Materials

General considerations

In nature, materials (chemical compounds, mixtures) are made of elements, and elements are made of isotopes.

These are the three main classes designed in Geant4.

G4Element and **G4Isotope** describe the properties of the atoms :

- atomic number
- number of nucleons
- mass of a mole
- shell energies
- quantities such as cross sections per atom, etc.

G4Material describes the macroscopic properties of matter:

- density
- state
- temperature
- pressure
- macroscopic quantities like radiation length, mean free path, dE/dx, etc.

The **G4Material** class is the one which is visible to the rest of the toolkit, and is used by the tracking, the geometry, and the physics.

It contains all the information relative to the eventual elements and isotopes of which it is made, at the same time hiding the implementation details.

Define a simple material

Liquid argon is created, by specifying its name, atomic number, mass of mole, density.

```
G4String name = "liquidArgon";
G4double atomicNumber = 18.;
G4double massOfMole = 39.95*g/mole;
G4double density = 1.390*g/cm3;

G4Material* lAr = new G4Material
            (name, atomicNumber, massOfMole, density);
```

The pointer to the material, lAr, will be used to specify the matter of which a given logical volume is made :

```
G4LogicalVolume* myLbox = new G4LogicalVolume
                          (aBox, lAr, "Lbox", 0, 0, 0);
```

Define a molecule

Water is built from its components, by specifying the number of atoms in the molecule.

```
G4Element* H = new G4Element (name="Hydrogen",symbol="H",
             atomicNumber=1., massOfMole=1.01*g/mole);
G4Element* O = new G4Element (name="Oxygen",symbol="O",
             atomicNumber=8., massOfMole=16.00*g/mole);

G4Material* H2O = new G4Material (name="Water",
                 density=1.0*g/cm3, nbComponents=2);

H2O->AddElement(H, nbAtoms=2);
H2O->AddElement(O, nbAtoms=1);
```

Define a mixture by fractional mass

Air is built from Nitrogen and Oxygen, by giving the mass ratio of each component.

```
G4Element* N = new G4Element ("Nitrogen", "N",
             atomicNumber=7., massOfMole=14.01*g/mole);
G4Element* O = new G4Element ("Oxygen", "O",
             atomicNumber=8., massOfMole=16.00*g/mole);

G4Material* Air = new G4Material (name="Air",
                 density=1.29*mg/cm3, nbComponents=2);

Air->AddElement(N, massRatio=0.7);
Air->AddElement(O, massRatio=0.3);
```

Define an element from its isotopes

Enriched Uranium is built from its isotopes, by giving the relative abundance of each component.

```
G4Isotope* U5 = new G4Isotope ("U235", atomicNumber=92,
                nbOfNucleons=235, massOfMole=235.01*g/mole);
G4Isotope* U8 = new G4Isotope ("U238", atomicNumber=92,
                nbOfNucleons=238, massOfMole=238.03*g/mole);

G4Element* U = new G4Element (name="enriched Uranium",
               symbol="U", nbComponents=2);

U->AddIsotope(U5, abundanceRatio=90.*percent);
U->AddIsotope(U8, abundanceRatio=10.*percent);
```

NB: abundance $\equiv$ number of atoms per volume.

Abundance

The number of atoms per volume is one of the basic quantities computed by G4Material for the needs of the physics processes.

For a simple material :

$$\text{nbOfAtomsPerVolume} = \frac{\text{AvogadroNumber} \times \text{density}}{\text{massOfMole}}$$

In a compound material :

$$n_{at}[i] = \frac{\mathcal{N}\ \rho\ w_i}{A_i} \quad \text{for the } i^{th} \text{ element}$$

`G4double*` n_{at} = `aMaterial -> GetVecNbOfAtomsPerVolume()`

Mixture of mixtures

```
G4Material* Aerog = new G4Material ( "Aerogel",
                    density=0.2*g/cm3, nbComponents=2);

Aerog->AddMaterial(SiO2, massRatio=62.5*percent);
Aerog->AddMaterial(H2O, massRatio=37.5*percent);
```

Gas in non STP conditions

For gas, it may be necessary to specify temperature and pressure. (dE/dx computation affected)

```
G4double density = 27.*mg/cm3;
G4double temperature = 325.*kelvin;
G4double pressure = 50.*atmosphere;

G4Material* CO2 = new G4Material ( "CarbonicGas",
                  density, nbComponents=2,
                  kStateGas, temperature, pressure);

CO2->AddElement(C, nbAtoms=1);
CO2->AddElement(O, nbAtoms=2);
```

Example of vacuum

Absolute vacuum does not exist. It is a gas at very low density.

```
G4double atomicNumber = 1.;
G4double massOfMole = 1.008*g/mole;
G4double density = 1.e-25*g/cm3;
G4double temperature = 2.73*kelvin;
G4double pressure = 3.e-18*pascal;

G4Material* vacuum = new G4Material ( "interGalactic",
                    atomicNumber, massOfMole, density,
                    kStateGas, temperature, pressure);
```

i.e. it is forbidden to define material with Z or A or $\rho = 0$.

Gas mixture by volume ?

```
Gas->AddElement(anElement, volumeRatio);
```

same signature as :

```
Gas->AddElement(anElement, massRatio);
```

would need a new function name :

```
Gas->AddElementPerVolume(anElement, volumeRatio);
```

Indeed we do not need it ! Example : Ar (80%) CO2 (20%)
In 10 moles of the mixture : 8 moles of Ar and 2 moles of CO2
$\Longrightarrow$ The mixture is equivalent to the molecule Ar8 C2 O4

the MaterialTable

It is the list of materials created so far.
More precisely, a STL vector : `G4std::vector<G4Material*>`.
An index is assigned to each material.

The MaterialTable is used by some physics processes to build and to access tables of quantities which are material dependent : cross-sections, mean free path, stopping power, range.

Therefore the MaterialTable must be completed before run initialisation.

```
const G4MaterialTable*
theTable = G4Material::GetMaterialTable();
G4Material* aMaterial = (*theTable)[J];
size_t J = aMaterial -> GetIndex();
```