within the uncertainty from the different isotope mixes. The elastic interaction is the main contributor to the total cross-section for n-N interactions.

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
- inelastic reaction at high energies (> a few MeV).

Only a few data are available in the literature for energies above 100 MeV. Thus, the verification by comparison is not accurate in the 100 MeV – 1 GeV energy range.
and the inelastic reaction at high energy,

\[ \begin{align*}
\text{• the order of magnitude of the cross-section is close to} \\
\text{the n-Ga one.}
\end{align*} \]

The resonance phenomena are smoothed by the sum or conjoint contribution of both interactions. The amplitudes of the n-Ga resonances are smaller, and those of the n-N have almost disappeared.

\[ \begin{align*}
\text{Fig. 4. Neutron – GaN cross-sections: this work.}
\end{align*} \]

### B. Energy partition functions in GaN

Fig. 5 and Fig. 6 show the partition damage energy as a function of the primary recoil energy of the two main PKAs: N and Ga. The displacement energy is the product of this distribution function with the PKA energy (E\(_r\)). The displacement threshold energy to use for GaN is not exactly defined. According to [39], the minimal energies of defect formation is 18 eV for Ga and 22 eV for nitrogen. [40] used a displacement energy of 21.8 eV for N in GaN obtained from an experiment [41] and a displacement energy of 22.0 eV for Ga in GaN which is a result of theoretical calculation [42]. SR-NIEL [3] proposes 21 eV for N and 21.5 eV for Ga. We choose to take \(-20\) eV as a medium value and \(+50\%\) for exploration. The LT(GaN/2) curves are close to each other for this difference in threshold displacement energy and these curves are similar to the corresponding TRIM results (cf. Fig. 5 and Fig. 6).

We investigated six methods to determine the energy partition functions:

- LR(K): where the Robinson function uses the average Z and A of the two target atoms, i.e., the “GaN/2” K atom.
- LR(GaN/2) is the average of the Robinson function of N and the Robinson function of Ga.
- LT(GaN/2 Ed = 20 eV): is the average of the Robinson function of N and the Robinson function of Ga, with a low displacement energy threshold of 20 eV. This threshold value is just below the SR-NIEL one.
- LT(GaN/2 Ed = 30 eV): is the average of the Lindhard-Robinson function of N and the Lindhard-Robinson function of Ga, with a high displacement energy threshold of 30 eV. This threshold value is \(+50\%\) above the previous value.
- SRIM: where nuclear stopping power from the SRIM database is used.
- TRIM: where the Monte Carlo results are used with the default displacement energy thresholds (25 and 28 eV).

We should mention that the Robinson method used for four energy partition functions is validated only for monatomic systems, which is not the case of GaN. But as can be seen between 100 eV and 1 MeV, all of the six results are close. At low energy, the oscillations of SRIM are caused by the limit of the number of significant digits on the output. Near the displacement threshold (~20 eV), the formulas differ slightly, depending on whether or not they take into account the threshold energy. As it was studied in [44], the damage energy functions of a polyatomic material are not a combination of those of the elements of this material. Indeed, depending on the nature of the PKA, one of the atoms of the target material will be privileged during the displacements. Thus, we believe that the presented approach should be complemented by molecular dynamics simulations in order to estimate the uncertainty of the functions.

\[ \begin{align*}
\text{Fig. 5. Partition function of displacement damage energy as a function of primary recoil energy of N in GaN for the six energy partition functions.}
\end{align*} \]

\[ \begin{align*}
\text{Fig. 6. Partition function of displacement damage energy as a function of primary recoil energy of Ga in GaN for the six energy partition functions.}
\end{align*} \]
Above 10 MeV, TRIM results are slightly above those from analytical models for this energy range. For the intermediate range of neutron-induced PKA energies, the results are close. With SRIM and TRIM, at high energy (above Lindhard model limit) the N ion shows an increase in the displacement deposit. That increase is not observed for the Ga ion, which is heavier and has a higher Lindhard model limit.

C. Displacement damage cross-section and NIEL

Fig. 7 presents the results of the Displacement damage cross-section in Si and GaN based on the production cross sections estimated with Geant4 and the six energy partition functions calculated following the different methods. Our calculations are compared to the new SR-NIEL GaN data.

As can be seen, the LR and LT assumptions have little influence on the result. Although the two LR formulas used are not identical, the obtained results are close (<~1 %) as for the LT and LR values. The threshold value has little influence on the results. The results for 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. The results for the TRIM function are slightly different: they are below for energies under MeV and above otherwise. At low energies, one would think that the different threshold energy assumptions would induce differences, but the $^{14}$N(n,p)$^{14}$C reaction predominates the other reactions on the lower energy range. The importance of the large neutron cross section from the N14(n,p) reaction was recently reflected in observed Single Event Effects in SRAMs [45] and is seen again in this analysis.

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.

One can convert displacement damage cross sections to NIEL with the following equation:

$$NIEL[MeV.cm^2/g] = D[MeV.mb] \times \frac{N_A[1/mol]}{M[g/mol]} \times 10^{-27}$$

Thus, for silicon with $M = 28.086$ g/mol the relation between D and NIEL is: $1$ MeV.mb = $2.144 \times 10^{-5}$ MeV.cm$^2$/g. For GaN with $M = 83.73$ g/mol, the relation between D and NIEL is: $1$ MeV.mb = $7.19 \times 10^{-6}$ MeV.cm$^2$/g.

By converting the displacement damage cross sections to NIEL (Fig. 8), the order of the curves changes. In contrast to the displacement damage cross section where silicon has the smallest values, the NIEL values of Si are larger than that of GaN between ~0.1 MeV and ~10 MeV.

D. Relative damage factors

The relative damage factor is a parameter used to estimate the 1 MeV equivalent fluence of a given neutron spectrum [19]. It is calculated from the NIEL curves or displacement damage cross section curves, which are normalized to 1.0 for an energy of 1 MeV. This factor makes it possible to carry out comparisons between experimental irradiations of electronic devices at fission-based neutron facilities where the effective neutron damage energy is above 0.1 MeV and where the dosimetry for displacement damage is expressed in 1 MeV equivalent neutron fluence in Si or GaN.
Fig. 9, 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 remarks are identical for the historical exponential \( a \cdot e^{(1 - exp(-A/E_n))} \) formula for silicon. By fitting Smits experimental data, Messenger obtained \( a = 1.02 \) and \( A = 3.6 \) MeV [2]. With other experimental data, [3] obtained different values: \( a = 1.0 \) and \( A = 2.8 \) MeV. These formulas smooth the resonance values.

In order to not underestimate the TNID level, it is then essential not to use the Silicon equivalence function for GaN components.

E. PKA contributions to the displacement damage

![Fig. 10. PKA contributions to the n-Si displacement damage cross-section (with LTE (21 eV) energy partition function).](image)

Fig. 10 and Fig. 11 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 1 GeV, 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 10 eV, the C ion is the first contributor and H the second. These ions come from the n+14N→p+14C reaction;
- between ~1 and 100 keV, the N ion is the first contributor (more than 70% weight) and Ga is 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; and
- 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.

The distributions of PKA types are very different between n-Si and n-GaN. For silicon, the Si PKA is the first contributor over a large part of the energy range. For GaN, we have to look at different types of PKA with different masses. Indeed, N and C are lighter than Ga and Zn. As seen in SiGe [47], it is likely that light and heavy PKAs have different responses. This will be investigated with further modelling such as molecular dynamics.

![Fig. 11. PKA contributions to the n-GaN displacement damage cross-section (with TRIM energy partition function).](image)

Fig. 11. PKA contributions to the n-GaN displacement damage cross-section (with TRIM energy partition function).

V. CONSEQUENCES IN TEST PROCEDURES

![Fig. 12. Ratio of relative damage factor in GaN on relative damage in Si as a function of neutron energy.](image)

As mentioned before, the tests are often performed using 1 MeV Silicon equivalent fluence. The ratio of relative damage factor in GaN on relative damage in Si as a function of neutron energy in Fig. 12 shows the error made if the Si curve is used instead of the GaN curve. The different modeling hypotheses give close results. We can observe that:

- between 10 MeV and 1 GeV, the error is between 2 and 10;
- between 0.1 MeV and 10 MeV, the error is less than
100%, which can be considered acceptable in many cases;
- between 100 eV and 100 keV, the error is about one order of magnitude (~10);
- and below 10 eV, the error is of the order of two orders of magnitude.

In summary, the error is reasonable for values close to 1 MeV, strong for high energies and very strong for low energies. It confirms that this is something to carefully take into account, because depending on the particle energy spectrum, the error can change from negligible to very high.

Table I

<table>
<thead>
<tr>
<th>Neutron Spectrum</th>
<th>NIEL in Si 1 MeV</th>
<th>NIEL in GaN 1 MeV</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 MeV</td>
<td>2.0 keV.cm²/g(Si)</td>
<td>0.47 keV.cm²/g(GaN)</td>
</tr>
<tr>
<td>25 meV</td>
<td>[1.0]</td>
<td>[0.024]</td>
</tr>
<tr>
<td>14 MeV</td>
<td>[0.024]</td>
<td>[0.16]</td>
</tr>
<tr>
<td>Watt distribution</td>
<td>[2.0]</td>
<td>[4.04]</td>
</tr>
<tr>
<td>Terrestrial spectrum</td>
<td>[2.1]</td>
<td>[1.05]</td>
</tr>
<tr>
<td></td>
<td>[1.4]</td>
<td>[2.34]</td>
</tr>
</tbody>
</table>

If we know a neutron spectrum, we can estimate the neutron NIEL in Si and in GaN. Table I displays the NIEL and ratio to 1 MeV in Si and GaN for different classic neutron spectra. NIEL at 1 MeV is also chosen as the reference because it is commonly used for Si even if for GaN another energy could be chosen. For 25 meV, in Si, the ratio is very low (~2.4%) and low in GaN (~16%). For 14 MeV, in Si, the ratio is x2 and x4 in GaN. For a Watt distribution, the ratio is equal to ~1 for Si and ~1.5 for GaN. For the terrestrial spectrum, the ratio is about 1.4 in Si and 2.34 in GaN. For these spectra, the ratios at 1 MeV are very different between Si and GaN. Neither the energy-dependent shape of the NIEL silicon displacement damage curve nor its 1 MeV reference normalization value are directly applicable to represent displacement damage in GaN.

VI. Conclusion

In this paper, we have presented and used a numerical method to evaluate the damage displacement damage cross section for GaN components under neutron irradiation in an energy range between 0.1 meV and 1 GeV.

After a quick presentation of the method models, we have chosen some of them for evaluations of the displacement damage cross section of the n-Si and n-GaN interactions. We have shown that using Si data for GaN components leads to underestimate the displacement levels. Between 0.1 MeV and 10 MeV, the error is less than 100%. Between 100 eV and 100 keV, the error is about one order of magnitude. Between 10 MeV and 1 GeV, the error is between two and ten. Below 10 eV, the error is around two orders of magnitude. For the characterization of displacement effects of GaN components, we strongly recommend to use the NIEL n-GaN values instead of other values.

Furthermore, we have shown that, contrary to Si, the PKA distributions are different according to the energy ranges. The main PKA is the C ion at very low energy (< 10 eV). Between ~1 and 100 keV, it is the N ion, while it is Ga at medium energy and a mix of different heavy ions at high energy. As has been done previously for Si [23][46], this work will be used as a starting point for future exhaustive studies based on atomistic modeling, in order to understand the radiation hardness of GaN components to displacement damage. For example, a study of the temporal evolution of cascades induced by N or Ga ions could allow a better understanding of the link between the displacement dose level and the number of stable residual defects that affect the relevant displacement damage modes.

These numerical data will be useful to validate experimentally the relative damage factor and to determine if this classical approach, used for silicon devices, is also suitable for GaN devices. This is the first step of an ambitious numerical and experimental study. The final goal is to reach an experimentally validated standard like the one in [4]. The following step will be to link this numerical data to the response of GaN devices after neutron irradiation.

APPENDIX

Watt distribution spectrum formula between 1 keV and 10 MeV:

\[
\frac{d\phi(E)}{dE} = 0.4865 \sinh(\sqrt{2E}) e^{-E}
\]

Terrestrial neutron spectrum between 1 MeV and 1 GeV [48]:

\[
\frac{d\phi(E)}{dE} = 1.006 \times 10^{-6} \exp(-0.35(\ln(E)^2)) + 2.1451\ln(E)) + 0.001011 \times 10^{-3} \exp(-0.4106((\ln(E)^2) - 0.667\ln(E))
\]

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References
