Displacement Damage Effects

WP1
Study Report

Literature Survey and Pre-Assessment of Methods

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1 Scope of the Document

The present Study Report represents the first outcome and deliverable as a result of Work Package 1 of the ESA-GSP Project "*Predicting Displacement Damage Effects in Electronic Components by Method of Simulation*". Objective of the project is the design and implementation of a pilot-type software simulation tool to calculate displacement damage effects due to non-ionising energy loss (NIEL) induced by an external radiation field, and to estimate the resulting parameter degradation in electronic circuit components.

The document comprises a literature survey on NIEL and displacement damage (Work Package 11), the selection and assessment of a suitable method and algorithm that shall form the basis of the planned simulation tool (Work Package 12), and the documentation of the relevant literature items on NIEL and displacement damage, that have been gathered in the course of WP11 (Work Package 13).

The Study Report is intended to be an aid for ESA to come to a consent concerning the final design of the planned simulation tool. The approval of the Agency is needed in order to continue with Work Package 2.

2 Introduction

The high energy space radiation environment consists of a variety of particle species, including solar, galactic, and trapped protons, trapped electrons, and heavy ions from Solar Particle Events and the Galactic Cosmic Radiation (GCR). A high energy particle interacts with matter in different ways depending on its energy, mass charge state and the species it interacts with. The main interaction mechanisms are elastic and inelastic scattering and nuclear reactions like spallation, fragmentation, and fission. The interaction of the primary radiation with the shielding or device material leads to secondaries such as neutrons, protons, mesons, atomic recoils, nuclear fragments, and electromagnetic radiation (due to bremsstrahlung and nuclear de-exitation). Depending on its origin the spatial distribution of the primary space radiation is more or less isotropic, and the particle flux varies slowly (e.g. the GCR with the solar cycle) or can increase largely within hours (e.g. during the passage of the radiation belts or due to a solar particle event).

Radiation effects in spacecraft electronics include:

- Transient ionisation effects due to the generation of electron-hole pairs. On one hand these effects are benificial, because they are used to detect the passage of high energy particles in particle detectors. However, if a critical charge in the sensitive volume of certain electronics components is exceeded, Single Event Effects may result in a catastrophic failure of the component (e.g. latchup, gate rupture, burnout).

- Long-Term ionisation effects. In insulating areas of a device charges produced by ionising radiation may be trapped and thus immobilised. This can affect electrical properties of the device and may result in permanent parameter changes (e.g. in a threshold voltage shift of a MOSFET).

- Displacement effects. The well-ordered crystalline lattice structure may be disturbed by radiation displacing some of the lattice elements. Important manifestations of displacement damage are i.a. the formation of mid-gap states, which facilitate the transition of electrons from the valence to the conduction band. Consequently the current of reversed-biased pn-diodes is increased or, in forward-biased junctions or non-depleted regions, recombination is facilitated resulting in a charge loss. Trapping is facilitated by radiation-produced states close to the band edges and the donor and acceptor density is changed.

Although only a small fraction (< 1 %) of the total energy deposited by a particle in a semiconductor is non-ionising resulting in non-transient atomic displacement and subsequent defect formation, this type of radiation damage has been identified as the main reason for serious parameter degradation and failure of certain components during space missions and becomes even more important with the extended use of optoelectronics components like LEDs, optocouplers and CCDs (tab. 1).

Component	Lifetime Degradation	Carrier Removal	Trapping	Mobility Degradation
Si MOS Transistors & ICs				S
CCDs	P		P	
Si Bipolar Transistors & Linear ICs	P	S		
Photodetectors	P			
LEDs & Laser Diodes	P			
pn Junctions	P	P	P	
JFETS		P	P	S
GaAs Transistors & ICs		P		S

Tab. 1: Mechanisms for the degradation via displacement damage in various technologies; P=primary, S=secondary [MAR99]

3 Displacement Damage

3.1 Defect Production

The bulk damage in semiconductor devices by hadrons or higher energetic leptons is caused primarily by displacing a *Primary Knock On Atom* (PKA) out of its lattice site resulting in an interstitial-vacancy pair (*Frenkel pair*). The PKA can leave its lattice site if its kinetic energy imparted during the collision exceeds the *displacement energy* E_d. In case of high energy particles a nuclear reaction can take place, resulting in a number of fragments of the target atom and possibly other secondary particles. The recoils, fragments or other secondaries lose their energy through ionisation (which will not result in any significant changes in the lattice) and additionally can give rise to further displacements. An atomic cascade takes place, until the displacement energy cannot be transferred any more. At the end of a heavy recoil range the non-ionising interactions are prevailing, leading to a dense agglomeration of defects (*clusters*). At room temperature a major part of the Frenkel pairs annihilate and will not cause any permanent damage. The remaining vacancies and interstitials migrate through the lattice and undergo numerous reactions (tending to create more complex defects), which are partly influenced by impurities present in the semiconductor material. The electrical properties of the resulting – relative stable – lattice defects influence the properties of the semiconductor material. The defects will have energy levels within the bandgap and can give rise to several basic effects [HOP96]: the generation or recombination of electron-hole pairs, the trapping of carriers, the compensation of donors or acceptors, and the tunneling of carriers.

The formation and evolution of the defects is a complex process and the interaction of different radiation fields with a semiconductor material may result in different defect types. The kind and the distribution of defects may even depend on the energy of a given particle impinging the semiconductor. Even for a well examined material like silicon not all electrically active defect types (and their relative importance) have been identified. At present, a first principles calculation of the radiation-induced degradation of a device parameter considering the entire damage process is generally not possible.

3.2 NIEL Scaling

For the prediction of radiation-induced parameter degradation it is fortunately (and somewhat surprisingly) often sufficient to consider the first step of the damage process only, i. e. the deposition of non-ionising energy in the semiconductor by the impinging particles and the produced secondaries. It has been experimentally shown, that in many cases the displacement-damage induced change of a device property scales linearly with the amount of non-ionising energy imparted in displacing collisions, irrespective of the spatial distribution of the introduced displacement defects in one PKA cascade, and regardless of the various annealing sequences taking place after the damage event. Therefore it is possible to extrapolate the parameter degradation of a device measured for a given particle and particle energy to other energies and other particles by comparing the non-ionising energy loss (NIEL) in the device material ("NIEL scaling").

4 Non-Ionising Energy Loss (NIEL)

4.1 Terms describing NIEL and related Quantities

During the last two decades a tremendous amount of papers have been published dealing with non-ionising energy deposition in semiconductor materials. Research was stimulated by the awareness of possible malfunctions of components in space and the need for radiation-hard electronics for future particle accelerator experiments. In contrast to the ionising energy deposition an obligatory terminology for the characterisation of non-ionising energy deposition has not been fixed yet. The "space community" and the "particle physics community" use slightly different approaches, however, the use of different names for the same physical quantity and – worse – of the same name for different quantities can be found among each "community".

According to NIEL scaling, a **hardness factor k_n** can be defined, allowing to compare the damage of an arbitrary particle field with a spectral distribution *f(E)* and fluence Φ to the damage that would have been produced by monoenergetic neutrons with an energy of E_n = 1 MeV:

$$\Phi_{eq}^{n,(1MeV)} = k_n \cdot \Phi \tag{1}$$

where

$$k_n = \frac{EDK}{EDK(n, E_n = 1\,MeV)} \tag{2}$$

with EDK being the energy spectrum averaged **displacement damage cross section**:

$$EDK = \frac{\int DK(E) f(E) dE}{\int f(E) dE} \tag{3}$$

where *f(E)* is the differential flux of the arbitrary particle field.

The displacement damage cross section *DK* (also called displacement KERMA) can be calculated using the cross section of an interaction leading to recoils, the energy distribution of recoils, the partitioning between ionising and non-ionising energy loss of the recoils and finally summing over all possible interaction channels for the initial particle.

$$DK(E) = \sum_k s_k(E) \cdot \int dT\, f_k(E,T)\, Q(T) \qquad (4)$$

where *k* is the index of an interaction between the incoming particle with energy *E* and the lattice atom, s_k is the cross section for interaction *k*, $f_k(E,T)$ is the probability for the production of a recoil with kinetic energy *T* by a particle with energy *E* undergoing reaction *k,* and *Q(T)* is the partition function, which gives the fraction of *T* lost in non-ionising energy loss. The integration is performed over all possible recoil energies and *Q(T)* is set to zero, if the energy of the recoil is less then the displacement energy: $Q(T < E_d) = 0$ [MOL99].

The displacement damage cross section is usually quantified in [MeV·millibarn]. A related magnitude, ***NIEL***, has been introduced [SUM87], which is analogous to, and has the same units as, ionising stopping power and Linear Energy Transfer (we use NIEL as an acronym for Non Ionising Energy Loss. *NIEL* – written in italics – denotes the physical quantity non-ionising energy loss rate). The displacement damage cross section and *NIEL* can be converted into each other by accounting for the number of atoms per gram (N_A / A), e.g. multiplying the damage cross section with Avogadro's number N_A and dividing by the molar mass *A*.

The value of the displacement damage cross section for neutrons with an energy of 1 MeV has been fixed [AST01]. For silicon, $DK(n, E_n = 1\ \text{MeV}) = EDK(n, E_n = 1\ \text{MeV}) =$ 95 MeVmb. With the molar mass of Silicon $A = 28.086$ g/Mol this corresponds to $NIEL(n, E_n = 1\ \text{MeV}) = 2.037$ keV·cm^2/g.

In terms of a differential partial cross section *ds/dT* for an impinging particle (with energy *E*) creating a given recoil the contribution of that kind of recoil to the total *NIEL* may be calculated [AKK01] by

$$NIEL(E) = \frac{N_A}{A} \int_{T_{\min}}^{T_{\max}} dT \, Q(T) \, T \left(\frac{ds}{dT} \right)_E \qquad (5)$$

Akkermann et al. [AKK01] assume a minimum energy transfer of $T_{min} = 2E_d$ and use for the upper integration limit the maximum recoil energy for a head-on collision where the lattice atom of mass *M* is directly hit by the impinging particle of mass *m*: $T_{max} = 4 \times E \times m \times M/(m+M)^2$.

Analogous to ionising dose the **Displacement Damage Dose D_d** can be defined, which is the product of *NIEL* and the particle fluence.

4.2 Applicability of NIEL Scaling

4.2.1 General

Although there is no real theoretical – microscopic – understanding, why radiation damage should scale with NIEL, the NIEL scaling hypothesis is generally accepted because it has agreed with most experimental data for bulk damage under various irradiation conditions. Using the NIEL concept the radiation damage in various semiconductor materials have been - at least qualitatively - examined (including diamond [LAZ98], germanium [MAR89], SiC [BAR91], SiGe [OHY97], InP ([SUM93], [WAL97]), InGaAs [BAR00], InGaAsP [OHY00], AlGaAs [REE00]). Of course the vast majority of investigations focus on damage in Si and - to a lesser extent - GaAs devices. On one hand, these studies showed the wide range of applicability of the NIEL concept, on the other hand they clearly demonstrated the limitations in certain cases.

4.2.2 GaAs and other II-V Semiconductor Compounds

NIEL scaling and the concept of Displacement Damage Dose has been proven to be very useful in describing the degradation of the maximum power of GaAs/Ge solar cells after irradiations with protons of energies of 0.2 to 9.5 MeV and electrons (0.6 to 12 MeV). Data points fall on a common (characteristic) curve, if the measured maximum power (normalised to pre-irradiation values) is plotted using the displacement damage dose as the abscissa of the plot [MES99]. However, the electron and proton characteristic curves derived for heteroepitaxial InP/Si solar cells did not coincide, unless the displacement damage dose for electrons had been divided by a constant factor. Radiation-induced defects that act to degrade the diffusion-length have maybe different characteristics in electron and proton irradiated material. Since the radiation-induced defect energy levels in InP appear to arise from complexes formed of impurity atoms and radiation-induced defects, the denser defect structure induced by proton irradiation might induce these defect energy levels more rapidly as compared with electron irradiation and results in more rapid cell degradation [WAL97].

Considering the entire proton energy range of interest, large discrepancies can be found between the energy dependence of NIEL in GaAs (and in other III-V compound semiconductors) and that of experimentally determined damage. Depending on how (at which energy) the damage factors are normalised to NIEL, it is reported that NIEL overestimates the damage at high energies or underestimates it at low energies.

Already early work on implanted resistors and JFETs showed that damage factors fall well below the NIEL curve when proton energy exceeds approximately 15 MeV [SUM88]. Since then, the existence of marked departures of experimental values from NIEL calculations have been confirmed e. g. by direct measurements of the minority carrier lifetime in amphoterically doped GaAs LEDs [BAR95] and by investigating the output power dependence on proton energy for AlGaAs LEDs [REE00]. NIEL scaling violations are not confined to proton irradiations and have also been reported for GaAs LEDs irradiated in several neutron environments [GRI91]. With respect to optocouplers, members of the NASA Electronics Radiation Characterisation Project have recently recommended that the use of NIEL scaling should be restricted to proton energies less than 30 MeV and supplemented by a couple of measured damage values at higher energies [REE01].

Because the major deviations from NIEL scaling appear at proton energies where nuclear reactions dominate and the corresponding cross sections are less well known, it might be suspected that NIEL calculations are not accurate in this energy region. However, a recent calculation of NIEL in GaAs [AKK01] agreed within a few percent (in the energy range of 40 to 150 MeV) with previous results obtained by Summers et al. [SUM88]. Akkermann et al. [AKK01] used the ENDF/B-VI library for the calculation of NIEL. This library does not contain any data for Ga and As, and the authors used cross sections of Cu instead for elastic and inelastic interactions. This will definitely introduce some uncertainty in the results, but does not explain the large discrepancies (up to some 100 percent) between calculation and experiment.

It has been considered that recoil equilibrium does not exist in the active areas of the devices examined. It has been shown [SUM88] that using a "restricted energy loss" approach to the calculation of NIEL in a very thin region close to the surface experimental data and the "restricted NIEL curve" were in line. The reasonable motivation for "restricted energy loss" calculations is, that the fragments from inelastic interactions can be many times the dimensions of the active region of a device. But the deviations have also appeared under experimental conditions where equilibrium could be assumed [BAR95].

Thus it appears that high energy protons are less damaging in GaAs than low energy protons (normalised to the same displacement damage dose). Barry et al. [BAR95] speculate that this could result from damage clusters of increasing size created by irradiation with high energy protons. They refer to the explanation of Luera et al. [LUE87] for the lower than expected carrier removal rate for 14 MeV neutrons, saying that such clusters are expected to have less effect on the electrical properties than the constituent defects acting individually. Griffin et al. [GRI91] propose a thermal spike mechanism, which has been extensively studied in metals, as the reason for the reduced efficiency of neutron-induced high energy recoils in GaAs. A thermal spike occurs when the cluster energy density is high enough to cause local melting and subsequent recrystallisation of the material, thus leading to an increased annealing of the defects. The saturation at high PKA energy is correlated with the production of defect clusters. As the PKA energy increases more clusters are generated (per neutron), but the cluster size (and cluster damage efficiency) stabilises. According to Griffin et al. the observation of a thermal spike phenomenon in GaAs and not in silicon is consistent with the fact that GaAs has a lower binding energy and a higher cascade energy density than does silicon.

Griffin et al. [GRI95] derived an empirical damage neutron efficiency function $x(T)$, which is dependent on the energy of the recoils. The efficiency function is applied by substituting the partition factor $Q(T)$ in equation (4) by the product $x(T) \times Q(T)$. In a recent paper [MES01] it has been shown that by adopting this concept for protons, the resulting modified NIEL calculation for protons in GaAs and LED carrier lifetime measurements [BAR95] are in agreement [MES01]. The efficiency function is stepwise defined [AST01]:

$$x(T) = 1.0 \quad \text{for } T < 0.1 \text{ keV},$$

$$x(T) = a_0 + a_1 \times \log(T) + a_2 \times T^2 \times \log(T) + a_3 \times [\log(T)]^2 \qquad \text{for } 0.1 < T < 500 \text{ keV},$$

$$x(T) = 0.01 \quad \text{for } T > 500 \text{ keV}$$

with $a_0 = 0.872670$, $a_1 = -0.187469$, $a_2 = 1.2371788 \cdot 10^{-7}$, $a_3 = -0.060753$.

The concept works by calculating an effective fraction of the recoils initial energy $x(T) \times Q(T)$, where $Q(T)$ is the Lindhard partition function. Is has not been shown yet that the empirical efficiency function is applicable to other GaAs devices nor to other III-V compound semiconductors. Following the thermal spike concept, most of the defects annihilate by recombinations during the thermal spike. Hashimoto et al. [HAS88] considered correlations of radiation induced microstructural changes in different metal alloy systems by accounting for the freely migrating defects. The fraction of defects which become free to migrate depends strongly on whether they are produced in cascade events or as isolated Frenkel pairs. The authors found, that the median energy $T_{1/2}$, with which the primary knock-on atoms recoil, is a suitable measure for estimating the number of freely migration defects and hence for the amount of microstructural changes induced in different metal alloy systems by a variety of irradiation particles. $T_{1/2}$ is computed by the evaluation of the primary-recoil spectrum weighted by the total number of Frenkel pair defects produced by each primary recoil. Larger values of $T_{1/2}$ imply, that a greater fraction of the total number of irradiation induced defects are produced in energetic displacement cascades and hence the damage efficiency is reduced. However, the effect of lower energy PKAs on enhancing radiation damage can be affected by a coexistence of displacement cascades by high energy knock-ons ([ARU99] and references therein).

It is interesting to note, that an even better agreement with the experimental data of [BAR95] can be achieved just by using a simpler model for the effective damaging recoil energy [MES01]. Prior to the Lindhard theory models were used, which assume a sharp ionisation limit E_i, above which a primary recoil loses all of its energy solely by ionisation. For an insulator E_i can be calculated by $E_i = M \times E_g / 8 \times m_e$, where

M is the atomic mass of the target, m_e is the mass of an electron and E_g is the optical width of the forbidden gap. This prescription by Seitz only contains well-known material parameters and might presumably be applicable not only for insulators but also for semiconductors. However, direct experimental evidence indicates that Lindhard's partition function does apply in GaAs as well as in silicon ([MES01] and references therein).

4.2.3 Silicon Devices

The CERN RD48 (ROSE) collaboration performed extensive investigations on the radiation damage of silicon detectors and on the details of defect formation and kinetics during annealing. Many experiments have shown that bulk damage parameters scale independent of particle type and energy with fluence if normalised to NIEL ([LIN00], [VAS00a]). Recently it was found that the NIEL scaling does not hold ideally when oxygen-enriched detectors are examined. In oxygenated silicon the change in effective doping concentration N_{eff} caused by high-energy protons or pions is considerable less than that due to MeV-neutrons of the same NIEL equivalent fluence. Present defect models attribute the oxygen effect especially to point defects; the low-energy recoils from Coulomb interactions are more likely to produce point defects, whereas the total NIEL in neutron damage is governed predominantly by the production of clusters. In fact gamma irradiations (creating only point defects due to the Coulomb interaction of the Compton electrons) support this explanation: the oxygen-enrichment had an even larger effect than for hadron irradiation ([LIN01] and references therein). Because the ratio between cluster-type defects and point defects varies with proton energy, notably below 10 MeV [FEI00], an examination of the dependence of effective doping change on proton energy would be another confirmation of the influence of defect types on damage. There is experimental evidence ([BIS00], [BIS00a] and references therein), that the acceptor creation rate cannot be scaled by NIEL even for standard silicon devices after low energy proton irradiations.

Comparing the damage effects of hadrons with that produced by electrons an example of an even worse breaking down of the NIEL scaling is reported by G. Lindström et al. [VAS00]: the current related damage of electrons with an energy of 1.8 MeV appears to be less damaging than that of hadrons (n, p, pions) by a factor of 40, although normalised to the same equivalent fluence. The authors state that the reason is most likely twofold: (1) the abundance of displacement clusters formed by hadron irradiations via nuclear interaction leading to a high generation current, whereas for electrons this part is almost negligible, and (2) in addition the higher ratio of close pairs among the primary Frenkel defects produced by electron irradiation (due to the lower mean recoil energy, because Coulomb interaction is the only interaction channel) leading to an enhanced recombination.

The observation of Lindström might be related to the findings of J. R. Srour and D. H. Lo [SRO00]. By evaluating a large amount of literature data, they succeeded in deriving a universal damage factor for radiation induced dark current in an arbitrary silicon device. The radiation induced increase in thermal generation rate per unit fluence scales linearly with NIEL for hadron (n, p, pion and heavy ion) irradiation but the authors found significant deviations from linearity for low-energy (< 2 MeV) electron and ^{60}Co irradiations (the latter being equivalent to low energy electron irradiation in that context). A quadratic dependence appears to describe the electron data reasonably well, but the authors found experimental evidence, both for linearity and deviations from linearity. In contrast to Summers et al., deviations from linearity have been found for p-type and n-type devices (whereas Summers et al. observed linearity for n-type and a quadratic dependence for p-type material [SUM93]). However, the study of Summers et al. involved diffusion length (i.e. recombination lifetime) degradation, whereas Srour and Lo considered generation lifetime changes. According to Srour and Lo, different defects generally dominate recombination compared to generation, and this might explain the different findings.

A compilation of *NIEL* data for neutron, protons, pions, and electrons in silicon can be found in [VAS00]. From the available literature those data were selected, which proved to be the most reliable ones (with respect to the physics approach behind and in comparison with experimental data).

4.2.4 Applicability of Ground Test Data to Space Conditions

Care has to be taken when using ground test data: despite the irradiation conditions (normal vs. isotropic; flux rate) the operating conditions of a device (supply voltage, bias, temperature, permanent/intermittent operation) might not appropriately reflect the situation during a mission and correction factors must be applied. Concurrent ionising dose effects must be taken into account, particularly with respect to the annealing behaviour. There may be a considerable device-to-device variation in radiation damage, especially for COTS (commercial-off-the shelf) devices. In contrast to ground tests, devices in space are simultaneously irradiated with different particles and continuos energy spectra. Possible synergetic effects (e.g. with respect to the formation of stable defects), are not yet sufficiently examined.

Some device properties are non-linear with fluence. E.g. at low fluences the degradation of solar cells is due to the introduction of non-radiative recombination centres, at (very) high fluences solar cells show additionally the effects of carrier removal. The annealing rate of certain defects in silicon for low proton fluence and/or density of primary damage sites is reduced [FEI00]. This may indicate a fluence dependence of radiation damage.

4.2.4.1 Geometry of the Device

Several geometry dependent effects have influence on the radiation damage of a device for a given radiation environment.

Recoil Equilibrium

Although an imperfect build-up of recoils could not generally explain the decreased parameter degradation of some GaAs devices measured for higher proton energies, it is definitely a matter of concern. For certain devices having a thin active volume near the surface recoil equilibrium may not be achieved, because e.g. for protons incident on a CCD, the primary recoils generated can have ranges larger than the depth to the CCD buried channel. If recoil equilibrium has not been reached, then *NIEL* would be expected to overestimate the displacement damage. However, compared to the case of isotropic irradiation behind spacecraft shielding, equilibrium conditions can be more violated during ground tests, where irradiations are usually performed with normally incident particles (furthermore, in some cases the de-lidding or de-packaging of devices during ground tests may prevent the build-up of equilibrium). A damage factor measured using normally incident irradiation and high proton energy applied to the space situation – disregarding the recoil build-up – may thus result in an underestimation of the radiation damage during a mission (cf. [DAL93], [DAL94]).

Local Variations of Energy Deposition

With shrinking dimensions of active volumes (e.g. a FET channel) fluctuations of the local energy deposition become important. In CCDs and CIDs, the variation of the dark current signal from one pixel to another due to the different energy deposition in such a microvolume is already a main concern (cf. e.g. [HOP96]). The use of *NIEL* alone only enables the prediction of the mean bulk damage. By using microdosimetry theory and *NIEL*, Robbins [ROB00] developed an improved analytical method for deriving the dark signal distribution induced by elastic and inelastic proton interactions. However, as shown in [DAL94], analytically obtained distributions can deviate significantly from those measured when the range of recoils become comparable with the dimensions of the depletion volume. Dale et al. [DAL94] performed Monte Carlo simulations and found that border crossers, which have crossed the active volume boundary and stopped outside, have a large effect on the inelastic variance. For 63 MeV protons the relative inelastic variance $(s/m)^2$ (where m is the mean damage energy and s is the standard deviation) sharply increases with decreasing depletion depth over a range relevant to device depths and that it decreases with increasing proton energy (this energy dependence flattens at high energies because the mean damage energy saturates due to the Lindhard partitioning).

Dale et al. used a modified version of the CUPID (Clemson University Proton Interactions in Devices) Monte Carlo code for the determination of the inelastic damage distribution. In CUPID, two nested volumes with identical shapes are specified. The smaller inner volume represents the sensitive volume. For any spallation reaction in either the sensitive volume or outer shell, CUPID follows all recoil fragments from the point of production to the end of range. If a particle crosses the boundary of the sensitive volume, only the damage energy deposited in this volume is counted. An event is defined as occurring whenever a particle with atomic number $z > 2$ enters the sensitive volume, or is generated within the sensitive volume [DAL94].

Slowing Down of Charged Particles and Secondary Particles

The range of low energy (< few MeV) charged particles in the space environment is often less than the shield thickness employed. However, due to the electronic stopping of high energy particles in the shielding and in the device itself low energy particles are present. Messenger et al. ([MES97], [SUM97]) showed that protons which have slowed down to energies below 0.1 MeV can contribute up to 30 % of the total displacement dose in GaAs solar cells. This is due to the fact that *NIEL* in GaAs peaks at a proton energy of about $4{\cdot}10^{-4}$ MeV and at this energy *NIEL* is four orders of magnitude higher than that at 100 MeV. To model proton displacement damage, it is necessary to know the proton energy spectrum down to the displacement threshold energy (≈150 eV; cf. chap. 4.3.1). Because energy spectra are often provided only down to 100 keV, which is generally sufficient for ionisation cases, Messenger et al. present a simple method for the calculation of the differential energy spectrum of the transmitted protons down to 100 eV [MES97].

In the case of heavier shielded (> some 5 millimetres Al equivalent material) devices, secondary particles generated in the shielding contribute significantly to the displacement damage dose. In heavy shielding applications where trapped and solar protons dominate, differences up to +25% where calculated, when the results of a Monte Carlo program (accounting for secondary particle generation) was compared to those obtained by a continuos slowing down approximation for the primary protons only [Jun01].

4.3 Monte Carlo Methods for the calculation of NIEL

4.3.1 Estimation of Particle Threshold Energies

It is instructive to consider the most simple case of an interaction with a lattice atom, i.e. a head-on collision where the lattice atom (mass *M*) is directly hit by the impinging particle of mass *m* and energy *E*. The recoil energy of the struck atom is

$$T_{\max} = 4 \cdot E \cdot \frac{m \cdot M}{(m+M)^2} \tag{6}$$

or in case of an impinging relativistic electron ($m_e << M$)

$$T_{\max} = 2 \cdot E \cdot \frac{m_e}{M} \cdot \left(2 + \frac{E}{m_e c^2} \right) \tag{7}$$

where m_e is the electron's rest mass ($m_e = 5.49 \cdot 10^{-4}$ amu) and $m_e \cdot c^2 = 0.511$ MeV.

The recoil can leave its lattice site, if its kinetic energy exceeds the displacement energy E_d. Consequently, a minimum energy of the incident particle E_{thr} is required to produce such an damage event. In the case of a relativistic electron and a head-on collision E_{thr} is given by [BRA94]

$$E_{thr} = m_e \cdot c^2 \cdot \left(\sqrt{1 + \frac{E_d}{2 \cdot m_e \cdot c^2} \cdot \frac{M}{m_e}} - 1 \right) \tag{8}$$

Using equation (8) and, after substituting $E \rightarrow E_{thr}$ and $T_{max} \rightarrow E_d$, equation (7) can be used to calculate the minimum energy of an incident particle required to dislodge an atom from its lattice site (tab. 2).

	Semiconductor Material					
			GaAs		SiC	
	Si	Ge	Ga	As	Si	C
E_d [eV]	21	27.5	7 to 11		21.8	
E_{thr} [keV] (electrons)	220	580	188 to 275	200 to 292	220	108
E_{thr} [keV] (protons)	0.15 (*)	0.5	0.12 to 0.19	0.13 to 0.21	0.15	0.065

(*) A value commonly used in the HEP community is E_{thr} *(neutrons)* ≈ 185 eV ([VAS97a], [MOL99]).

Tab. 2: Threshold energies E_{thr} for different particles and semiconductor materials (after [BRA94]).

It should be noted here that the kinematical limit imposed by the elastic threshold does not exclude damage effects by less energetic neutrons due to nuclear reactions. E.g. in silicon, E_{thr} corresponds to a minimum of the displacement damage cross section, but *DK(E)* increases below the threshold energy with decreasing neutron energy due to an (n,γ) reaction resulting in Si recoils with an energy of approx. 1.28 keV, well above E_d [VAS97a].

The displacement energy E_d is the minimum energy required to produce a Frenkel pair. A higher energy is required for the production of defect clusters, about 5 keV in silicon ([LIN87]). With (7) and (8) one can deduce that a neutron must have at least a kinetic energy of 35 keV, and an electron more than approx. 8 MeV, to produce a cluster. Photons of a ^{60}Co-source will mainly interact with the silicon via Compton electrons having a maximum energy of approx. 1 MeV [MOL99], which is not sufficient to create clusters, but a relatively uniform distribution of isolated point defects (MARLOWE simulations by Woods et al. [WOO81] lead to a different description of the dependence of the defect structure on the recoils energy T: recoils in Si with $E_d < T < \approx 2$ keV produce only point defects. For recoils with ≈ 2 keV$< T < \approx 12$ keV one defect cluster is formed and for recoils with $T > \approx 20$ keV a tree like defect structure is formed. Further investigations – including also other semiconductor materials – would be interesting).

4.3.2 Heavy Charged Particles

Interaction with a Target Nucleus

A particle of atomic number z approaching a nucleus of atomic number Z will, at large distances, experience only the Coulomb potential

$$V_c(r) = \frac{z \cdot Z \cdot e^2}{4\pi\varepsilon_0 \cdot r} \tag{9}$$

at distances r from the centre of the nucleus. This situation is changed when the particle comes within the range of the nuclear forces. However, there is a Coulomb potential barrier V_b to be surmounted whose value is approximately

$$V_b(r) = \frac{z \cdot Z \cdot e^2}{4\pi\varepsilon_0 \cdot R} \tag{10}$$

where R is the nuclear radius. There is a finite chance of penetrating the barrier for energies less than V_b, but if the energy is well below the barrier height then this effect is negligible and the incident particle will be simply elastically scattered by the

Coulomb potential (Rutherford scattering). In the case of an incident proton approximate values for V_b are e.g. 3 MeV for Z=6 (carbon) and 17 MeV (Z=82; lead). According to (10) the Coulomb barrier will be much larger for heavy ions.

At present, a description of nuclear reactions derived from fundamental principles covering the variety of observed phenomena in the entire energy range does not exist. Several models are used, which describe the interaction of an incident particle with the nucleus rather well in a certain energy range, but may fail for other energies.

An optical model can be used to describe the situation, when the energy of the incident particle is sufficiently high, so that the distance of the closest approach brings it within the range of nuclear forces. The optical model, developed by Feshbach, Porter and Weisskopf in 1954, describes the interaction of the incident particle with a nuclear potential $V + iW$, where the imaginary part is introduced to account for all nonelastic processes by leading to a damping of the projectile wavefunction. This is analogous to the imaginary term in the refractive index introduced in optics to take account of absorption. In fact, the regular fluctuations of the differential cross section ds/dW as a function of the scattering angle, which are observed for a wide range of nuclei (and also for incident neutrons), are reminiscent of a "smeared out" diffraction pattern and can be interpreted as approximating to Fraunhofer diffraction due to an absorbent sphere [BLI91]. While the optical model predicts the total reaction cross section, it does not provide information on the subsequent nonelastic partial cross sections for various decay channels.

Various possibilities exist, if a direct collision with a nucleon takes place. The nucleon may be exited to a higher state and the incident particle leaves the nucleus with reduced energy (inelastic scattering). Alternatively the incident particle may give enough energy to the nucleon so that this nucleon is knocked out from the nucleus. Depending on how much energy the incident particle retains it may escape the nucleus or it is captured. A composite incident particle may lose some of its component nucleons which remain in the target nucleus (stripping reaction) or, conversely, it may pick-up a nucleon from the target (pick-up reaction). Such direct interactions take place in a time of the order of that taken by the incident particle to cross a nucleus ($\approx 10^{-22}$ s).

The collision of the incident particle with the nucleus may result in a series of further random collisions within the nucleus. The state of the nucleus after it has captured the incident particle and in which many internal collision processes are occurring was first discussed by Niels Bohr and is referred to as the compound nucleus. The de-excitation of the compound nucleus may be described statistically and results in the emission (evaporation) of single nucleons or more complex clusters of nucleons. If less energy has been imparted to the nucleus during the collision the de-exitation of the nucleus may be achieved through the emission of gamma rays. The resulting nucleus recoils with energies in the range of a few hundred keV to a few MeV. A compound nucleus process can thus be represented as taking place in two stages - formation of the compound nucleus and its decay. The compound nucleus exists for approximately 10^{-16} to 10^{-18} s and the evaporation stage proceeds almost independently of the mode of the compound nucleus formation.

A particle emission can take place with a time scale longer than the very rapid direct reactions but much shorter than the slower compound nucleus reactions These emission processes are known as pre-equilibrium or multistep reactions, and they are characterised by particles emitted with relatively high energies and with angular distributions that are peaked in the forward direction. Numerous models have been developed to account for the high-energy pre-equilibrium particles that make up the "continuum" region of the secondary particle emission spectra above the evaporation peak (for incident energies above approximately 10 MeV). Beginning in the 1940s, intranuclear cascade (INC) models were developed that use Monte Carlo techniques to simulate nucleon-nucleus reactions in terms of individual successive nucleon-nucleon collisions. The INC theory makes use of free nucleon-nucleon experimental cross sections, and it accounts for Fermi motion and Pauli blocking in a semiclassical manner. Perhaps the most questionable assumption within the INC model is the utilisation of free-space nucleon-nucleon cross sections for scattering events that take place within a nuclear medium, which is most accurate only at high incident energies (above approximately 100-200 MeV). However, some authors have had some success with INC calculations even at energies as low as 20 MeV [CHA02].

Some general relations hold for hadron-nucleon interactions [FIL92]:

- the non-elastic cross section is almost constant above 100 MeV,
- the multiplicity of high energy secondary particles increases approximately with ln(*E*), with *E* being the energy of the incident particle
- the residual excitation energy (and thus the multiplicity for the production of low energy [< 20 MeV] hadrons) increases slowly with the energy of the incident particle.

Calculation of Damage Cascades and *NIEL* using TRIM

The well known Monte Carlo code TRIM calculates the final 3D distribution of the ions impinging an arbitrary material. All target atom cascades in the target are followed in detail (fig. 1). TRIM considers the interaction of an incident ion with atomic number Z_1, and energy E, having a collision within the target with an atom of atomic number Z_2. After the collision, the incident ion has energy E_1 and the struck atom has energy E_2. Previously specified for the target are the displacement energy E_d , the binding energy of a lattice atom to its site E_b, and E_f, the final energy of a moving atom, below which it is considered to be stopped. A displacement occurs if $E_2>E_d$. A vacancy occurs if both $E_1>E_d$ and $E_2>E_d$ (both atoms have enough energy to leave the site). Both atoms then become moving atoms of the cascade. The energy E_2 of atom Z_2 is reduced by E_b before it has another collision. If $E_2<E_d$, then the struck atom does not have enough energy and it will vibrate back to its original site, releasing E_2 as phonons. If $E_1<E_d$ and $E_2>E_d$ and $Z_1 = Z_2$, then the incoming atom will remain at the site and the collision is called a replacement collision with E_1 released as phonons. The atom in the lattice site remains the same atom by exchange. This type of collision is common in single element targets with large recoil cascades. If $E_1<E_d$ and $E_2>E_d$ and $Z_1 \neq Z_2$, then Z_1 becomes a stopped interstitial atom. Finally, if $E_1<E_d$ and $E_2<E_d$, then Z_1 becomes an interstitial and E_1+E_2 is released as phonons. If a target has several different elements in it, and each has a different displacement energy, then E_d will change for each atom of the cascade hitting different target atoms [ZIE96].

Since TRIM calculates the vacancy production rate, i.e. the average number of produced vacancies along a path of an ion, it is possible to derive *NIEL* using the modified Kinchin-Pease relationship between the number of atomic displacements N_d and a given quantity of non-ionising energy E_n

$$N_d = \frac{E_n}{2.5 \cdot E_d} \tag{11}$$

which holds for $E_n>2.5 \cdot E_d$; $N_d = 1$ for $E_d < E_n < 2.5 \cdot E_d$, else $N_d = 0$.

Recently the use of TRIM has been proposed for the calculation of *NIEL* for heavy ions [MES99]. However, TRIM does not include any nuclear reaction analysis, thus the validity of the results is constrained to the energy range where Rutherford scattering dominates. The TRIM code is suitable for transport calculations of the produced recoils, which typically have energies less than 10 MeV. Consequently, for a detailed analysis of damage cascades in silicon, Huhtinen [HUH01] followed the lines of the TRIM code given in [ZIE85] (with some

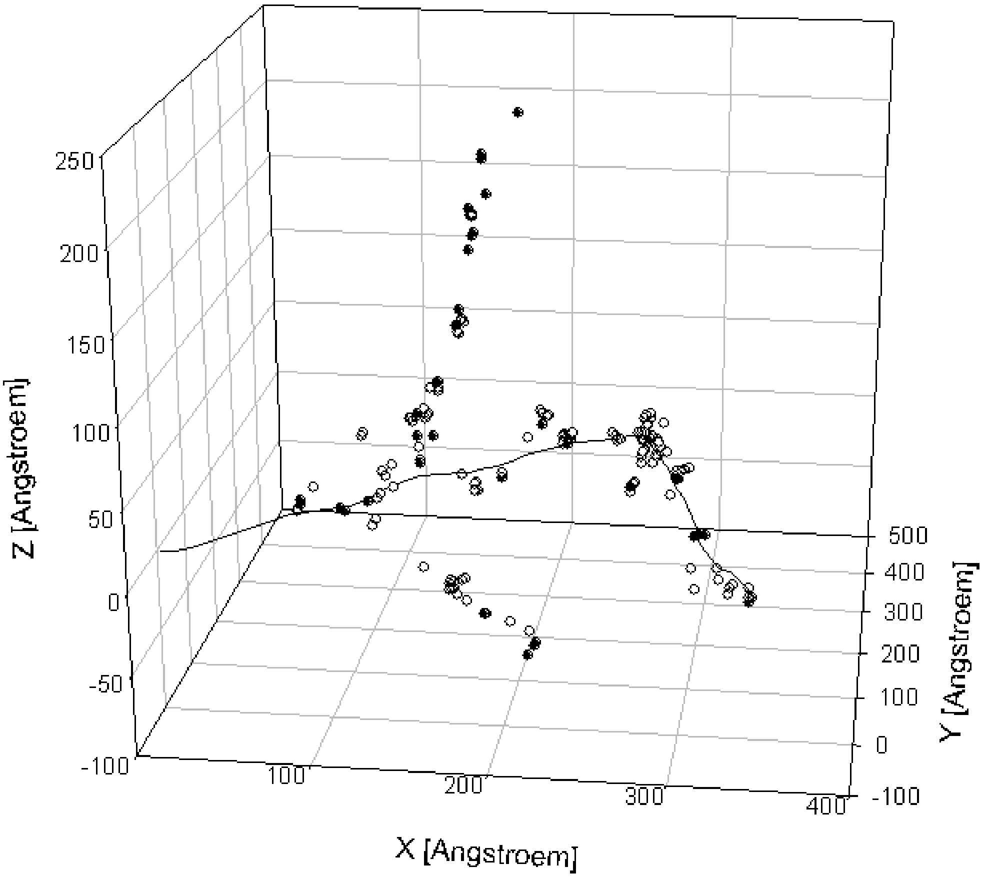

Fig 1: Track of a Si-recoil in a SiC lattice. The primary recoil (line) was generated at (*X,Y,Z*) = (0,0,0) with initial energy *T* = 30 keV. In this example the recoil gave rise to 343 displacements. Moving or stopped C-atoms are denoted with filled circles, moving or stopped Si-atoms with open circles. Simulation with TRIM (SRIM 2000.40).

modifications allowing the explicit production of secondary recoils when the ion collides with lattice atoms). A related method has been applied by Chilingarov et al. [CHI00]. They calculated the total non-ionising energy loss for a variety of ions during their slowing down to rest in carbon, silicon, and GaAs. The incident ion was followed in small steps through the material and in each step the ionisation energy loss, assumed to be continuos, was computed and the discontinuous energy loss due to Rutherford scattering was simulated. In the latter case, the energy of each nucleus recoiling from both primary and secondary interactions was stored.

Recently Applied Methods for the Calculation of Proton *NIEL*

Various approaches to calculate proton *NIEL* are undertaken in the following publications:

[AKK01]: Approximation of the elastic ds/dW cross section data, which are tabulated in the ENDF/B-VI library, by a sum of a few Gaussians. The recoil energy is calculated using two body kinematics. Inelastic ENDF/B-VI library data include direct, pre-equilibrium, and compound nucleus reaction mechanisms and are suitable up to approximately 200 MeV. Contains only a selection of target atoms. Library data are used up to 150 MeV and a semi-empirical model is used for higher energies.

[ALU91]: A modified version of the cascade-evaporation model of the High Energy Transport Code (HETC) is used to calculate the interactions of protons from 70 to 600 MeV in Si. Calculations of localised displacement cascades are done with the MARLOWE-12 code, which uses the binary collision approximation (BCA).

[HUH01]: A pre-equilibrium model is used for energies less than 1.3 GeV; for elastic scattering a simple Glauber optical model is used. It has the drawback, that it tends to overestimate scattering at large angles. To avoid unphysically high values a maximum of 10 MeV is imposed on the contribution of the recoils from elastic scattering.

[Jun01]: *NIEL* data below 200 MeV are taken from [SUM93]. The authors use the relativistic differential cross section for the PKA spectrum for Coulomb scattering formulated by [SEI56] and present a corrected form of equations; Cross section for the inelastic contribution and the recoil energy spectrum from MCNPX version 2.1.5.

4.3.3 Neutrons

Interaction with Matter

Together with protons, neutrons form the most important contribution to the secondary particle flux in a heavy shielded device. Some aspects of hadron interaction with matter have been already discussed in the previous chapter. Due to the missing charge, neutrons do not experience the Coulomb repulsion and thus exothermal nuclear reactions can take place even for low energy neutrons. With decreasing velocity of the neutron v the probability increases that it is in the vicinity of a nucleus, thus one expects a $(1/v)$-dependence of the neutron capture cross section. This dependence can be observed for low energy neutrons and most nuclei, however, particularly in the energy range 1 to 100 eV it is superimposed by large resonances (see tab. 3 for a compilation of the most important nuclear reactions). Neutron capture reactions (n, γ) are important wrt radiation damage, because they generate recoils with energies high enough to dislodge a lattice atom. This happens in a neutron energy range, where recoils generated by elastic scattering have not sufficient energy for producing a displacement (cf. chap. 4.3.1).

Energy Range of Incident Particle	Main Nuclear Reactions for	
	Neutrons	Protons
0 to 1 keV	(n,γ)	–
1 to 500 keV	(n,γ)	(p,n), (p,γ), (p,α)
0.5 to 10 MeV	(n,α), (n,p)	(p,n),(p,α)
10 to 50 MeV	(n,2n), (n,p), (n,np), (n,2p), (n,α)	(p,2n), (p,n), (p,np), (p,2p), (p,α)

Tab. 3: Main nuclear reactions of neutrons and protons with medium heavy nuclei (25<A<80) [LIE91].

Recently Applied Methods for the Calculation of Neutron *NIEL*

A review of neutron *NIEL* calculations, which have been performed until 1997, can be found in [VAS97]. More recently Jun [JUN01] considered the contribution of secondary neutrons to the displacement damage in silicon for a typical space proton environment. Below a neutron energy of 150 MeV, the damage cross sections were computed by NJOY97 [FAR97] based on the recently evaluated Los Alamos National Library high energy cross section library [CHA99a]. Above 150 MeV, *NIEL* was computed by using a thin target approximation. A 1-cm slab of silicon with a normalised density of 0.01 atoms/barn/cm was modelled, and a pencil beam of neutrons through this slab was considered. The history tape of the Monte Carlo program MCNPX was analysed to calculated the mean damage energy per source particle. Using this method, at the 150 MeV boundary an approx. 25 % larger damage energy cross section was calculated than that obtained by NJOY97. This was attributed to spallation effects, which are included in MCNPX, whereas NJOY97 only accounts for elastic and inelastic scattering, and other types of particle emanating reactions such as (n,p), (n,α). This highlights the importance of spallation reactions when computing *NIEL* in high neutron energy range.

4.3.4 Electrons

Over the energy range of interest only coulombic events are important. Several approximations for Mott's formula, which describes the elastic cross section $d\sigma/d\Omega$, are used. For low Z materials (including silicon), Summers et al. [SUM93] used the McKinley-Feshbach approximation [MCK44], and for higher Z (> approx. 24) material the Curr form [CUR55] and the approximation of Dogget et al. [DOG56] were applied.

Lijian et al. [LIJ95] developed a fitting formula for the Mott differential cross section, which is based on the Rutherford cross section. A modified version of this formula has been employed in recent electron *NIEL* calculations and is given in [AKK01]. The modifications account for the screening effect of the electrons of the scattering atom.

4.3.5 ^{60}Co Gamma Rays

In order to compare radiation induced effects due to the ionising and non-ionising energy deposition, electronic components are sometimes irradiated with ^{60}Co gamma rays and protons. However, ^{60}Co gamma quanta interact primarily via Compton scattering, and the secondary electrons have sufficiently high energies (up to 1 MeV) to displace a lattice atom. The calculation of *NIEL* for ^{60}Co radiation can be reduced to the calculation of electron *NIEL*, if the energy spectra of the secondary electrons generated in the device and the shielding are known. Akkermann et al. [AKK00] use the Heitler form of the differential cross section *ds/dT* for an energy transfer *T* to a free electron in a solid and account for the slowing down of the Compton electrons. The calculated electron spectra behind shieldings of thicknesses from 100 µm to 2 mm deviate markedly from prior calculations by Summers et al. [SUM93].

4.3.6 Partition Function

The fractions of energy imparted to ionisation and displacing collisions were calculated by Lindhard in the LSS (Lindhard screened potential scattering) theory [LIN63]. Several approximations for the Lindhard partition function *Q(T)* are used. An appropriate formulation has been noted by Robinson (cf. [AKK01], [JUN01],[VAS97]):

$$Q(T) = \frac{1}{1 + F_L \cdot (3.4008 \cdot \boldsymbol{e}^{1/6} + 0.40244 \cdot \boldsymbol{e}^{3/4} + \boldsymbol{e})} \qquad (12)$$

for $T \geq E_d$ and *Q(T)*=0 elsewhere; with

$$\boldsymbol{e} = \frac{T}{E_L}$$

and

$$E_L = 30.724 \cdot Z_R \cdot Z_L \cdot \left(Z_R^{2/3} \cdot Z_L^{2/3} \right)^{1/2} \cdot \frac{A_R + A_L}{A_L}$$

$$F_L = \frac{0.0793 \cdot Z_R^{2/3} \cdot Z_L^{1/2} \cdot (A_R + A_L)^{3/2}}{(Z_R^{2/3} + Z_L^{2/3})^{3/4} \cdot A_R^{3/2} \cdot A_L^{1/2}}$$

A_R and Z_R are the atomic weight and number of the moving particle and A_L and Z_L the corresponding quantities for the lattice atoms.

4.3.7 Displacement Energy

An appropriate choice of the displacement energy E_d seems to be important, at least for the calculation of electron *NIEL* at energies near displacement threshold. The low energy portion of the *NIEL* curve is shifted to higher energies as the displacement energy is increased (cf. fig. 9 in [MES99]). However, in their calculations of the total displacement energy for various ions in semiconductor materials Chilingarov et al. [CHI00] did not observe a strong dependence on the threshold energy.

Tab. 4 contains a compilation of commonly used values for E_d. The displacement energy is related to the binding energy of the atomic bond and is about twice the binding energy ([BRA94]; the accurate relationship can be found in [BAR91]). A first order value of the displacement energy may be calculated using an empirical relationship between E_d and the reciprocal lattice constant (Corbet and Bourgain; a revised form is given in [BAR91]).

Element/ Compound	**Z**	**Displacement Energy [eV]**							
		[AKK01]	[BAR91]	[BRA94]	[CHI00] (c)	[MES99] (a)	[SUM93] (b)	VAS97a (d)	
C	6		35		50	35			
Si	14	21		21	(12.9); 21	21	(12.9); 21	25	
SiC			21.8 ± 1.5 (e)						
P	15					8.7			
Ga	31					10			
GaAs	31.33	10			10	10			
Ge	32			27.5		27.5			
As	33					10			
Y	39					20			
In	49					6.7			

(a) taken from [Bau62] and [BOE90]; GaAs calculated using Bragg's rule; values for Y and In are those for elements which are in a compound.
(b) upper value (21 eV) fits data much better than 12.9 eV.
(c) Si: 21 eV used in calculations and 12.9 eV used to estimate the accuracy of calculations.
(d) taken from [LIN87]; commonly used in the HEP community.
(e) experimentally determined.

Tab. 4: Displacement Energies E_d for various materials and compounds.

5 Outline of a Simulation Tool Prototype

5.1 Calculation of Non-ionising Energy Deposition

There are many question marks concerning the general applicability of NIEL scaling. The uncertainty already starts when comparing the results of present *NIEL* calculations (involving e.g. different computer codes, various models for the interaction processes, and basic quantities). The existing proton *NIEL* data for silicon deviate by a factor of two in certain energy regions [MES01], even if only those data are selected, which have been gained by accounting for all major interaction processes (including inelastic events). It is even more difficult to assess *NIEL* curves for different materials, which have been obtained using different algorithmic approaches or different cross section libraries. Few or no *NIEL* calculations have been performed for other semiconductor materials, which become increasingly important (e.g. SiGe, GaAs, InP and related compounds). Obviously there is a need for a consistent set of *NIEL* data.

A data base containing pre-calculated *NIEL* data for different semiconductor materials could be used to predict parameter degradation of a device during a mission for the most simple case, when recoil equilibrium exists (i.e. the dimensions of the sensitive volume and the layers surrounding this volume are large compared to the range of recoils) and provided, that linear *NIEL* scaling holds.

The evaluation will comprise the following steps:

1. irradiate device with monoenergetic particles
2. measure parametric degradation
3. calculate device degradation versus displacement damage dose (assuming that the parameter degradation and *NIEL* have the same energy dependence)
4. determine radiation environment for mission (or time intervals of the mission)
5. calculate particle spectra behind shielding
6. calculate displacement damage dose for mission
7. predict onboard parameter degradation based on calculations (3) + (6).

In cases where large gradients of the non-ionising energy deposition can be expected (because recoil equilibrium does not exist) or local fluctuations of the energy deposition are interesting (e.g. the pixel-to-pixel variation in a CCD), the use of the material-specific *NIEL* is not sufficient for a reliable prediction of onboard performance. In such cases the total non-ionising energy deposition in a specified sensitive volume (or in multiple volumes) must be calculated, possibly both for an isotropic (or given) angular distribution of incident particles and normally incident particles (this will allow the comparison of the expected damage measured during ground tests and during flight). A suitable method will be discussed in chap. 5.3.

5.2 Calculation of Parameter Degradation

Recently simulation studies [HUH01] on NIEL and defect formation in silicon (exposed to various types of hadron irradiation) lead to a fairly consistent description of the radiation effects in oxygenated silicon. However, the applied model makes use of many uncertain input parameters and *ad hoc* assumptions, and the standard Shockley-Read-Hall theory could not be applied. With respect to the present state of theoretical understanding, attempts to predict macroscopic device parameters by the detailed simulation of the entire damage process (including primary defect generation, annealing and migration, formation of stable defects and their occupancy, possible charge exchange reactions) might be generally not fruitful, even more when semiconductor materials with less known properties than that of silicon are considered. Furthermore such simulations require a detailed knowledge of the underlying physical processes and a simulation tool could only partly assist the user, thus being a research tool rather than an engineering tool (however, an engineering tool might provide the basis for further analysis by the calculation of the damage cascades and the resulting defect structure). Therefore empirical relations between the non-ionising energy loss and the resulting parameter degradation presently seems to be the most promising solution.

Empirical Relations Between NIEL and Degradation of Device Parameters

- In many cases a simple linear *NIEL* scaling can be applied (if recoil equilibrium is achieved). It has been shown that the radiation induced dark (or leakage) current in silicon devices is independent of particle type and impurity concentration in the semiconductor, provided that *NIEL* exceeds approx. 10^{-4} MeV·cm^2/g, i.e. with respect to dark current increase the linear NIEL scaling holds for neutron, proton, pion and heavy ion radiation. Using the universal damage factor K_{dark} [SRO00] it is even possible to estimate the dark current increase during a space mission without any ground testing.

- There seems to be a quadratic dependence of radiation induced parameter changes on electron *NIEL* in certain cases. However, the situation is somewhat unclear ([SUM93] versus [SRO00]). In the case of GaAs solar cells and electron irradiation a good correlation was found, if *NIEL* was raised to the power of 1.7.

- Applying an efficiency function to the non-ionising part of the primary recoils energy lead to a good correspondence between the calculated dependence on the energy of incident protons and the energy dependence of measured minority lifetime damage coefficients of GaAs solar cells.

The relationship between NIEL and the resulting damage is dependent on the considered damage parameter and on the type of incident irradiation. At present a universal description is not possible and the simulation tool should provide (i) a power function scaling: (parameter degradation) $\propto NIEL^{x}$, (ii) the possibility to apply an efficiency function. Obviously there is some correlation – additionally to *NIEL* – between the energy of the primary recoils and the damage efficiency (reflecting the different annealing and evolution of defects due to the defect distribution). For further investigations the simulation tool should deliver the energy distribution of the recoils and some statistics (mean, median), allowing an estimation of the fraction of defects produced in energetic displacement cascades and in primary defects. A possible further "spin-off" of the simulation tool would be an output of the spatial three-dimensional defect distribution, which could be processed by other tools for the calculation of defect migration and the formation of electrically active defects.

5.3 Algorithmic Approach for the Calculation of NIEL

The core of the simulation tool will calculate the non-ionising energy deposition in a semiconductor material by accounting for the energy of the primary recoils generated in the material by elastic and inelastic events (if any) and

(a) applying the Lindhard partition $Q(T)$ and additionally a given damage efficiency function $x(T)$ to the primary recoils energy T ; a binned energy distribution will be stored,

(b) following up the history of each recoil in a given sensitive volume and its vicinity until the recoil energy decreases below the threshold energy E_{thr} for displacing an lattice atom. Only Rutherford scattering will be taken into account for the production of NIEL.

Option (b) will be applied, if the geometry of the device (sensitive volume and the covering layers) must be taken into account. It is possible to extend option (b) by following up the history of each recoil until it comes to rest (within the sensitive volume) and by storing the (x,y,z)-positions of primary defects (vacancies and interstitials).

The calculations related to option (b) are very time-consuming, because a lot of recoils have to be considered. Furthermore in this case a Monte Carlo simulation is rather inefficient for two reasons:

(1) because the heavy recoils may have ranges up to approx. 100 µm (α-particles), the detailed calculation of recoil paths must be performed in a volume with dimensions of that size, and only a small part of the recoils will hit the (relatively small) sensitive volume. In order to improve statistics a grid of target volumes can be used, which are sufficiently spaced, such that events generated by the same particle in more than one target volume are negligible,

(2) inelastic events are relatively rare, but they are the main reason for fluctuations of the local non-ionising energy deposition. In order to improve statistics, a common practice in such cases is to sample each event channel with equal probability and assign statistical weights according to the true partial cross section.

Methods for the calculation of the primary recoil energy, the Lindhard partition function and an efficiency function are given in the literature and a selection is presented in chap. 4.3. However, a main concern is still the choice of a suitable model and the definition of required extensions to GEANT4 for the calculation of recoil energies due to high-energy hadron (particularly: proton) interactions. The still rapidly changing implementation status of interaction models and cross sections in GEANT4 has to be taken into account as well as the completeness wrt to target atoms considered, the energy range considered and the accuracy for that energy range.

5.4 Basic Functions of the Simulation Tool Prototype

The prototype of the simulation tool shall primarily allow the assessment of the core functionality, i.e. the calculation of the non-ionising energy deposition, and the dependence of the results on basic parameters (e.g. the displacement energy E_d).

The user interface shall support the generation of *NIEL* curves (*NIEL* versus particle energy) for an arbitrary semiconductor material. This will allow the comparison with literature *NIEL* data.

It shall be possible to select a damage efficiency function.

It shall be possible to scale pre-calculated *NIEL* curves by applying a function $C \cdot NIEL^x$, where C is a constant. This will support the comparison of the calculated *NIEL* curves with the energy dependence of experimental damage factors.

It shall be possible to define a simple device geometry (sensitive volume/covering layers). This will allow to check the calculations of the local ionising energy deposition and its variance.

In view of the limited timeframe for the development of the prototype and the required amount of validation steps it might be reasonable to constrain the investigations to the most important (and most difficult) case, i.e. the radiation damage due to protons.

Appendix: Documentation of the Literature Survey

The following section summarises the reference outcome of the literature survey, that was found to be related to the project objectives. Appendix I is a list of all references found. Appendix II gives the filtered publications related to theory and algorithms that are preferably dealing with NIEL, displacement damage, SEUs and particle interaction in general.

Appendix I: Project Related References

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ANG99 - Angarano, M. M., Bder, A., de Palma, M., Raso, G.; Characteristics and SPICE simulation of an n+ on n type Si strip detector before and after neutron irradiation. submitted to NIM A (1999)

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AST01 - American Society for Testing and Materials; Standard practice for characterizing neutron energy fluence spectra in terms of an equivalent monoenergetic neutron fluence for radiation-hardness testing of electronics. ASTM Standard E722-94 (2001)

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