A simulation tool for the calculation of NIEL in arbitrary materials using GEANT4
- Some new results -

Hans-Herbert Fischer and Klaus Thiel
Nuclear Chemistry Dept.
University of Köln, FRG

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Overview

- The Simulation Tool (ST)
  - Objectives
  - Main modules
- New results (*NIEL* data)
- Possible integration under SPENVIS
Tool Objectives

- Develop a S/W tool prototype allowing to:
  - calculate displacement damage effects in semiconductors induced by non-ionising energy loss (NIEL) during a space mission
  - estimate the resulting performance degradation of electron. circuit components

- **Aim**: Facilitate qualification procedure for new electronic devices used in space missions
ST Main Modules

GUI (input)

NIEL
NIEL Calculation

PRED
Prediction of param.
degradation

GUI (output)

General Tool Features

• Modular structure
  (easy maintenance)

• Designed as internet application
  (remote or local use of ST)

• Modules NIEL and PRED
  partly use GEANT4

• Running under MS Windows
  (portable to other platforms)
Two options of running module NIEL

(a) NIEL calculation by applying the Lindhard partition function to the initial energy of the recoils (not for high-energy projectiles, not for compounds with high $\Delta Z$, no information about 3D defect distribution)

(b) NIEL calculation by MC simulation of the damage cascade step by step in the vicinity of the active volume (validity of algorithms and models in Geant4 limited at low energy; e.g. binary collision model rather should be replaced by a molecular dynamics code)
Algorithmic basics for Lindhard approximation

• Contribution of a given recoil type to NIEL:

\[
NIEL(E) = \frac{N_A}{A} \int_{T_{\text{min}}}^{T_{\text{max}}} dT \ Q(T) \ \xi(T) \ \frac{d\sigma}{dT} \ E
\]

- **E**: Kinetic energy of impinging particle
- **T**: Kinetic energy of recoil or fragment
- **d\sigma/dT**: Differential partial cross section for recoil creation
- **Q(T)**: Fraction of T being lost by non-ionising processes (Lindhard partition)
- **\xi(T)**: Empirical efficiency function (optional)
- **N_A/A**: Number of atoms per gram

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Prediction of parameter degradation

**Input:**
- NIEL curves ($NIEL$ vs. particle energy)
- ground test data (experimental damage factors)

**Algorithm:**
- Extrapolation of ground test data over the required energy range using empirical power function scaling:
  
  \[
  \text{(parameter degradation)} \propto NIEL^x \quad (x=\text{adjust. exponent})
  \]
- *Alternative option:* Use a modified NIEL curve calculated by applying an efficiency function
- Fold particle spectra with the energy dependence of the damage factors

**Output:** Expected parameter degradation for a given mission radiation environment
Observation

- In many cases surprisingly good relationship between NIEL and device degradation (damage factor) of electronic components (e.g. max. power output of solar cells)

- For the same NIEL value, device degradation often is the same, independent of particle type and energy.
GEANT4 presently contains only algorithms for multiple Coulomb scattering without recoil generation.

To obtain the energy of the Coulomb recoils and to follow up single displacement events within the damage cascade, binary elastic Coulomb scattering had to be included in ST.

We decided to implement an algorithm developed at Vanderbilt University (by courtesy of the authors)

* Advantage: Already successfully validated

NIEL due to elastic Coulomb scattering of $p$, $\alpha$ and Si in silicon

![Graph showing NIEL vs. Ion Energy]

Dependence on projectile properties as expected.

Symbols:
- Relativistic effects for $E_p > 100$ MeV
- Curves: Non-relativistic analytical method

Validating Module NIEL (1)

Proton NIEL for Silicon
(Lindhard-Approximation, $E_d = 21$ eV)

Energy, MeV

NIEL, MeV cm$^2$/g

Hadronic-elastic
Hadronic-nonelastic
Coulombic
Total

Validation Module NIEL (1)

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ST separately yields contributions of different types of interactions and recoils
Validating Module NIEL (2)

Hadronic elastic NIEL for p in silicon

Hadronic-elastic Proton NIEL for Silicon
(This work: Lindhard-Approximation, $E_d = 21$ eV)

Using Geant4 (this work)
Using MCNPX [Jun03]

Somewhat unexpected curve shape at low E. Underlying G4 process (G4LELastic) presently being revised (cf. bug reports #534 & #601). Lit. reference*)

Validating Module NIEL (3)

Hadronic non-elastic NIEL for p in silicon

Data & curve shape largely correspond to reference *).

Coulomb and Total Proton NIEL for Silicon

(Lindhard-Approximation, $E_d = 21$ eV)

NIEL due to screened Coulomb elastic scattering of $p$ in silicon

Coulomb and Total Proton NIEL for Silicon

(Lindhard-Approximation, $E_d = 21$ eV)

Total NIEL for p in GaAs – Hadronic and Coulomb contribution

Proton NIEL for GaAs
(Lindhard-Approximation, $E_d = 10$ eV)

Using Module NIEL (1)
Using Module NIEL (2)

NIEL for p in GaAs – Hadronic contribution and total NIEL

Proton NIEL for GaAs
(Lindhard-Approximation, $E_d = 10$ eV)

Essentially in agreement with Lit. data. Hadronic contribution too high compared to Jun et al. Lit. reference*)

Proton NIEL for InP

(Lindhard-Approximation)

Total NIEL for p in InP – Hadronic and Coulomb contribution

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ST under SPENVIS (1)

**SPENVIS**
- Orbit generator
- Radiation environment
- S/C shielding + MULASSIS

*Mission particle spectra on device level*

**Ground Test Irrad.**
- Irradiate device with one particle type and energy

*Parameter degradation for one particle type & energy*

**Simulation Tool**
- NIEL calculation for each particle type
- NIEL scaling of parameter degradation

*Prediction of mission parameter degradation*

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How to integrate ST under SPENVIS? – Some issues

- The Simulation Tool (ST) and SPENVIS already worked successfully together by off-line data exchange
- Complete integration of ST under SPENVIS would be difficult
- Part of the ST functionality already exists in SPENVIS (e.g. damage prediction using pre-calculated NIEL curves)
- It would be feasible to
  - integrate only those algorithms of ST that are missing in SPENVIS
  - extend existing modules in SPENVIS (MULASSIS) to enable NIEL calculation in 1D geometry
  - extend modules that are planned to be integrated (e.g. GRAS) to enable NIEL calculation in 3D geometry

Presently, a requirements document is worked out to integrate ST algorithms under SPENVIS
Summary

- ST runs much more reliable with GEANT4 version 7.1 than with version 5.x (e.g. no longer problems with nucleus de-excitation; see bug report #540)
- Validity of hadron elastic scattering process in G4 still doubtful (routine G4LELastic)
- Choice and applicability of ionisation processes for hadrons at very low energies poorly documented in G4 (options Standard/Low-Energy)
- Binary elastic Coulomb scattering code (needed for ST) still missing in G4 → Implementation of the Vanderbilt code in ST (turned out to be useful in ST and should be considered for G4)
- The Simulation Tool yields NIEL data for various projectiles and arbitrary targets in good agreement with literature data (as far as available)