Defining Materials in Geant4

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Single Element Materials

Need G4Material* in order to instantiate G4LogicalVolume

```
G4Material(name, atomic_number, atomic_weight, density);
G4Material(name, density, number_of_components);
```

Defining a simple material:

```
G4double atomic_weight = 39.95*g/mole;
G4double density = 1.390*g/cm3;
G4Material* lAr =
  new G4Material("liquidArgon", Z=18,atomic_weight, density);
```

Molecules

Molecules are defined from instances of the G4Element class.

Defining the components of H2O:

```
G4Element* hydrogen =
  new G4Element("Hydrogen", symbol="H", z=1, a=1.01*g/mole);

G4Element* oxygen =
  new G4Element("Oxygen", symbol="O", z=8, a=16.00*g/mole);
```

Assemble elements into H2O molecule:

```
G4Material* H2O =
  new G4Material("Water", density=1.000*g/cm3,n_comps=2);

G4int number_of_atoms;
H2O->AddElement(hydrogen, number_of_atoms=2);
H2O->AddElement(oxygen, number_of_atoms=1);
```

Isotopes

Elements can comprise different components, just like molecules

```
G4Isotope* isoU235 =
  new G4Isotope("U235", Z=92, A=235, a=235.044*g/mole);

G4Isotope* isoU238 =
  new G4Isotope("U238", Z=92, A=238, a=238.051*g/mole);

G4Element* enrichedU =
  new G4Element("enriched U", symbol="U", n_comp=2);

enrichedU->AddIsotope(isoU235,abundance=80.*perCent);
enrichedU->AddIsotope(isoU238,abundance=20.*perCent);
```

The element is then added to a single-component material:

```
G4Material* mat_enrichedU=
  new G4Material("enr. U",density, ncomp = 1);

mat_enrichedU
  ->AddElement( enrichedU, fraction_mass = 1 );
```

Compounds

Compounds are mixtures of elements not bound into molecules and can be specified by fraction of mass:

```
G4Element* nitrogen  =
  new G4Element("Nitrogen",symbol="N",z= 7., a=14.01*g/mole);
G4Element* oxygen  =
  new G4Element("Oxygen",symbol="O",z=8., a=16.00*g/mole);

G4Material* Air =
  new G4Material("Air",density=1.290*mg/cm3,ncomp=2);
  Air->AddElement(nitrogen, fracMass=70.0*perCent);
  Air->AddElement(oxygen, fracMass=30.0*perCent);
```

Mixtures

Mixtures allow the combination of G4Materials and G4Elements into a single G4Material instance, allowing the combination of molecules, isotopes and elements:

```
G4Element* elC  = …;    // define "carbon" element
G4Material* SiO2 = …;   // define "quartz" material
G4Material* H2O = …;    // define "water" material

density = 0.200*g/cm3;
G4Material* Aerog =
  new G4Material("Aerogel",density,ncomponents=3);
  Aerog->AddMaterial(SiO2,fractionmass=62.5*perCent);
  Aerog->AddMaterial(H2O ,fractionmass=37.4*perCent);
  Aerog->AddElement (elC ,fractionmass= 0.1*perCent);
```

The NIST Material Database

- The National Institute of Standards (NIST) provides a detailed database of material properties, particularly:
  - Density
  - Excitation potential
  - Element composition
  - Isotope composition

- More than 3000 isotopes and their properties are being tracked

- A version of this database is part of the Geant4 distribution

The NIST Material Database - Si

- The table to the right shows the physical porperties of 20 known Si isotopes
- The table also provides natural isotope abundances and a single „average isotope“
- Various molecules and compounds are also provided

Z		A	m	error	(%)	A_{eff}
14	Si	22	22.03453	(22)		28.0855(3)
		23	23.02552	(21)		
		24	24.011546	(21)		
		25	25.004107	(11)		
		26	25.992330	(3)		
		27	26.98670476	(17)		
		28	27.9769265327	(20)	92.2297 (7)	
		29	28.97649472	(3)	4.6832 (5)	
		30	29.97377022	(5)	3.0872 (5)	
		31	30.97536327	(7)		
		32	31.9741481	(23)		
		33	32.978001	(17)		
		34	33.978576	(15)		
		35	34.984580	(40)		
		36	35.98669	(11)		
		37	36.99300	(13)		
		38	37.99598	(29)		
		39	39.00230	(43)		
		40	40.00580	(54)		
		41	41.01270	(64)		
		42	42.01610	(75)		

Using NIST Materials - I

Database access is managed by a singleton manager class:

```
G4NistManager* manager = G4NistManager::GetPointer();
```

G4Element and G4Material can both be loaded straight from the database:

```
G4Element* elm = manager->FindOrBuildElement(symbol="H", G4bool iso);

G4Element* elm = manager->FindOrBuildElement(G4int Z, G4bool iso);

G4Material* mat = manager->FindOrBuildMaterial(name="G4_Air", G4bool iso);
```

Using NIST Materials - II

A compound can be build by specifying a vector of atomic numbers and weights to retrieve NIST elements:

```
G4Material* mat = manager->ConstructNewMaterial("name",
                            const std::vector<G4int>& Z,
                            const std::vector<G4double>& weight,
                            G4double density, G4bool iso);
```

The database can also be queried for isotope masses:

```
G4double isotopeMass = manager->GetMass(G4int Z, G4int N);
```

Finally, the UI commands to list defined elements/materials are:

```
 /material/nist/printElement   --- print defined elements
 /material/nist/listMaterials    --- print defined materials
```

Conclusions

- Simple materials can be defined directly by using the *G4Material()* constructor

- Molecules are defined by declaring multi-component materials and using *AddElement(...)* method to add *G4Element* instances

- Mixtures are arbitrary combinations of elements and *G4Material* objects

- The NIST database can be used to obtain precise physical data for elements and their isotopic composition as well as molecules