Geant4-DNA for solid state materials

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Extensions of G4-DNA to solid state materials

Previous work

- G4-DNA was first extended to gold by Sakata et al.
- Documented in
    - Sakata et al, Physica Medica, 63, pp. 98-104, 2019
    - Sakata et al, Medical Physics, 45 (5), pp. 2230-2242, 2018.
    - Sakata et al, Journal of Applied Physics, 120 (24), art. no. 244901, 2016.
    - Sakata et al, Physica Medica, 62, pp. 152-157, 2019

This is in addition to models for silicon (MuElec)

This Work

- Further extend G4-DNA to include other solid state materials
- Currently graphite and later gadolinium and platinum
- Activity within the Geant4-DNA effort

Uses of Carbon/Graphite

- Possible applicability to carbon multi-layer nanotubes with applications of
  - Radiation shielding
  - Transistors (single event upset studies which depend on accurate description of track structure)

Electron processes

- Elastic scattering: ELSEPA
- Plasmon excitation: Cross section from atomic state using Quinn model
- Ionisation and atomic de-excitation: Relativistic Binary Encounter Bethe Vriens
- Electronic excitation: ACE

C. Plasmon excitation

Plasmon excitation refers to the excitation of dynamic oscillations in the conduction electrons of a material. In gold, free electrons can lose energy by exciting volume plasmon excitations. Cross-sections and energy losses in volume plasmon excitation are given by Quinn.[36]

The cross section for volume plasmon excitation from the Quinn model can be calculated from the number of atoms per unit volume n and the mean free path λ via the equation

$$\sigma_{\mathrm{PE}} = \frac{1}{n\lambda} = \frac{1}{n}\frac{\hbar\omega_p}{2a_0E}\ln\left(\frac{\sqrt{p_0^2 + 2m_e\omega_p\hbar} - p_0}{p - \sqrt{\omega_p\hbar(p^2 - 2m_e)}}\right), \quad (1)$$

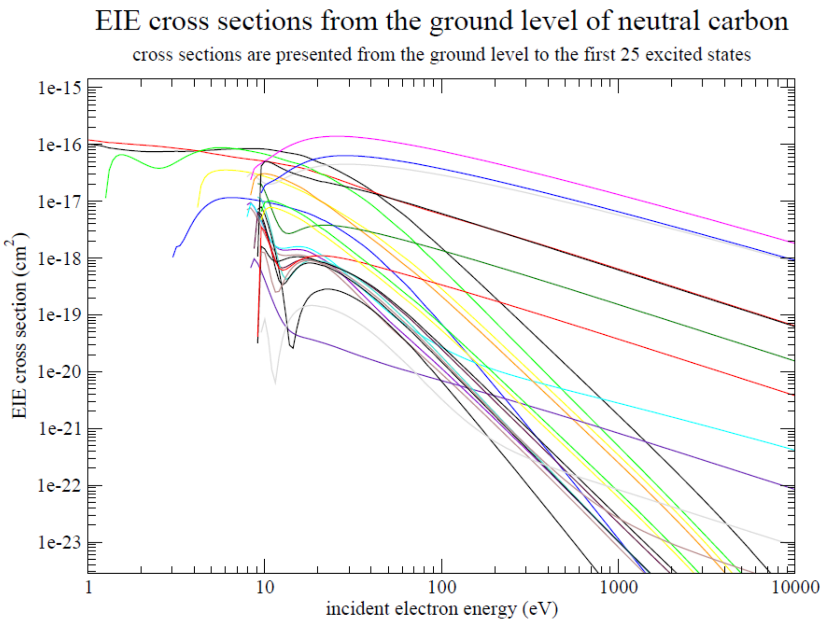
where E is the energy of the incident electron, $\hbar$ is the reduced Planck constant, a_0 is the Bohr constant, m_e is the mass of an electron, and ω_p is the plasmon frequency given by $\sqrt{(n_v e^2)/(\epsilon_0 m_e)}$ where e is the electron charge, ϵ_0 is the electrical field constant, n_v is the density of valence electrons, and p and p_0 are the incident electron momentum and Fermi momentum, respectively. The density of valence electrons can be calculated from

$$n_v = \frac{\rho N_A N_v}{M_{\mathrm{mol}}}, \quad (2)$$

https://journals.aps.org/pr/abstract/10.1103/PhysRev.126.1453

Electronic Excitation

- Currently working on using the ACE (Another Collisional Excitation) code, produced by Los Alamos to include more channels (currently 25 channels for graphite out of 3151)
- ACE calculates the cross sections using distorted-wave approximations
- Provided Cross-sections are from 1-10^4 eV, above this the Dirac B-Spline R-Matrix method is used
- Collaboration with Christopher Fontes, Los Alamos National Laboratory



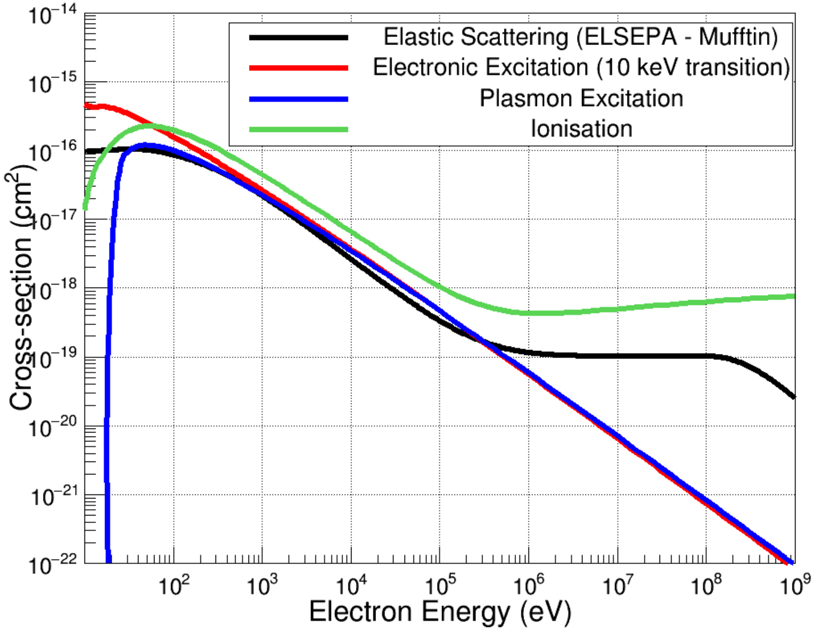
Fontes et al, J. Phys. B 48, 144014 (2015)

https://www.osti.gov/servlets/purl/6861416

Geant4 classes

- **Elastic Scattering**
  - G4DNAELSEPAElasticModel
- **Electronic Excitation**
  - G4DNADiracRMatrixExcitationModel
- **Plasmon Excitation**
  - G4DNAQuinnPlasmonExcitationModel
- **Ionisation and atomic de-excitation**
  - G4DNARelativisticIonisationModel

Summary of cross-sections for graphite



Same approach of Sakata et al, Journal of Applied Physics, 120 (24), art. no. 244901, 2016.

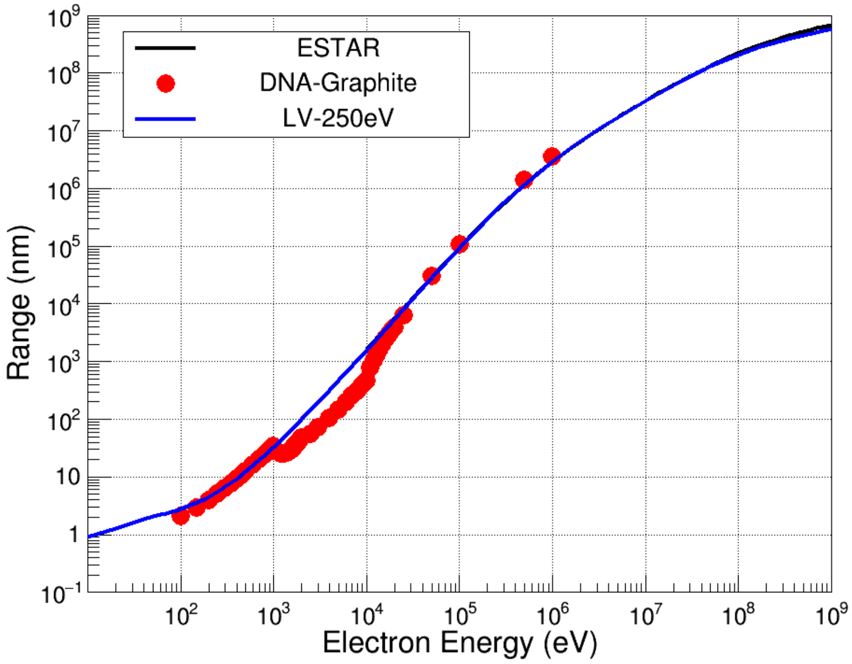
Testing

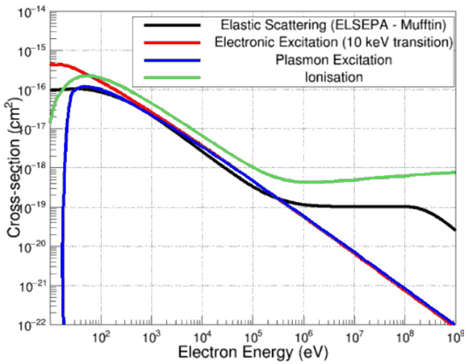
Calculation of

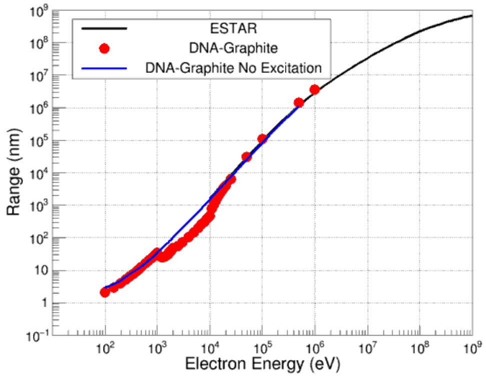
- **Range** - using /dna/range example
- **Stopping power** - using /dna/spower example
- **Backscattering** - using /EM/TestEM5 example

Graphite Range Testing

- Abrupt change between 1-10 keV
- Cross-section of each process has no abrupt changes
- Maybe caused by Excitation class - still updating for ACE input

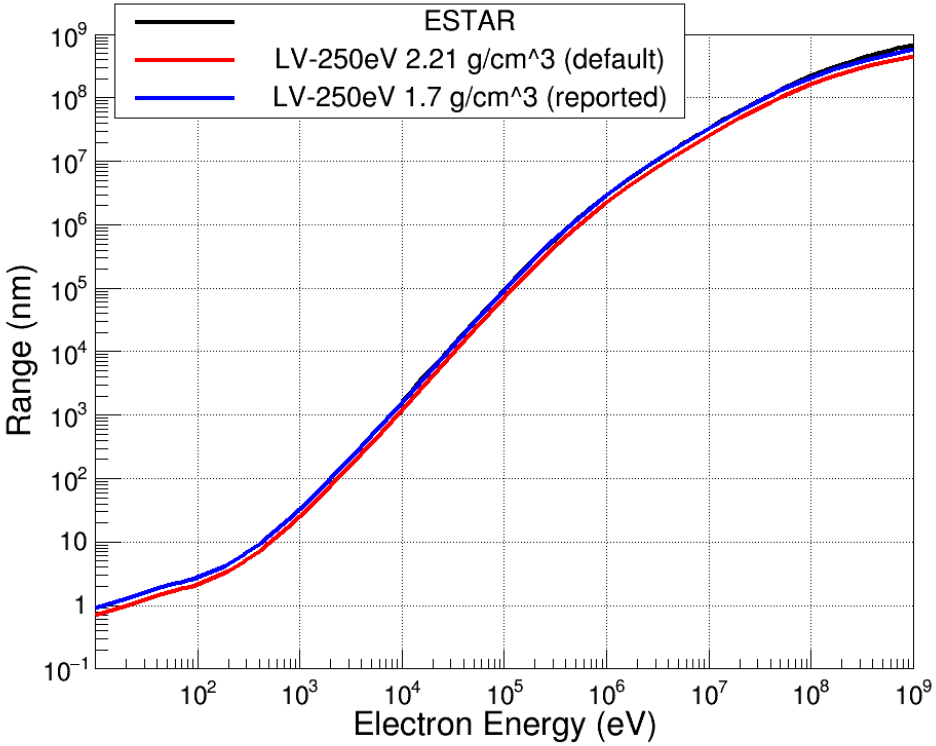




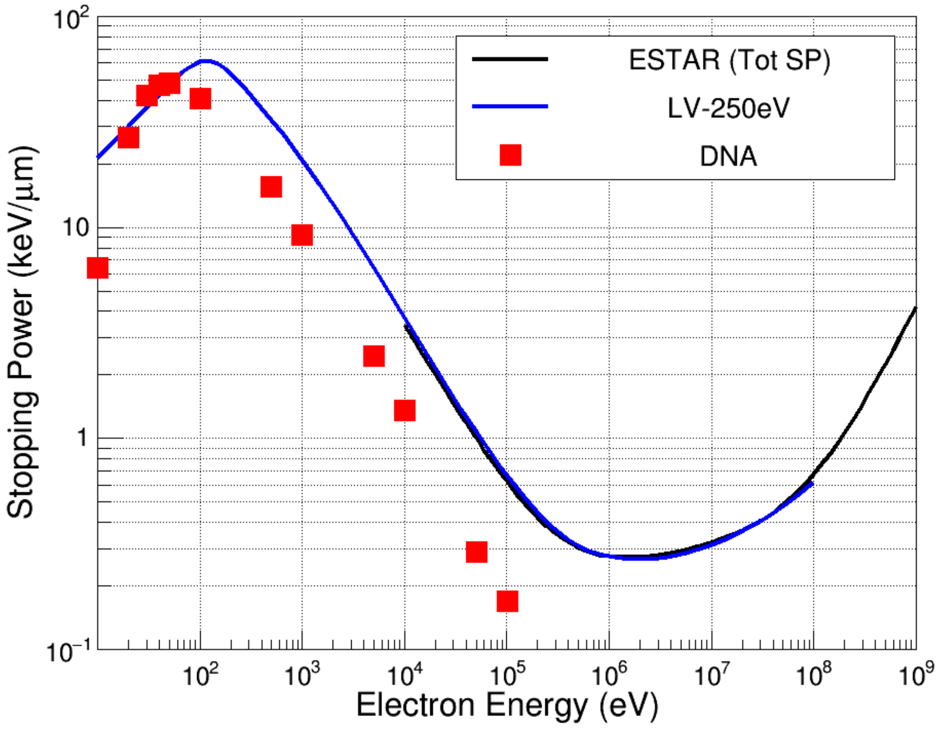


Graphite density

- NIST Material database lists
  - graphite density: **1.7 g/cm^3**
  - amorphous carbon as **2.0 g/cm^3**
- Geant4 NIST material: **2.21 g/cm^3**
- ICRU90 report: 2.265 g/cm^3



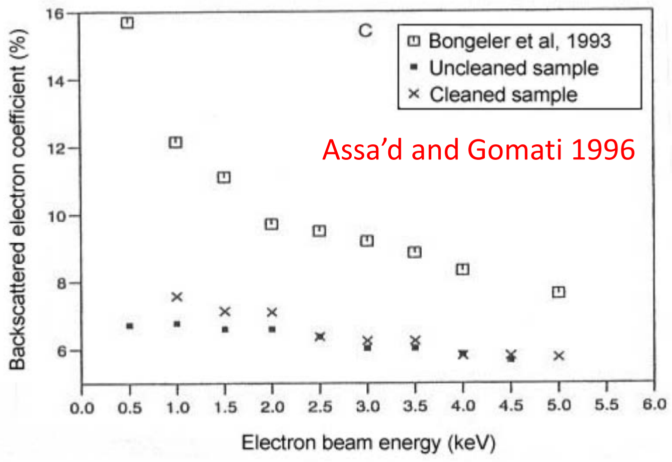
SP of Graphite

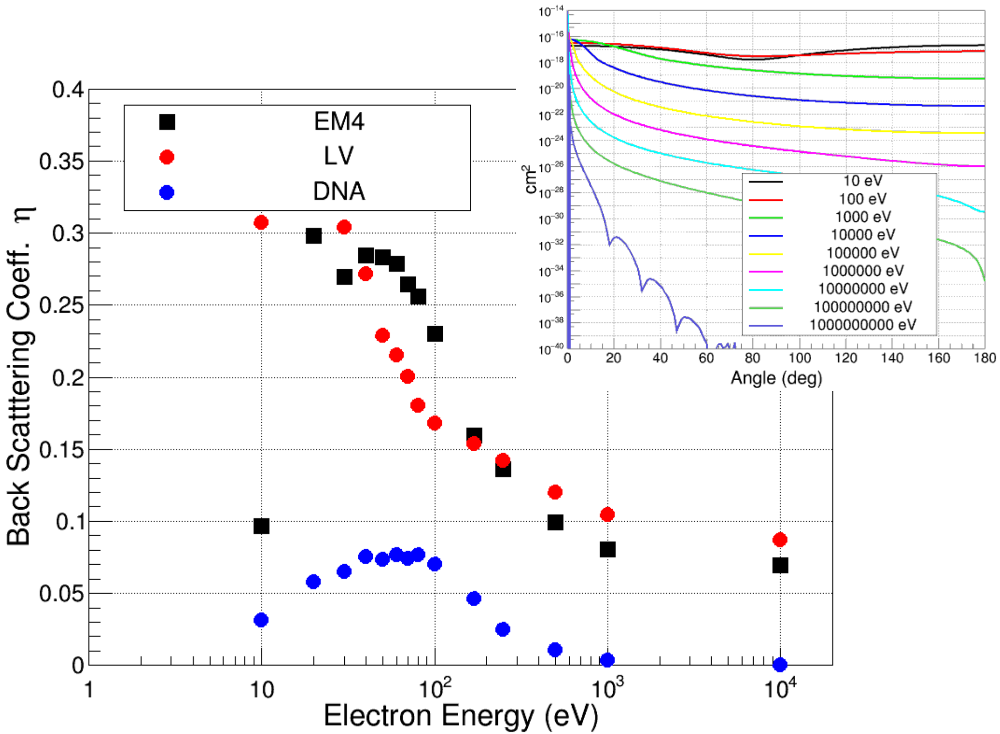


Graphite backscattering

Differential cross-section for elastic scattering

- Comparing using 0.5 mm thick target
- Need to investigate cross-sections more





Conclusions

- Cross sections for graphite implemented in Geant4
- Problems:
  - Disagreement in terms of stopping power and backscattering coefficient
- We will continue to work on this
  - Any suggestion very welcome