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GEANT4 MicroElec module
2021 update

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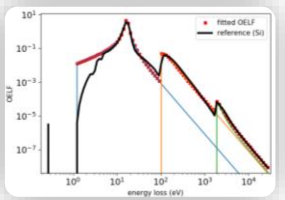
GEANT4 MicroElec module : current state 1/3

Cross section calculation based on the dielectric function formalism (OELF)

$$\boldsymbol{OELF}(\boldsymbol{\omega},\vec{\boldsymbol{0}}) = Im\left[-\frac{1}{\varepsilon(\omega,\vec{0})}\right] = \frac{2nk}{(n^2+k^2)^2}$$

$$]Im\left[-\frac{1}{\varepsilon(\omega,\vec{0})}\right] = \sum_j F(\omega)A_j Im\left[-\frac{1}{\varepsilon_M(\omega,\vec{0},E_j,\gamma_j)}\right]$$

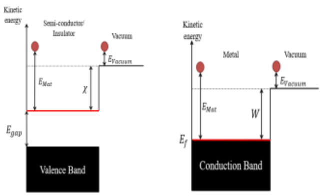
$$\frac{d\sigma}{d(\hbar\omega)}(E,\hbar\omega) = \frac{Z_{eff}^2}{\pi N a_0 E'}\int_{q-}^{q+}\sum_j F(\omega)A_j\, Im\left[-\frac{1}{\varepsilon(\omega,q)}\right]\frac{dq}{q}$$

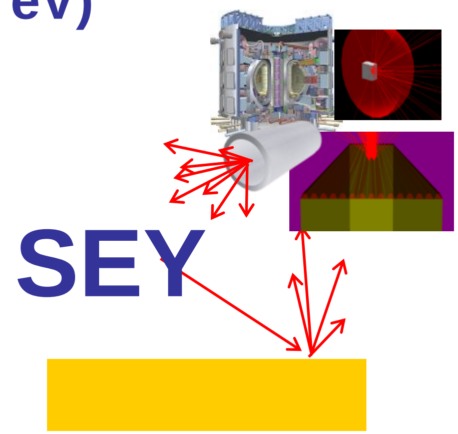


[~eV, ~keV] electrons typically Workfunction (~5 eV)
~100 eV/amu protons & ions

G4MicroElecSurface : $T(\theta,E) = 1 - \frac{\sinh^2(\pi a(k_i - k_f))}{\sinh^2(\pi a(k_i + k_f))}$

material-material interfaces
(discrete process)





Model have been extended to 16 materials, 11 are available in the june release

- **Be, C, Al, Si, Ti, Fe, Ni, Cu, Ge, Ag, W, Au**
- **SiO_2, Kapton ($C_{22}H_{10}N_2O_5$), Al_2O_3, BN**

- **In the future :**
- **GaAs, CuO, Cu2O, TiO2, TiN, MgO**

GEANT4 MicroElec module : current state 2/3

Elastic e-/e- interaction database for 92 elements

ELSEPA partial wave solution of Shrödinger equation

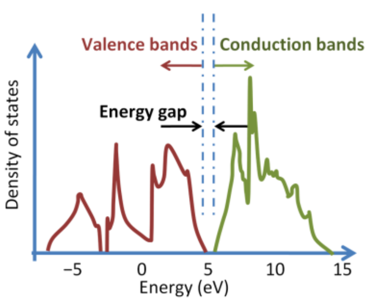
Large gap materials (Insulators) : Work function < GAP

Transport must be performed down to few eV where the dynamic is driven by elastic scattering.

Phonons have to be and are taken into account in microelec

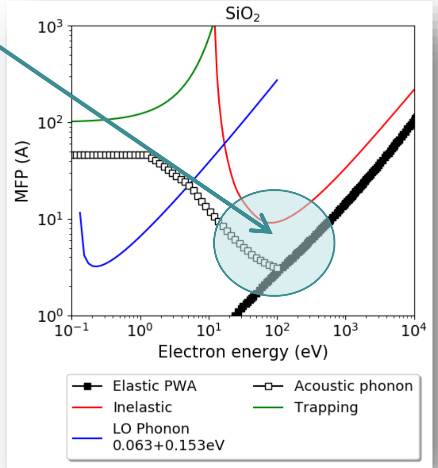
- Optical and accoustic phonons

Below typically some tens of eV ELSEPA cross sections are replaced case by case as a function of the materials

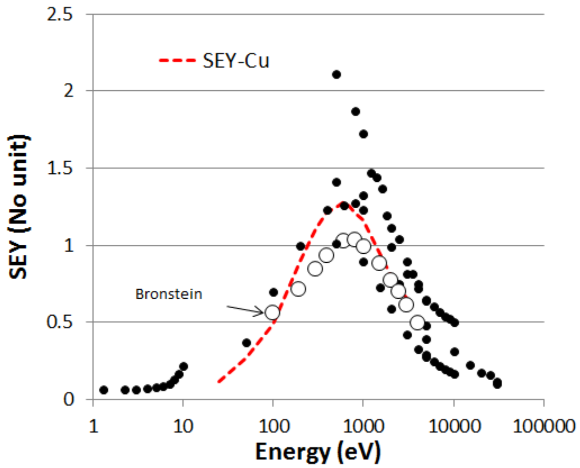


The density of state is taken into account by means of an average energy <E> of the electrons in the valence band. This parameter serves as an adjusting parameter to optimize SEY

Gap + <E> = 2,85 eV for Si (3,6 eV)



GEANT4 MicroElec module : current state 3/3



Both Secondary Electron Emission Yield And Backscattering Emission Yield are Faithfully Reproduced

This work have been published in 6 papers

"Monte-Carlo simulation and analytical expressions for the extrapolated range and transmission rate of low energy electrons [10 eV - 10 keV] in 11 monoatomic materials" Q. Gibaru, C. Inguimbert, M. Belhaj, M. Raine, D. Lambert
Applied Surface Science 2021

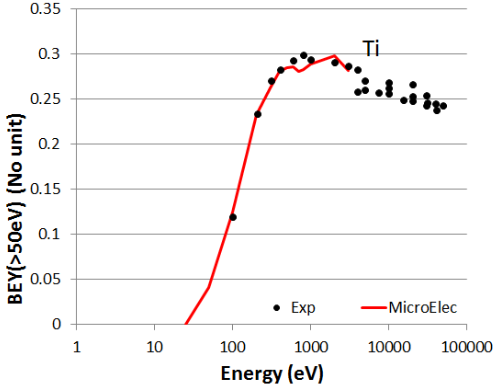
"Role of Electron-induced Coulomb Interactions to the Total SEU Rate during Earth and JUICE Missions" P. Caron, C. Inguimbert, L. Artola, N. Balcon, R. Ecoffet
IEEE Trans. Nucl. Sci. 68, no. 8, (2021), 1607–1612.

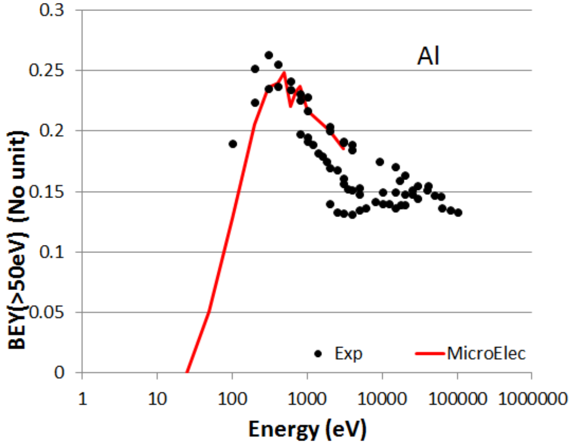
"Geant4 physics processes for microdosimetry and secondary electron emission simulation: Extension of MicroElec to very low energies and 11 materials (C, Al, Si, Ti, Ni, Cu, Ge, Ag, W, Kapton and SiO2)"
Q. Gibaru, C. Inguimbert , M. Belhaj, J. Puech, M. Raine **Nucl. Instr. And Methods 487, (2021), 66-77.**

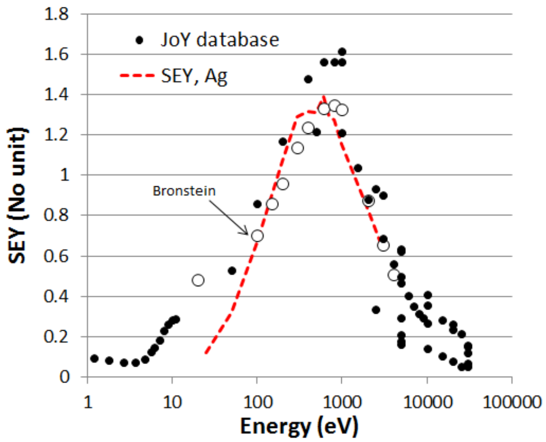
Surface ionizing dose for space application estimated with low energy spectra going down to some hundreds of eV"
C. Inguimbert, P. Caron, Q.Gibaru, A. Sicard, N. Balcon, R. Ecoffet **IEEE Trans. Nucl. Sci. 68, no. 8, (2021), 1754–1763.**

"New SEU modeling method for calibrating target system to multiple radiation particles" P. Caron, C. Inguimbert, L. Artola, F. Bezerra, R. Ecoffet
IEEE Trans. Nucl. Sci. 67, no. 1, (2020) 1558–1578.

"Physical Mechanisms of Proton-Induced Single-Event Upset in Integrated Memory Devices" P. Caron ; C. Inguimbert ; L. Artola ; R. Ecoffet ; F. Bezerra
IEEE Trans. Nucl. Sci. 66, no. 7, (2019),1404–1409.







GEANT4 MicroElec correction of bugs

- **SAMPLING ERROR in the Integrated cross sections**
  occuring when the random number is lower than sampling precision : Aborting interaction

  -> FIXED by adding the exception :

  if (isnan(secondaryElectronKineticEnergy)) secondaryElectronKineticEnergy = PrimaryEnergy - currentMaterialStructure->GetLimitEnergy(shell);

- **SAMPLING ERROR for electrons of the valence band.**
  When E = T - (Egap+Initial energy in the band) if T can be sampled down to the gap energy which provide : E< 0 values

  -> FIXED by adding an exception : if T < Egap+Initial energy in the band E is chosen equal to **E = T - Egap assuming the electron coming from the Fermi level**

- **ENERGY PARTITION in the CAPTURE PROCESS**
  when particle come at rest :

  -> FIXED G4ElectronCapture has been derivated for the G4dielectricModel The residual energy of the particle was formerly proposed as ionizing energy. The partitioning between Ionizing and Non ionizing is performed now for both electrons protons and heavy ions.

  - **Protons and heavy ions use the Lindhard energy partition function.**
  - **Electrons :**

    in metals the Non ionizing deposited energy is chosen equal to zero

    in large gap materials the following partition is made:

```
int c = (int)((aTrack.GetKineticEnergy()) / (Egap+Initial energy);
pParticleChange>ProposeNonIonizingEnergyDeposit(aTrack.GetKineticEnergy() - (Initial energy)*c);
```

- **Segmentation fault in the G4MicroElecInelasticModel destructor related to the use of maps (Geant4-11.00.b01)**
  fixed

  But this bug could be related to important memory consumption (Under analysis)

GEANT4 MicroElec examples

- **Jun. 2021 G4 10.11 release**
  - The 11 elements have been added to G4EMLOW7.13
  - New model files (quoted « NEW ») available in G4source (Beta version)
- **Dec. 2021 release**
  - Analysing possible excessive memory consumption (Under analysis)
  - Improvement of the existing microelec example

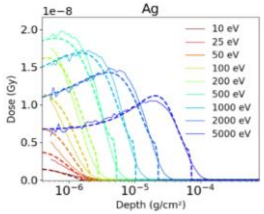
    (in order to show the use of the 11 elements of the new material list)

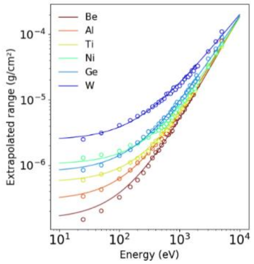
In the future :

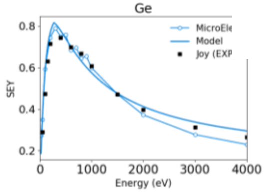
- **Extending the material database (GaAs, CuO, Cu2O, TiO2, TiN, MgO, …)**

- **Providing new examples**

  - **Calculation of the dose depth profile for low energy electrons and protons**
  - **Calculation practical range of low energy electrons**
  - **Calculation of Secondary Electron Emission Yield for the different materials of the list**







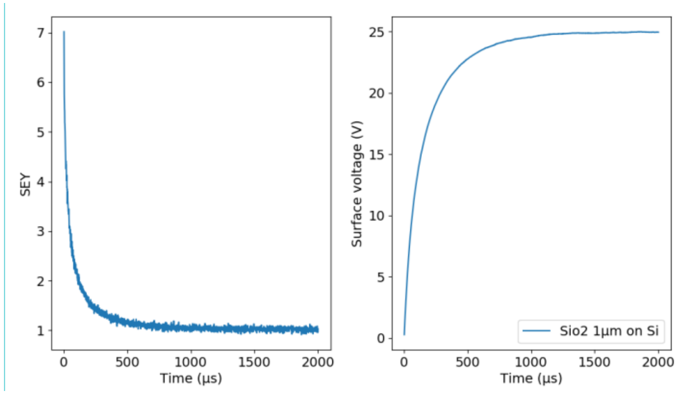
Publications are currently under writing and/or in a submission process. The examples will be released when this work will be published.

Future developments (PHD Q. Gibaru)

Transport of Electrons in dielectric materials strongly depends on the charging equilibrium state.

- Holes and electrons can move under the effect of the electric field that is built up during irradiation

- Drift diffusion process occurs for both electrons and holes
- Trapping and detrapping effects (Tunneling and Phonon Assisted Tunneling, Poole Frenkel)
- Recombination of electrons and thermalized electrons with holes



- 1D Poisson solver
- New particles : DriftElectrons, DriftHoles
  (derivated from G4Electrons)
- G4Electrons are tracked down to ~1eV, become drift electrons and start the new diffusion process
- The Drift diffusion process handled by means of **DriftManager**
  - The native G4 Electric field,
  - Iterative process following the charge build up in the volume
- A single level of energy for trapps