Material Definition

University of Pennsylvania Geant4 Tutorial
15 May 2011
Dennis Wright
Outline

- Materials in Geant4
- Material definition
- NIST material database
Materials in Geant4

• Materials in the real world
  ▪ are made up of elements, compounds (or molecules), mixtures of elements and/or compounds
  ▪ can be solid, liquid or gas (sorry, no plasma)
  ▪ exist under various pressures, temperatures and densities

• Geant4 allows the custom definition of materials
  ▪ starting with elements: use G4Element class
  ▪ compounds or molecules can be built by assigning two or more instances of G4Element to an object of the G4Material class
  ▪ mixtures can be built by assigning two or more compounds or elements to an instance of G4Material
  ▪ A G4Material can also be built from a single G4Element
  ▪ Optionally, you may define your own G4Element by assigning to it one or more instances of the class G4Isotope
Materials in Geant4

- Geant4 requires you to set at least one material condition
  - density

- The rest are optional
  - state (default is solid or gas, depending on density)
  - temperature (default = STP temperature = 273.15 K)
  - pressure (default = STP pressure = 100 kPascals = 1 atm)

- Along with normal stuff, you can define some strange things
  - gases far from STP
  - high pressure solids
  - low density liquids

- And there's a shortcut => NIST material database
• Let's start with a single-element material:

\[
\begin{align*}
\text{G4double } & \text{ density } = 4.506*\text{g/cm}^3; \\
\text{G4double } & \text{ a } = 47.867*\text{g/mole}; \\
\text{G4Material* } & \text{ ti } = \\
& \text{ new G4Material("pureTitanium", z=22., a, density);}
\end{align*}
\]

• Vacuum is also useful

\[
\begin{align*}
\text{G4double } & \text{ density } = 0.001*\text{g/cm}^3; \\
\text{G4double } & \text{ a } = 14.007*\text{g/mole}; \\
\text{G4Material* } & \text{ vacuum } = \\
& \text{ new G4Material("labVacuum", z=7., a, density);}
\end{align*}
\]

– for vacuum, low-density materials are preferred rather than density = 0
– “average” materials (e.g. z = 25.7) are not allowed
Definition of Materials: molecules

- A molecule is made of several elements, with the composition specified by the number of atoms

```c++
G4double a = 1.01*g/mole;
G4Element* elH = new G4Element("Hydrogen","H", z=1., a);
a = 16.00*g/mole;
G4Element* elO = new G4Element("Oxygen","O", z=8., a);
G4double density = 1.000*g/cm3;

G4int ncomp = 2;
G4Material* H2O =
    new G4Material("Water", density, ncomp);
G4int nAtoms;
H2O->AddElement(elH, nAtoms=2);
H2O->AddElement(elO, nAtoms=1);
```
Definition of Materials: mixture (alloy)

- A mixture is similar to a molecule, except that materials and elements are combined instead of just elements

```cpp
G4Element* elC = ...;  // define carbon
G4Material* H2O = ...;  // define molecule (previous page)
G4Material* SiO2 = ...;  // define another molecule

G4double density = 0.20*g/cm3;
G4int ncomp = 3;
G4double fracMass;
G4Material* Aerog = new G4Material("Aerogel", density, ncomp);
Aerog->AddMaterial(SiO2, fracMass = 62.5*perCent);
Aerog->AddMaterial(H2O, fracMass = 37.4*perCent);
Aerog->AddElement(elC, fracMass = 0.1*perCent);
```
Elements and Isotopes

- If you define an element, it is treated by default as if it has the natural isotope abundance
  - even if the g/mole value you enter is quite different from the natural abundance
  - hadronic code only knows how to deal with specific nuclides, not elements

- You can define an element with non-natural abundance by assigning to G4Element a list of G4Isotope instances

- Example: making nuclear fuel – start with isotopes
  ```
  G4int z; G4int a;
  G4Isotope* isoU235 = new G4Isotope("U235", z=92, a=235, 235.044*g/mole);
  G4Isotope* isoU238 = new G4Isotope("U238", z=92, a=238, 238.051*g/mole);
  ```
• Example: use the isotopes to define enriched uranium for power generation:

```cpp
G4int ncomp;
G4double abundance;
G4Element* enrichedU =
    new G4Element("EnrichedU", U", ncomp=2);
enrichedU->AddIsotope(isoU235, abundance=5.0*perCent);
enrichedU->AddIsotope(isoU238, abundance=95.0*perCent);
```

• Make some fluorine, too

```cpp
G4Element* elF =
    new G4Element("Fluorine", F", 9., 18.998*g/mole);
```
Elements and Isotopes (continued)

- Example: now use F and enriched U to make nuclear fuel (UF$_6$):

  G4double density;
  G4Material* fuel = new G4Material("NuclearFuel", density =
          5.09*g/cm3, ncomp=2,
          kStateSolid, 640*kelvin, 1.5e7*pascal);
  fuel->AddElement(elF, 6);
  fuel->AddElement(enrichedU, 1);

- Note the red line: state, temperature, pressure
  - these are optional parameters which default to STP if not specified
Using the NIST Material Database

- Most of the materials you will want to define are already done for you
  - also all elements with natural isotopic abundance
  - more than 3000 isotopes defined

- Since 2005 Geant4 has included pre-defined materials from the NIST database
  - physics.nist.gov/PhysRefData
  - provides the best accuracy for major parameters:
    - density
    - isotopic composition of elements
    - elemental composition of materials
    - mean ionization potential
    - chemical bonds
  - standardization is very useful
# NIST Elemental Composition

<table>
<thead>
<tr>
<th>Z</th>
<th>A</th>
<th>Z</th>
<th>error</th>
<th>(% comp)</th>
<th>A_{eff}</th>
</tr>
</thead>
<tbody>
<tr>
<td>14</td>
<td>Si</td>
<td>22</td>
<td>22.03453</td>
<td>(22)</td>
<td>28.0855(3)</td>
</tr>
<tr>
<td>23</td>
<td>Li</td>
<td>23</td>
<td>23.02552</td>
<td>(21)</td>
<td></td>
</tr>
<tr>
<td>24</td>
<td>Be</td>
<td>24</td>
<td>24.011546</td>
<td>(21)</td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>B</td>
<td>25</td>
<td>25.004107</td>
<td>(11)</td>
<td></td>
</tr>
<tr>
<td>26</td>
<td>C</td>
<td>26</td>
<td>25.992330</td>
<td>(3)</td>
<td></td>
</tr>
<tr>
<td>27</td>
<td>N</td>
<td>27</td>
<td>26.986704/6</td>
<td>(1)</td>
<td></td>
</tr>
<tr>
<td>28</td>
<td>O</td>
<td>28</td>
<td>27.9769265327</td>
<td>(20)</td>
<td>92.2297(7)</td>
</tr>
<tr>
<td>29</td>
<td>F</td>
<td>29</td>
<td>28.97649472</td>
<td>(3)</td>
<td>4.6832(5)</td>
</tr>
<tr>
<td>30</td>
<td>Ne</td>
<td>30</td>
<td>29.97377022</td>
<td>(5)</td>
<td>3.0872(5)</td>
</tr>
<tr>
<td>31</td>
<td>Na</td>
<td>31</td>
<td>30.97536327</td>
<td>(7)</td>
<td></td>
</tr>
<tr>
<td>32</td>
<td>Mg</td>
<td>32</td>
<td>31.9741481</td>
<td>(23)</td>
<td></td>
</tr>
<tr>
<td>33</td>
<td>Al</td>
<td>33</td>
<td>32.978001</td>
<td>(17)</td>
<td></td>
</tr>
<tr>
<td>34</td>
<td>Si</td>
<td>34</td>
<td>33.978576</td>
<td>(15)</td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>P</td>
<td>35</td>
<td>34.984580</td>
<td>(40)</td>
<td></td>
</tr>
<tr>
<td>36</td>
<td>S</td>
<td>36</td>
<td>35.98659</td>
<td>(11)</td>
<td></td>
</tr>
<tr>
<td>37</td>
<td>Cl</td>
<td>37</td>
<td>36.99300</td>
<td>(13)</td>
<td></td>
</tr>
<tr>
<td>38</td>
<td>Ar</td>
<td>38</td>
<td>37.00598</td>
<td>(29)</td>
<td></td>
</tr>
<tr>
<td>39</td>
<td>K</td>
<td>39</td>
<td>39.00230</td>
<td>(43)</td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>Ca</td>
<td>40</td>
<td>40.00580</td>
<td>(54)</td>
<td></td>
</tr>
<tr>
<td>41</td>
<td>Sc</td>
<td>41</td>
<td>41.01270</td>
<td>(64)</td>
<td></td>
</tr>
<tr>
<td>42</td>
<td>Ti</td>
<td>42</td>
<td>42.01610</td>
<td>(75)</td>
<td></td>
</tr>
</tbody>
</table>
### Elementary Materials from the NIST Database

<table>
<thead>
<tr>
<th>Z</th>
<th>Name</th>
<th>ChFormula</th>
<th>density(g/cm^3)</th>
<th>I(eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>G4_H</td>
<td>H(_2)</td>
<td>8.3748e-05</td>
<td>19.2</td>
</tr>
<tr>
<td>2</td>
<td>G4_He</td>
<td></td>
<td>0.000166322</td>
<td>41.8</td>
</tr>
<tr>
<td>3</td>
<td>G4_Li</td>
<td></td>
<td>0.534</td>
<td>40</td>
</tr>
<tr>
<td>4</td>
<td>G4_Be</td>
<td></td>
<td>1.848</td>
<td>63.7</td>
</tr>
<tr>
<td>5</td>
<td>G4_B</td>
<td></td>
<td>2.37</td>
<td>76</td>
</tr>
<tr>
<td>6</td>
<td>G4_C</td>
<td></td>
<td>2</td>
<td>81</td>
</tr>
<tr>
<td>7</td>
<td>G4_N</td>
<td>N(_2)</td>
<td>0.0011652</td>
<td>82</td>
</tr>
<tr>
<td>8</td>
<td>G4_O</td>
<td>O(_2)</td>
<td>0.00133151</td>
<td>95</td>
</tr>
<tr>
<td>9</td>
<td>G4_F</td>
<td></td>
<td>0.00158029</td>
<td>115</td>
</tr>
<tr>
<td>10</td>
<td>G4_Ne</td>
<td></td>
<td>0.000838505</td>
<td>137</td>
</tr>
<tr>
<td>11</td>
<td>G4_Na</td>
<td></td>
<td>0.971</td>
<td>149</td>
</tr>
<tr>
<td>12</td>
<td>G4_Mg</td>
<td></td>
<td>1.74</td>
<td>156</td>
</tr>
<tr>
<td>13</td>
<td>G4_Al</td>
<td></td>
<td>2.6989</td>
<td>166</td>
</tr>
<tr>
<td>14</td>
<td>G4_Si</td>
<td></td>
<td>2.33</td>
<td>173</td>
</tr>
<tr>
<td>N</td>
<td>Name</td>
<td>ChFormula</td>
<td>density (g/cm³)</td>
<td>I (eV)</td>
</tr>
<tr>
<td>---</td>
<td>---------------------</td>
<td>-----------</td>
<td>----------------</td>
<td>--------</td>
</tr>
<tr>
<td>13</td>
<td>G4_Adipose_Tissue</td>
<td></td>
<td>0.92</td>
<td>63.2</td>
</tr>
<tr>
<td>1</td>
<td>0.119477</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>0.63724</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>0.00797</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>0.232333</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>0.00005</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>2e-05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>0.00016</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>0.00073</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>0.00119</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>0.00032</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>2e-05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>26</td>
<td>2e-05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>2e-05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>G4_Air</td>
<td></td>
<td>0.00120479</td>
<td>85.7</td>
</tr>
<tr>
<td>6</td>
<td>0.000124</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>0.755268</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>0.231781</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>0.012827</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>G4_CsI</td>
<td></td>
<td>4.51</td>
<td>553.1</td>
</tr>
<tr>
<td>53</td>
<td>0.47692</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>55</td>
<td>0.52308</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
How to Use NIST Database

- User interfaces to C++ code:
  ```
  G4NistManager* manager = G4NistManager::GetPointer();
  G4Element* elm =
      manager->FindOrBuildElement("chem symbol", G4bool iso);
  G4Element->FindOrBuildElement(G4int z, G4bool iso);
  G4Material->FindOrBuildMaterial("name", G4bool iso);
  G4Material->ConstructNewMaterial("name",
      const std::vector<G4int>& Z,
      const std::vector<G4double>& weight,
      G4double density, G4bool iso);
  G4double isotopeMass = manager->GetMass(G4int Z, G4int N);
  ```

- **G4bool iso = true**: element is built of isotopes with natural abundance
- **G4bool iso = false**: isotopes not explicitly built
How to Use NIST Database

• User interfaces to G4 command line
  – list all NIST-defined elements:
    material/nist/printElement
  
  – list all NIST-defined materials
    material/nist/listMaterials
Summary

• Geant4 allows you to define materials in terms of
  – isotopes (G4Isotope)
  – elements (G4Element)
  – materials (G4Material)

• And to set material conditions
  – density
  – state
  – temperature
  – pressure

• Whenever you can, use the pre-defined NIST database elements and materials
  – accurate
  – standardized