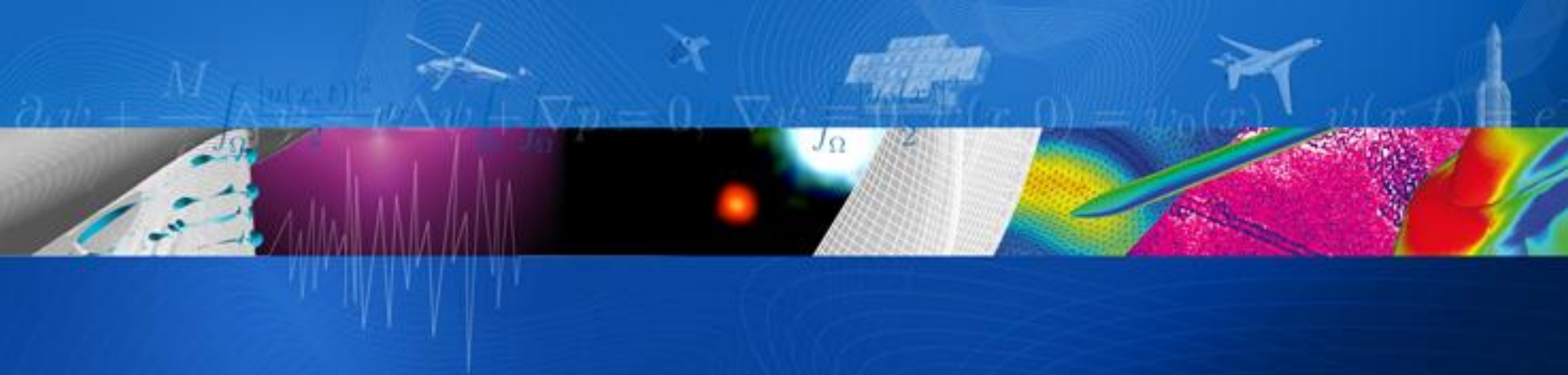


ONERA

THE FRENCH AEROSPACE LAB

retour sur innovation

www.onera.fr

GEANT4 MicroElec module
2020 update

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

C. Inguimbert
P. Caron
Q. Gibaru

ONERA THE FRENCH AEROSPACE LAB

GEANT4 A SIMULATION TOOLKIT

cea

Q. Gibaru
M. Raine
D. Lambert

ONERA- DPHY, Toulouse center, France.

CEA-DAM DIF - 91297 ARPAJON, France

retour sur innovation

GEANT4 MicroElec module : current state

MICROELEC :

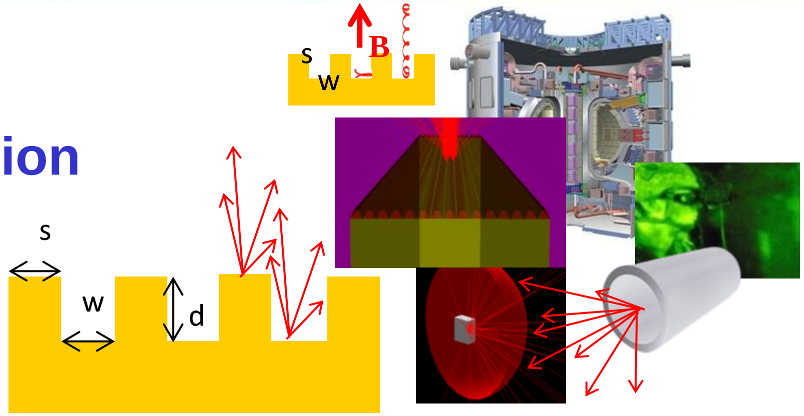
- Low energy transport module
- [~eV, ~keV] electrons
- > ~50 keV/amu protons & ions
- Based on complex dielectric function (OELF),
- Extended Drude model
- Silicon material
- low energy limit : 16 eV

NEEDs :

- Extending to other materials
- Extending to other applications (≠ microelectronics)
- Improving the reliability specially for protons & ions

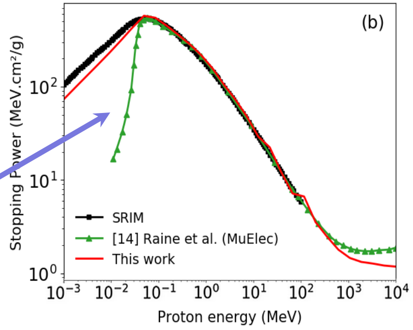
GEANT4 MicroElec : GOALs & main issues

Ex : modelling the
Secondary Electron Emission
is necessary for many
applications



Scientific problem :

- **Modelling material/material interfaces (Workfunction solid/vacuum)**
- **Dielectric materials**
    - large gap,
    - importance of phonons,
    - trapping effect,
    - electric field,
- **Stopping power for protons not good at low energy with the Drude model**



New developments (1)

- Mermin complex dielectric function

$$\epsilon_M(k,\omega;E_p,\gamma) = 1 + \frac{\left(1+\frac{i\gamma}{\hbar\omega}\right)\left(\epsilon_L(k,\omega+i\gamma)-1\right)}{1+\frac{\left(\frac{i\gamma}{\hbar\omega}\right)\left(\epsilon_L(k,\omega+i\gamma)-1\right)}{\epsilon_L(k,0)-1}}$$

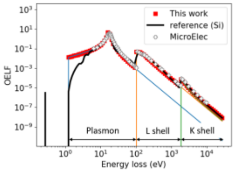
- Dependence on the wave vector

$$\epsilon_L(k,\omega;E_p) = 1 + \frac{\chi^2}{z^2}\left(f_1(u,z)+if_2(u,z)\right)$$

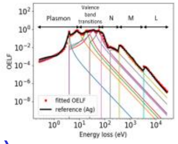
$$z = k/2k_F$$

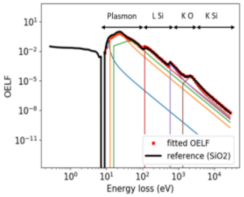
- Dispersion relation of the Drude model REMOVED

- Principle remains the same

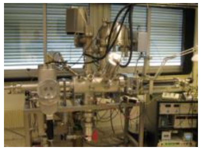


- Fit of OELF function according to the energy of the different shells
- Weakly bound electrons treated analogously to core electrons
  - *Plasmon Damping : systematic production of a secondary electron*
  - *introduction of a « mean » initial energy for electrons (valence & cond. bands)*
- Interband transition taken into account
- Decay : G4 Auger cascade
- Optimisation of the fitting procedure:



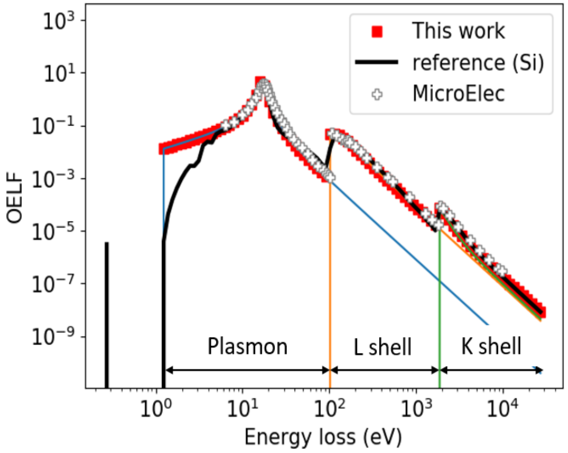


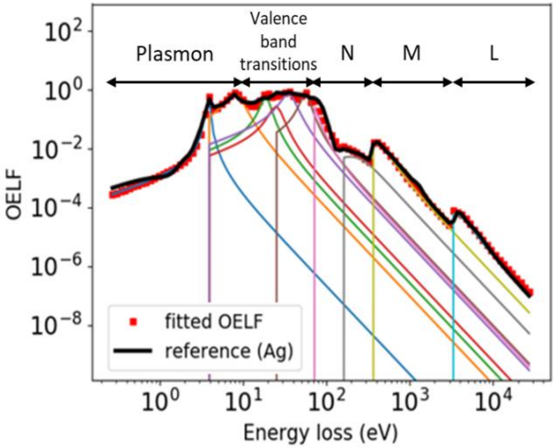
Trade off
Sum rules (mean ionizing potential + valence)
vs.
Secondary electron emission yield
experimental data
ONERA measurements)

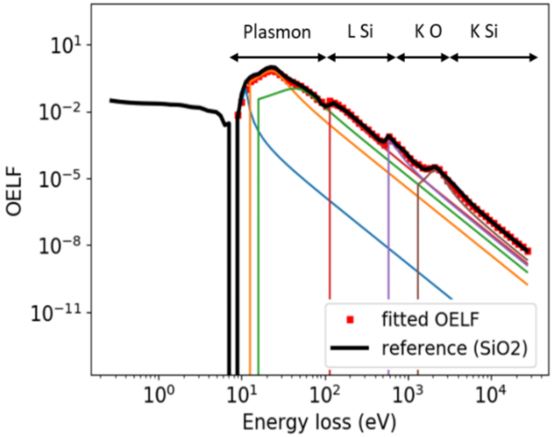


I.M. Bronshtein, B.S. Fraiman, VTORICHNAYA ELEKTRONNAYA EMISSIYA. (Secondary Electron Emission)., 1969, 1969.

New developments (2)







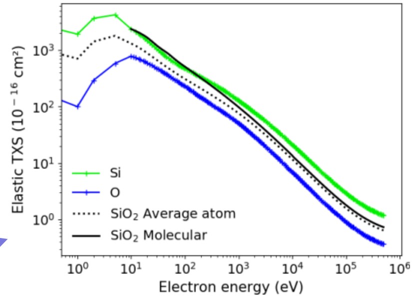
- **11 materials**

  C, Al, Si, Ti, Ni, Cu, Ge, Ag, W, Kapton and SiO_2

- **2 dielectrics**

  Kapton and SiO_2

- **Low energy limit extended to the work function ~5 eV**



- **ELECTRONS : Elastic cross sections re-calculated following PW formalism using ELSEPA** (1 eV to 500keV)

F. Salvat, A. Jablonski, C.J. Powell, ELSEPA—Dirac partial-wave calculation of elastic scattering of electrons and positrons by atoms, positive ions and molecules, Computer Physics Communications. 165 (2005) 157–190.

Material interface potential barrier

- Exponential potential barrier with an height W or χ and a transmission probability

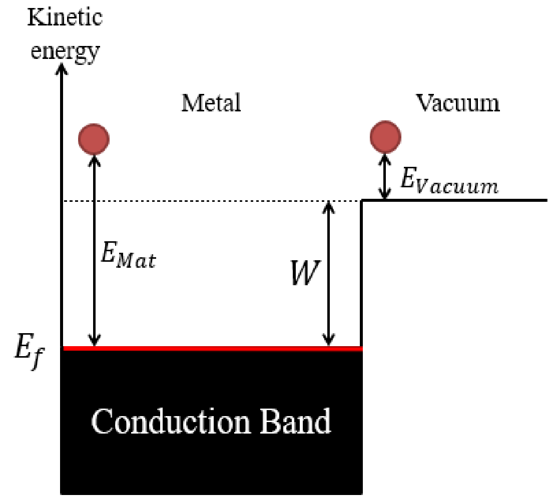
$$T(\theta,E) = 1 - \frac{\sinh^2\left(\pi a\left(k_i - k_f\right)\right)}{\sinh^2\left(\pi a\left(k_i + k_f\right)\right)}$$

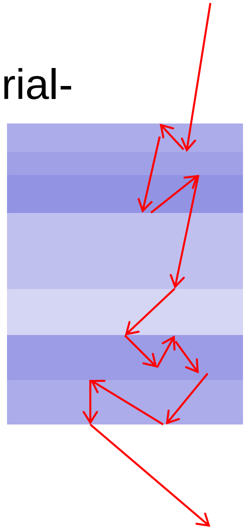
- Low energy electrons or high incidence angles may be reflected by the surface

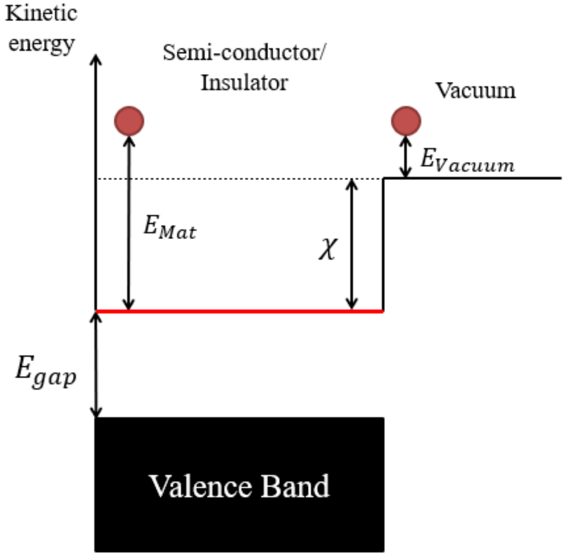
- Model usable for vacuum-material and material-material interfaces
    - Simulation of Multilayers

- Handled by the new discrete process

G4MicroElecSurface







Electron-phonon interactions in SiO2

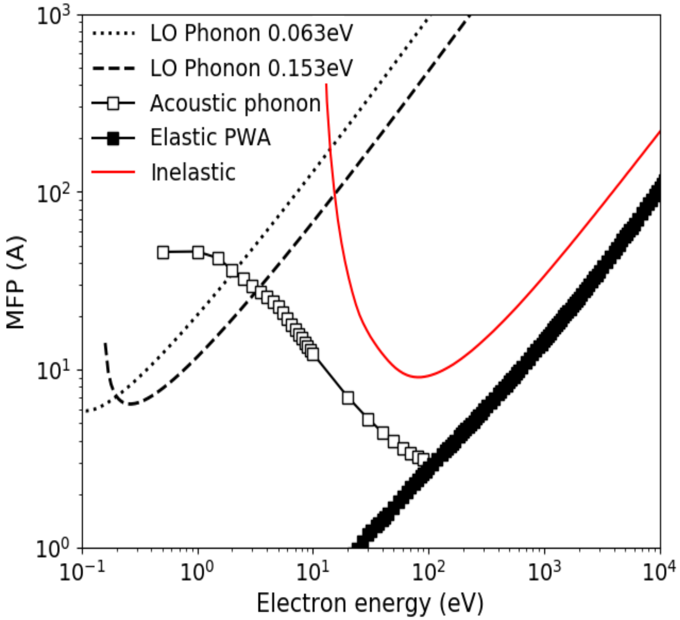
New discrete process: G4LOPhononModel

Optical phonons

- Fröhlich theory [1]
- Energy loss for incident electrons below the band gap (9eV)
- Monoenergetic loss of the phonon mode $\hbar\omega_{LO}$, 2 modes for SiO2: 63 and 153meV

Acoustic phonons

- Bradford screened model [2]
- Isotropic angular distribution
- Substitute to the partial wave cross sections below 100eV
- Transition between the 2 models handled in G4MicroElecElasticModel



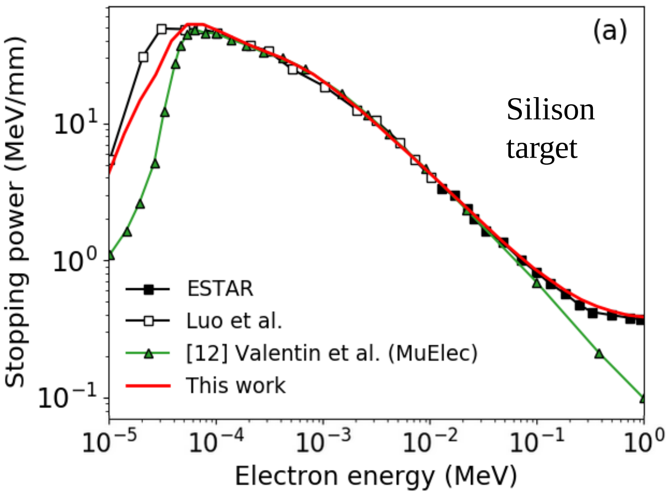
[1] J. Llacer, E.L. Garwin, Electron-Phonon Interaction in Alkali Halides. I. The Transport of Secondary Electrons with Energies between 0.25 and 7.5 eV, Journal of Applied Physics. 40 (1969) 2766–2775. https://doi.org/10.1063/1.1658075.

[2] J.N. Bradford, S. Woolf, Electron-acoustic phonon scattering in SiO2 determined from a pseudo-potential for energies of E≳Ebz, Journal of Applied Physics. 70 (1991) 490–492. https://doi.org/10.1063/1.350254.

Validations : Stopping powers

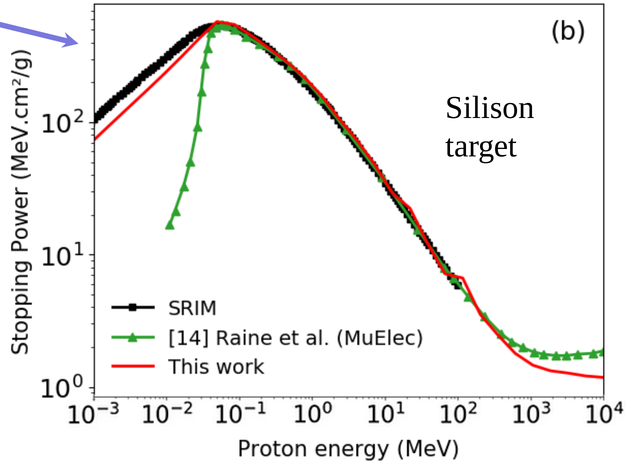
Improvement of the Mermin approach compared to former Drude treatment

Electrons



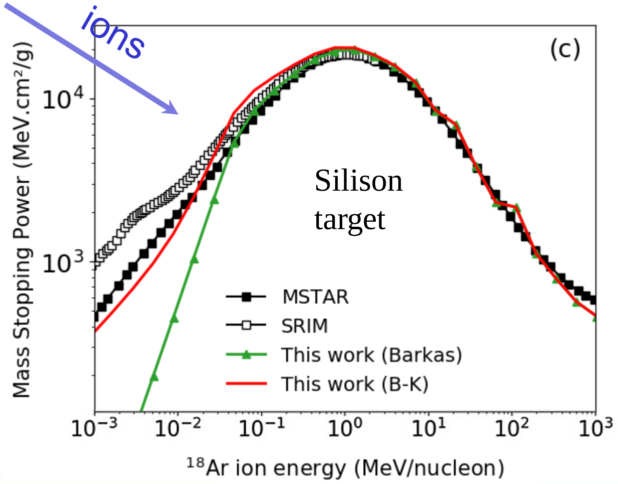
Good agreement with the stopping power of SRIM for both protons

Protons



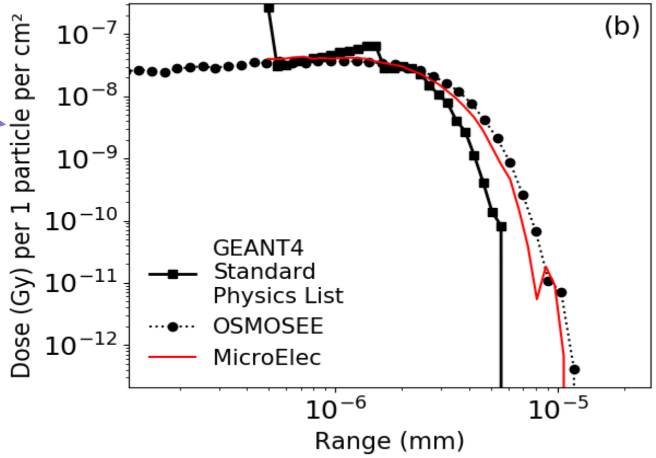
And heavy ions
improvement of the Kaneko approach

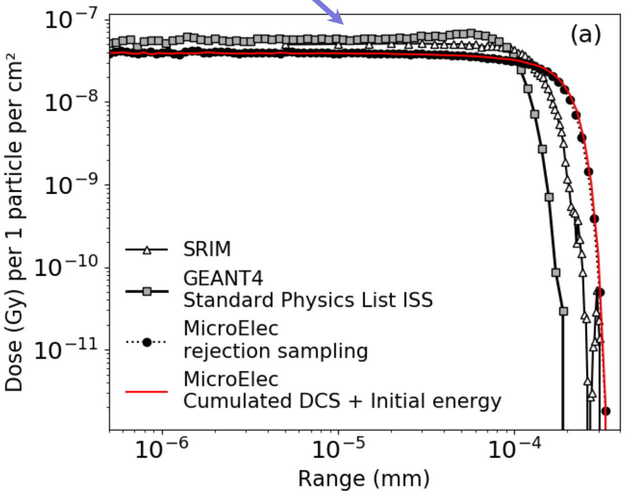
ions

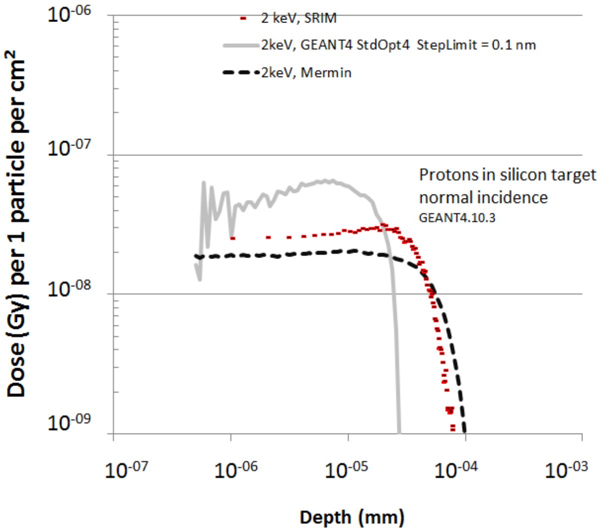


Validation : Silicon dose-depth profile

- ELECTRONS (200 eV): Good agreement between OSMOSEE* and µELEC
- PROTONS (2 keV) : 25 % difference with SRIM (formerly valid > 50keV)
- PROTONS (10 keV) : satisfying when compared to both SRIM & Std ISS physics







---

* J. Pierron, C. inguimbert, M. Belhaj, T. Gineste, J. Puech, Electron emission yield for low energy electrons: Monte Carlo simulation and experimental comparison for Al, Ag, and Si Electron emission yield for low energy electrons: Monte Carlo simulation and experimental comparison for, Journal of Applied Physics. 121 (2017) 215107. https://doi.org/10.1063/1.4984761.

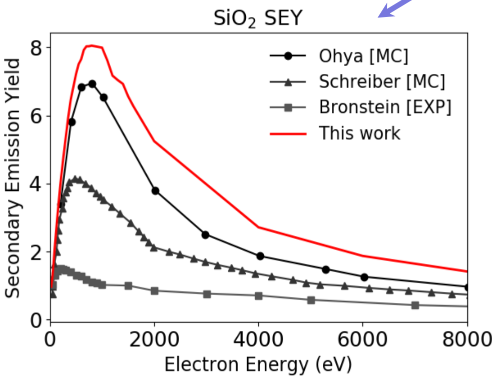
Electron emission yield calculations

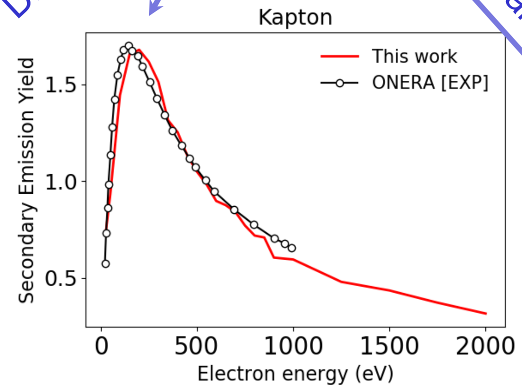
Good agreement with experimental data for most materials

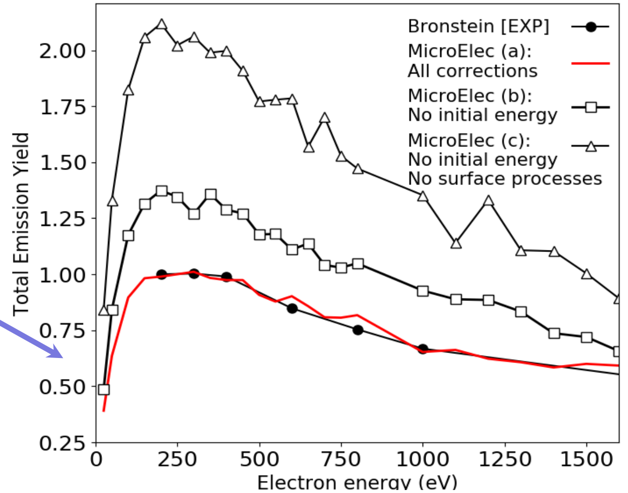
Dielectrics

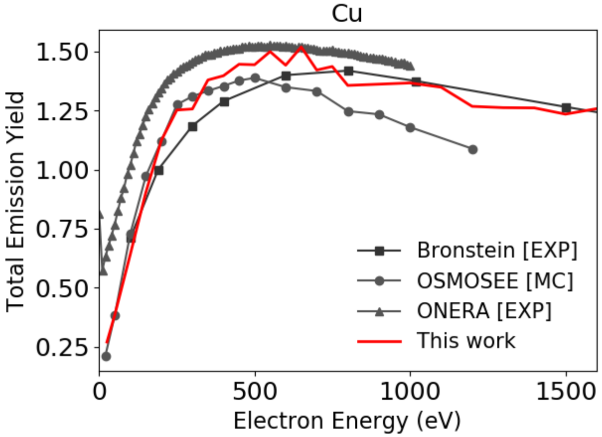
Silicon target

Metals : Cu









Very low energy production threshold for secondary electrons (4-5eV, 9eV for SiO_2 due to the band gap)

Difference for SiO_2 probably due to charging effect (electric field establishing)

Undergoing developments

- Trapping and charge effects to be added to get accurate SEY calculations for insulators

- Generalized Oscillator Strength (GOS) formalism to improve deep shells for certain materials for which Lorentzian fits of OELF fail.
- Improving cross sections for low energy ions

- Extending the list of materials :
  - Al_2O_3
  - BN,
  - Au
  - Etc…
- Publication submitted to Nucl. Instr. Method. This work will be available in G4 Dec 2020 release.