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Review of a energy loss simulation for negatively charged particles in Geant4

G4QAOLowEnergyLoss

In Geant4 there is a class to simulate stopping power of low energy negatively charged hadrons: processes/electromagnetic/lowenergy/G4QAOLowEnergyLoss

S. Chauvie, P. Nieminen, M.G. Pia. Geant 4 Model for the Stopping Power of Low Energy Negatively Charged Hadrons. IEEE Trans. Nucl. Sci. 54 (2007) 578
A model for a calculation of the stopping power by regarding the target atom as an ansemble of quantum harmonic oscillators is implemented

Motivation:

The class doesn't work in the context of current EM design

Plan:

1) Migration of anti-proton energy-loss at low energies to current EM design
2) Modification and development of the class
3) Application to other negatively charged particles
4) Tests

2

The Quantal Harmonic Oscillator Model

Stopping power can be calculated from Bohr-Bethe-Bloch theory with the expression

$$S=\frac{-dE}{dx}=N Z_2 \frac{4\pi e^4}{mv^2} Z_1^2 L = N Z_2 \frac{4\pi e^4}{mv^2}\left(Z_1^2 L_0 + Z_1^3 L_1 + Z_1^4 L_2 + \ldots\right)$$

The dimensionless stopping number L can be expanded in powers of Z_1:

1st term – well-known Bethe formula, 2nd – the Barkas correction (of Z^3).

The presence of terms with odd powers in Z leads to a different stopping behaiviour of positevely and negatively charged particles.

Bohr: the model of atoms as a collection harmonic oscillators for the description of inelastic collisions of charged particles

Sigmund and co-workers considered a harmonic oscillator target treated within the framework of quantum mechanics

The stopping number of an atom $L_{atom}=\sum_n f_n L\left(\frac{2mv^2}{\hbar\omega_n}\right)$, ω_n, f_n – resonance frequencies (excitation energies) and the optical oscillator strengths

The excitation energies and oscillator strengths must satisfy the sum rules: $\sum_n f_n = Z_2$, $\sum_n f_n \ln(\hbar\omega_n) = Z_2 \ln(I)$

G4QAOLowEnergyLoss:

1) the oscillator strength is set equal to the number of electrons in the n-th atomic shell $f_n = Z_n$

2) the resonance frequencies can be obtained from $\hbar\omega_n = \sqrt{(aU_n)^2 + \frac{2}{3}\frac{f_n}{Z_2}(\hbar\omega_p)^2}$, $\hbar\omega_p = \sqrt{\frac{4\pi\hbar^2 e^2 N Z_2}{m}}$,

where U_n is the ionization energy of the n-th shell, $\hbar\omega_p$ – the nominal plazmon energy

3) there are in literature table sets ω_n, f_n calculated from Optical Constatnts of Solids only for 6 materials

processes/electromagnetic/standard/G4BraggPbarModel – new class

```
class G4BraggPbarModel : public G4VEmModel
public:
  G4BraggPbarModel
  virtual ~G4BraggPbarModel
  virtual void Initialise                                  virtual G4double MinEnergyCut
  virtual G4double ComputeCrossSectionPerElectron          virtual G4double ComputeCrossSectionPerAtom
  virtual G4double CrossSectionPerVolume                   virtual G4double ComputeDEDXPerVolume
  virtual void SampleSecondaries                           virtual void CorrectionsAlongStep

private:
  inline void SetParticle
  G4double DEDX


  G4int GetNumberOfShell        G4double GetShellEnergy          G4double GetOscillatorEnergy
  G4double GetShellStrength     G4double GetOccupationNumber
  G4double GetL0            // terms in Z^2
  G4double GetL1            // terms in Z^3
  G4double GetL2            // terms in Z^4
```

processes/electromagnetic/standard/G4BraggPbarModel – II

```
// Z of element at now avaliable for the model
static const G4int materialAvailable[6];
//"Aluminum", "Silicon", "Copper", "Tantalum", "Gold", "Platinum"

// number, energy and oscillator strenghts for an harmonic oscillator model of material
static const G4int nbofShellForMaterial[6];
static G4double alShellEnergy[3]; static G4double alShellStrength[3];
static G4double siShellEnergy[3]; static G4double siShellStrength[3];
static G4double cuShellEnergy[4]; static G4double cuShellStrength[4];
static G4double taShellEnergy[6]; static G4double taShellStrength[6];
static G4double auShellEnergy[6]; static G4double auShellStrength[6];
static G4double ptShellEnergy[6]; static G4double ptShellStrength[6];
```

TABLE I. Oscillator strengths w and energies E used in the harmonic-oscillator model calculations.

	Al	Si	Cu	Ta	Pt	Au
w_K	0.1349	0.1222	0.0505	0.0126	0.0129	0.0139
E_K (keV)	2.795	3.179	16.931	88.926	95.017	96.235
w_L	0.6387	0.5972	0.2561	0.0896	0.0745	0.0803
E_L (keV)	0.202	0.249	1.930	18.012	25.590	25.918
w_M	0.2264	0.2806	0.4913	0.2599	0.2295	0.2473
E_M (keV)	0.0169	0.0203	0.199	3.210	4.063	4.116
w_N			0.2021	0.3413	0.4627	0.423
E_N (keV)			0.0396	0.575	0.576	0.599
w_O				0.2057	0.1324	0.1124
E_O (keV)				0.1087	0.0819	0.0873
w_P				0.0908	0.0879	0.1231
E_P (keV)				0.0308	0.0314	0.0369
I (keV)	0.164	0.168	0.322	0.709	0.764	0.800

```
// variable for calculation of stopping number of L's term
static const G4double L0[67][2];
static const G4double L1[22][2];
static const G4double L2[14][2];
```

$L_i\left(\frac{2mv^2}{\hbar\omega_n}\right)$ is evaluated by means of linear interpolation in the tables of L_i

```
static const G4int nbOfElectronPerSubShell[1540] → G4AtomicShells::fNumberOfElectrons[1540]
static const G4int fNumberOfShells[101]          → G4AtomicShells::fNumberOfShells[101]

G4int sizeL0;
G4int sizeL1;
G4int sizeL2;
```

G4BraggPbarModel - Plans

Planning implementation:

- introduce delta-electron poduction threshold (cut) above cut
- simulation of energy loss for complex material by using of Bragg's rule
- set spline interpolation under calculation of of L_i in the tables instead of linear intepolation
- plasma energy is supposed to take from G4DensityEffectData::GetPlasmaEnergy() instead of to calculate by formula
- values of nbOfElectronPerSubShell[1540] and NumberOfShells[101] is supposed to take from G4AtomicShells::fNumberOfElectrons[1540], G4AtomicShells::fNumberOfShells[101] instead of to contain inside the class the same arrays

Planning tests:

- comparison of energy loss simulation by harmonic oscillator model for 6 materials: shell energies and shell strengths from tables (2 set of parameters) and from formulas
- comparison of energy loss simulation by oscillator model and by Bethe-Bloch formula for different particles and different materials especially for energy region 2 – 10 MeV
- study of alternative publications concerning stopping number calculation