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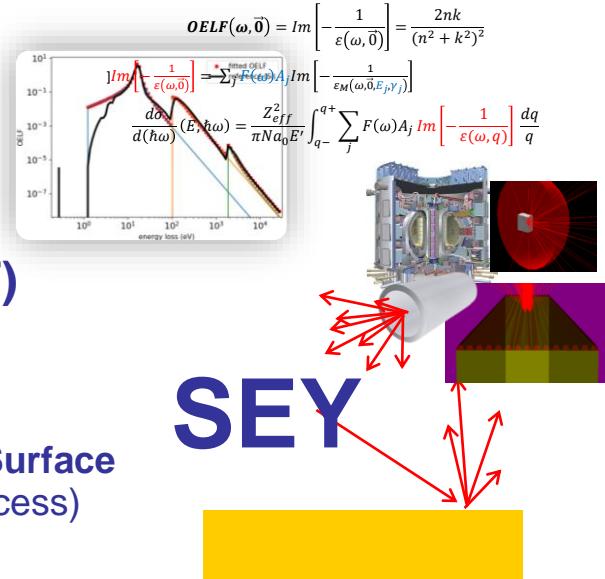


# GEANT4 MicroElec module 2022 update

C.Inguimbert, Q.Gibaru, D. Lambert, M. Raine, P. Caron

# GEANT4 MicroElec module : overview

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



Cross section deduced from dielectric function (OELF)

Quantum reflection at material-material interfaces (discrete process)

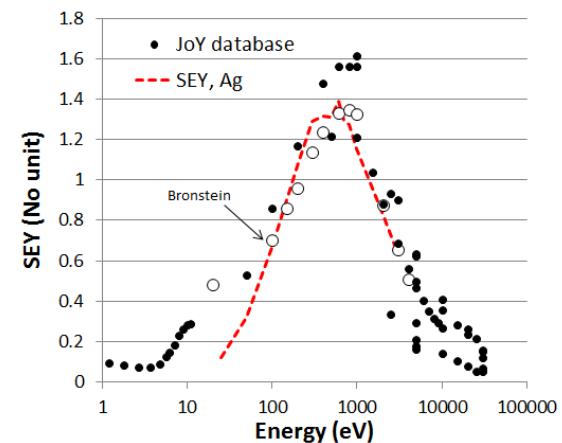
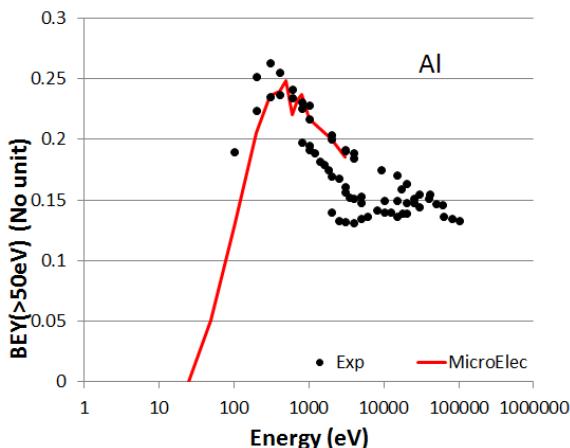
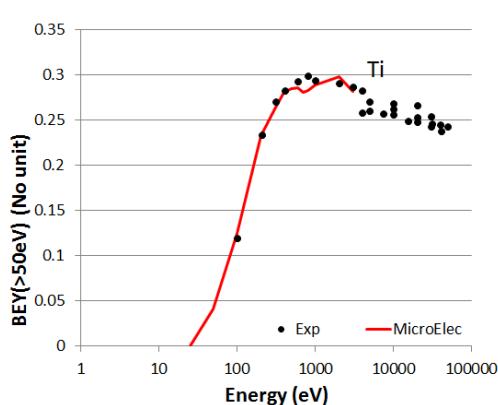
G4MicroElecSurface  
For dielectrics phonon (acoustic & optical) interaction models are implemented  
(SiO<sub>2</sub>)

Electron trapping in insulators handled by mean of a Capture process

Model extended to 17 materials, 11 are available in the june 2022 release

- Be, C, Al, Si, Ti, Fe, Ni, Cu, Ge, Ag, W, Au
- SiO<sub>2</sub>, Kapton (C<sub>22</sub>H<sub>10</sub>N<sub>2</sub>O<sub>5</sub>), Al<sub>2</sub>O<sub>3</sub>, BN, TiN

# GEANT4 MicroElec module : validation using Secondary Electron emission measurements



"Use of combined linear and nonlinear formalisms applied to the transport of protons and secondary electrons in a Monte-Carlo code: applications for space missions"

P. Caron, C. Inguimbert, Q. Gibaru, M. Pinson

JAP 2022 accepted

"Modelling the impact on the secondary electron yield of carbon layers of various thicknesses on copper substrate"

C. Inguimbert, Q. Gibaru, P. Caron, M. Angelucci, L. Spalino, R. Cimino

NIMB, Volume 526, 1 September 2022, Pages 1-8

"Surface ionizing dose deposited by low energy electrons (10eV-10keV) in eleven monoatomic materials: Monte Carlo calculations and analytical expression"

Q. Gibaru, C. Inguimbert, P. Caron, M. Belhaj, M. Raine, D. Lambert

Applied Surface Science, 576, Part A, (2022) 151813

"Monte-Carlo simulation and analytical expressions for the extrapolated range and transmission rate of low energy electrons [10 eV - 10 keV] in 11 materials"

Q. Gibaru, C. Inguimbert, M. Belhaj, M. Raine, D. Lambert

Applied Surface Science 570, (2022), 151154

"Surface Ionizing Dose for Space Applications Estimated With Low Energy Spectra Going Down to Hundreds of Electronvolt"

C. Inguimbert, P. Caron, Q. Gibaru, A. Sicard, N. Balcon, et R. Ecoffet

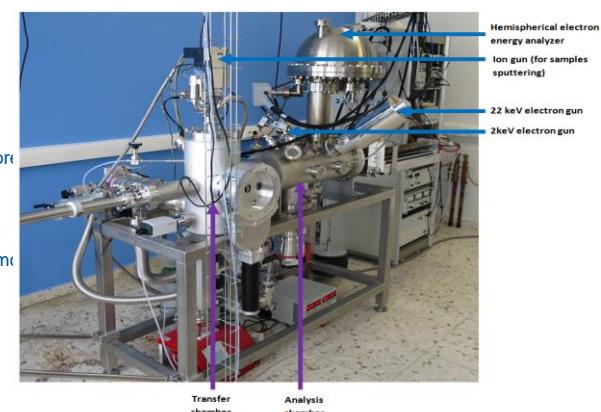
IEEE Transactions on Nuclear Science, vol. 68, no 8, p. 1754 1763, aug. 2021

"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 SiO<sub>2</sub>)

Q. Gibaru, C. Inguimbert, P. Caron, M. Raine, D. Lambert, et J. Puech

NIM B, vol. 487, p. 66 77, jan. 2021



# GEANT4 MicroElec changes and bugs correction

# Weakly bound electrons treatment simplification

Weakly bound electrons handled now similarly to core electrons

limitEnergy  $\Leftrightarrow$  binding energy

```
G4double G4MicroElecMaterialStructure::GetLimitEnergy(G4int level)
{
    G4double E = LimitEnergy[level];
    //correction CI 07/02/2022 the following line is commented following one is ok
    if (IsShellWeaklyBound(level)) { E = energyGap+ initialEnergy; } ←
    // correction CI 09/03/2022 : the following line is commented previous one is ok
    //if (IsShellWeaklyBound(level)) { E = energyGap; }
    return E;
}
```

InitialEnergy is a mean energy level of the electrons in the band

The minimal transferable energy is the gap + the mean energy level in the band

Changes have been brought to

**G4MicroElecInelasticModelNew** class

In the functions

```
void G4MicroElecInelasticModel_new::SampleSecondaries(...)
G4double RandomizeEjectedElectronEnergyFromCumulatedDcs(...)
```

It has also required to modify

**G4MicroElecMaterialStructure**

# Other bugs found and fixed

**correction of the shell enumerator values in the structure file (eadl vs. G4 nomenclature)**

# 4 EADL noUnit -1 -1 3 1 corresponding G4shell defined below  
4 EADL noUnit -1 -1 1 0

# G4MicroElecCapture improvement

The NON IONIZING DEPOSITED ENERGY is accounted for by means of Lindhard energy partition

```
if ((IncPartName == "Generacion") || (IncPartName == "alpha") || (IncPartName == "He3") ||  
(IncPartName == "deuteron") || (IncPartName == "triton") || (IncPartName == "proton")) {  
    pParticleChange->ProposeNonIonizingEnergyDeposit(NIEdep);  
    pParticleChange->ProposeLocalEnergyDeposit(aTrack.GetKineticEnergy());  
}
```

G4VParticleChange\* G4MicroElecCapture::PostStepDoIt(const G4Track& aTrack,  
const G4Step&)

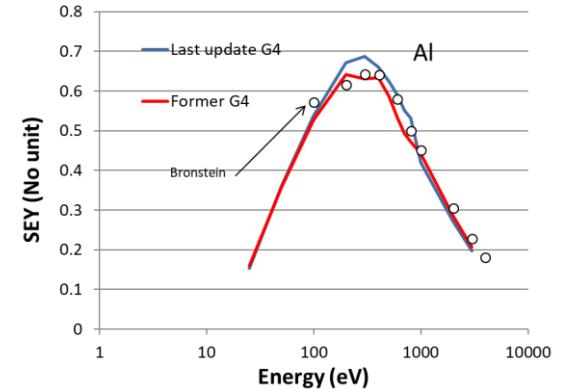
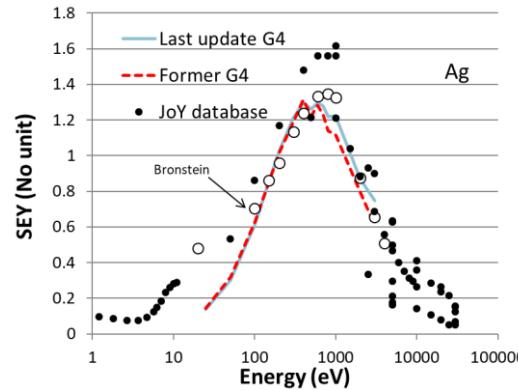
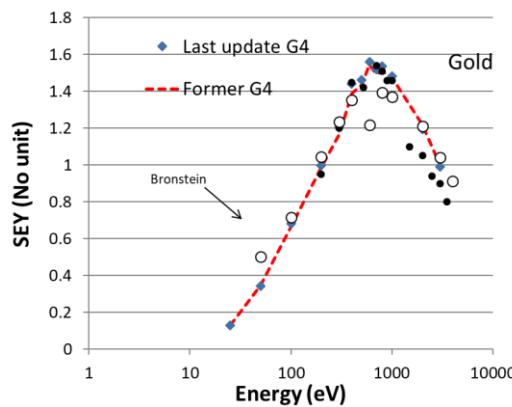
# Crosssection database for incident electrons

Database recalculated for the full list of materials

Be, C, Al, Si, Ti, Fe, Ni, Cu, Ge, Ag, Au, W  
Kapton, SiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, TiN, BN

Erroneous data below the low limit energy have been removed  
File size devided in average by a factor ~ 5

REGRESSION TESTS for the full list of materials (SEY metric)



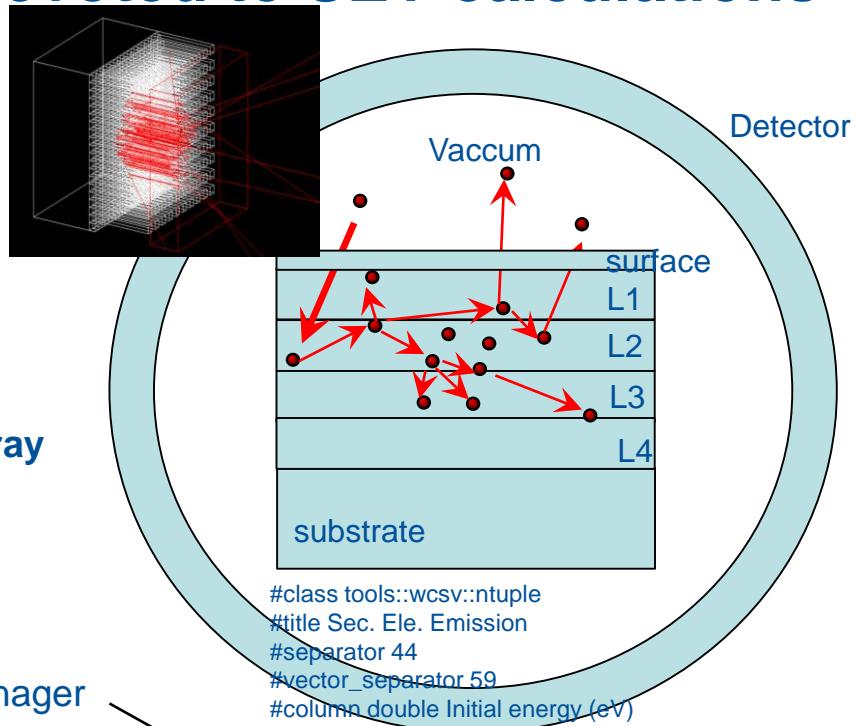
# GEANT4 MicroElec examples devoted to SEY calculations

microelectronics-SEYv5-G4v11

## Geometry

### - stack of 6 layers

user defined thicknesses and materials via messenger  
and macro commands,  
lateral dimensions = default square = user defined length



### - Spherical detector with an automatically adapted ray

4 counters : primaries  
secondaries  
electrons with  $E > 50$  eV  
total

Output data : CSV file generated with G4VAnalysisManager

### - Database for 17 materials

**Be, C, Al, Si, Ti, Fe, Ni, Cu, Ge, Ag, Au, W  
Kapton, SiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, TiN, BN**

### - Compiled with GEANT4 v11

### - Multi threading mode

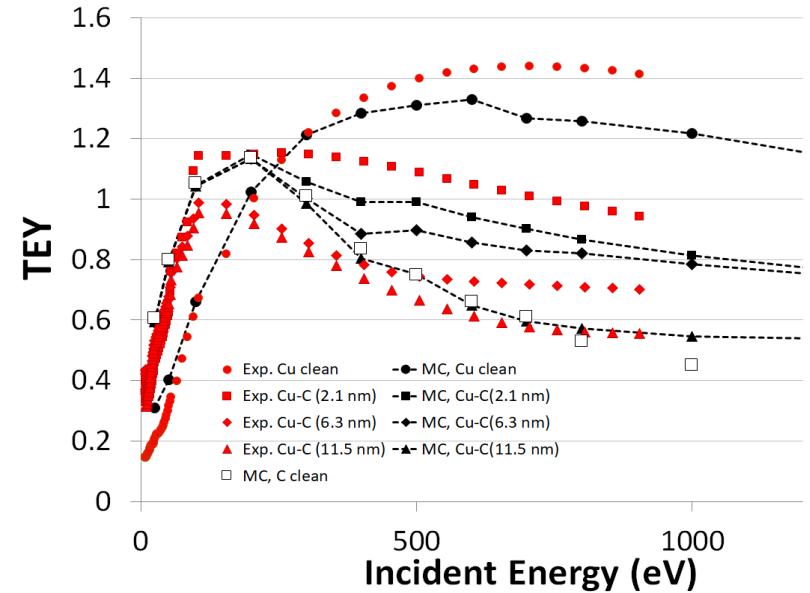
# microelectronics-SEYv5-G4v11 : macro command file

```
#Substrat (Green)
#/testem/det/setMat G4_Be
#/testem/det/setMat G4_C
#/testem/det/setMat G4_Al
#/testem/det/setMat G4_Si
#/testem/det/setMat G4_Ti
#/testem/det/setMat G4_Fe
#/testem/det/setMat G4_Ni
#/testem/det/setMat G4_Ge
#/testem/det/setMat G4_Ag
#/testem/det/setMat G4_Au
#/testem/det/setMat G4_W
#/testem/det/setMat G4_KAPTON
#/testem/det/setMat G4_SILICON_DIOXIDE
#/testem/det/setMat G4_ALUMINUM_OXIDE
#/testem/det/setMat G4_BORON_NITRIDE
#/testem/det/setMat G4_TITANIUM_NITRIDE
/testem/det/setMat G4_Cu
/testem/det/setSize 500 nm
/testem/det/setWidth 500 nm

#Layer4 (Red)
/testem/det/setMatLayer4 G4_Cu
testem/det/setSizeLayer4 4 nm
#Layer3 (Red)
/testem/det/setMatLayer3 G4_Cu
/testem/det/setSizeLayer3 4 nm
#Layer2 (Red)
/testem/det/setMatLayer2 G4_Cu
testem/det/setSizeLayer2 2 nm
#Layer1 (Red)
/testem/det/setMatLayer1 G4_Cu
/testem/det/setSizeLayer1 5 nm
#Surface (Red)
/testem/det/setMatSurf G4_Al
/testem/det/setSizeLayer1 5 nm

/testem/det/update
```

```
#-----
# General particle source GPS
#-----
/gps/pos/type Plane
/gps/pos/shape Square
/gps/pos/halfx 0.00 mm
/gps/pos/halfy 0.00 mm
/gps/pos/centre 0.000 0 -50.0 nm
/gps/ang/type cos
/gps/ang/mintheta 0.000 deg
/gps/ang/maxtheta 0.000 deg
/gps/ang/minphi 0.000 deg
/gps/ang/maxphi 0.000 deg
/gps/pos/rot1 0 1 0
/gps/pos/rot2 1 0 0
/gps/particle e-
/run/numberOfThreads 2 #
/run/printProgress 100
/run/initialize
#-----
Energy loop
#-----
/control/loop loop_ekin.mac Ekin 25 50 25
/control/loop loop_ekin.mac Ekin 100 800 100
/control/loop loop_ekin.mac Ekin 1000 3000 1000
```



"Modelling the impact on the secondary electron yield of carbon layers of various thicknesses on copper substrate"  
C. Inguimbert, Q. Gibaru, P. Caron,  
M. Angelucci, L. Spalino, R. Cimino  
**NIMB**, Volume 526, 1 September  
2022, Pages 1-8

↓  
**/gps/ene/mono {Ekin} eV**  
**/run/beamOn 3000**

# In the future :

- Extending the material database (GaAs, GaN, CuO, Cu<sub>2</sub>O, TiO<sub>2</sub>, MgO, ...)
- Providing new examples
  - Calculation of the dose depth profile for low energy electrons and protons
- Below the energy needed to excite a plasmon (~ some tens of eV)  
**BINARY collisions**  
becomes the main interaction process. A binary collision model has been implemented in order to replace interaction cross sections for incident protons.

“Use of combined linear and nonlinear formalisms applied to the transport of protons and secondary electrons in a Monte-Carlo code: applications for space missions”  
P. Caron, C. Inguimbert, Q. Gibaru, M. Pinson  
**JAP 2022** accepted
- Cross sections must be recalculated for heavy particles protons and ions following **BINARY approach** (+ regression test)

# Future developments (PHD Q. Gibaru)

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

- Incident electron transport is impacted by the charge build up during irradiation recombination with holes

- DriftManager

- Drift diffusion process occurs for both electrons and holes
- Trapping and detrapping effects

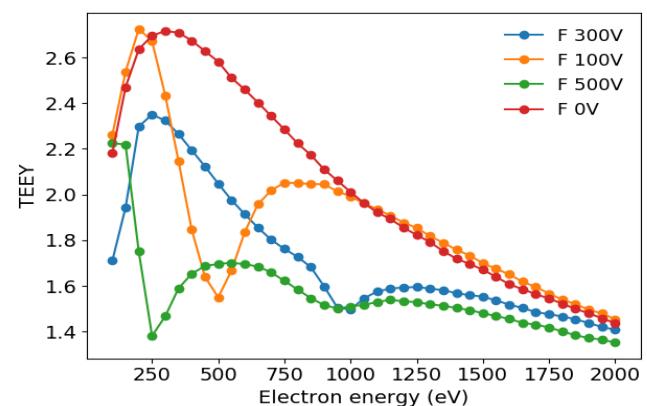
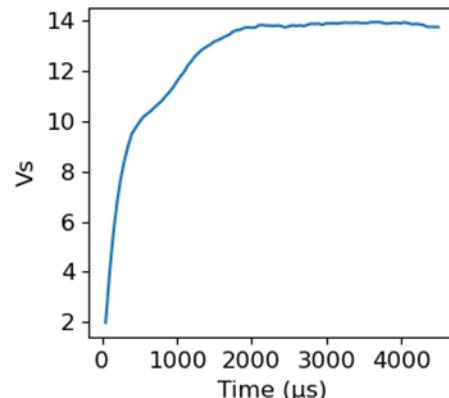
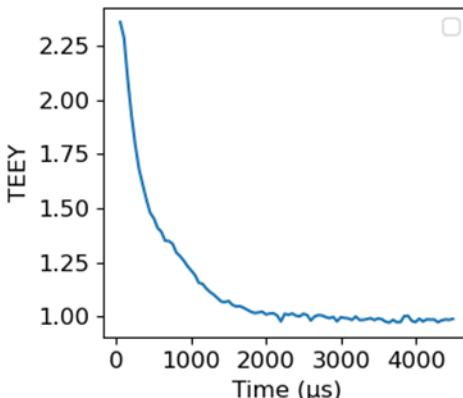
- Recombination

- Tunneling and Phonon Assisted Tunneling, Poole Frenkel

- Recombination

- 1D Poisson solver

- DriftElectrons, DriftHole (derived from G4Electrons)



Article submitted to  
J. Of Elec. Spectroscopy