Prove that the atomic packing factor for the FCC structure is \(0.74\).

From lecture:

Atoms per unit cell: 
\[8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 4\]  

In the hard packed spheres model, atoms touch along the face diagonal.

\[
\sqrt{2} a = 4r 
\rightarrow a = \frac{4r}{\sqrt{2}} = 2\sqrt{2}r
\]

\[\text{Packing efficiency } PE\]

\[
PE = \frac{4 \text{ atoms/unit cell} \times \frac{4}{3} \pi r^3}{\text{volume of the unit cell}}
\]

\[
= \frac{\frac{8}{3} \pi r^3}{(2\sqrt{2})^3 r^3} = 0.74
\]
Problem 2 [12]

Using the table below, estimate the densities of Vanadium, Lead, and Polonium. Compare to measured densities.
1 pt for a, 1 pt for n, 1 pt for density, 1 pt for comparison to measured density

density[element_, A_, r_, xstc_, actualdensity_] := Module[{Vc, NA, \[rho]_, a, n},
  Switch[xstc,
    "BCC",
    a = 4 \[Theta] r / Sqrt[3]; (*m*)
    n = 2; (*2 atoms per cell in a BCC unit cell*)
    , "FCC",
    a = 2 Sqrt[2] \[Theta];
    n = 4;
    , "SC",
    a = 2 \[Theta];
    n = 1;
  ];
  Vc = a^3; (*m^3*)
  Vc = Vc \[times] (10^2)^3; (*cm^3*)
  NA = 6.022 \[times] 10^23; (*atoms*)
  \[rho] = (n \[times] A) / (Vc \[times] NA); (*equation 3.5, units = g/cm^3*)
  {element, A, r \[times] 10^12, xstc, \[rho], actualdensity}]

Grid[Transpose[{{"Element", "Atomic weight", "Radius (pm)"},
  "Crystal structure", "Computed density (g/cm^3)", "Actual density (g/cm^3)"},
  density["V", 50.9415, 134. \[times] 10^-12, "BCC", 6.0],
  density["Pb", 207.2, 175. \[times] 10^-12, "FCC", 11.34],
  density["Po", 209, 168 \[times] 10^-12, "SC", 9.196}]]

<table>
<thead>
<tr>
<th>Element</th>
<th>V</th>
<th>Pb</th>
<th>Po</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atomic weight</td>
<td>50.9415</td>
<td>207.2</td>
<td>209</td>
</tr>
<tr>
<td>Radius (pm)</td>
<td>134.</td>
<td>175.</td>
<td>168</td>
</tr>
<tr>
<td>Crystal structure</td>
<td>BCC</td>
<td>FCC</td>
<td>SC</td>
</tr>
<tr>
<td>Computed density (g/cm^3)</td>
<td>5.70885</td>
<td>11.3491</td>
<td>9.1493</td>
</tr>
<tr>
<td>Actual density (g/cm^3)</td>
<td>6.</td>
<td>11.34</td>
<td>9.196</td>
</tr>
</tbody>
</table>
\( \text{Rh} \)

\[
\text{atomic} = 0.1345 \ \text{nm} \quad A_{\text{Rh}} = 102.91 \ \frac{\text{g}}{\text{mol}}
\]

\[ \text{density} = 12.41 \ \frac{\text{g}}{\text{cm}^3} \]

(3.8) \[ \rho = \frac{n A_{\text{Rh}}}{V_c N_A} \]

\[ \Rightarrow \text{assume } \text{FCC, } n = 4, \ V_c = 16 R^3 \sqrt{2} \]

\[
12.41 \ \frac{g}{cm^3} = \frac{(4)(102.91 \ \frac{g}{mol})}{16(0.1345 \ \text{nm})^3 \sqrt{2} \ (6.022 \times 10^{23} \ \text{atoms/mol})}
\]

\[ = 1.24 \times 10^{-20} \ \frac{g \cdot \text{mol}}{\text{mol} \cdot \text{nm}^3} \left( \frac{1 \times 10^7 \ \text{nm}}{1 \ \text{cm}} \right)^3 \]

\[ = 12.42 \ \frac{g}{cm^3} \]

\[ \Rightarrow \text{assume } \text{BCC, } n = 2, \ V_c = \left( \frac{4R}{\sqrt{3}} \right)^3 \]

\[
12.41 \ \frac{g}{cm^3} = \frac{(2)(102.91 \ \frac{g}{mol}) X^3 \sqrt{2}}{(4^3)(0.1345 \ \text{nm})^3 \ (6.022 \times 10^{23} \ \text{atoms/mol})}
\]

\[ = 1.14 \times 10^{-20} \ \frac{g \cdot \text{mol}}{\text{mol} \cdot \text{nm}^3} \left( \frac{1 \times 10^7 \ \text{nm}}{1 \ \text{cm}} \right)^3 \]

\[ = 11.40 \ \frac{g}{cm^3} \]

\( \Rightarrow \boxed{\text{FCC}} \)
All cubic, simplify by thinking of all edges as length 1

i) intercepts: \[
\begin{array}{ccc}
  x & y & z \\
  1 & \infty & 1
\end{array}
\]

reciprocal (plane \((1\ 0\ 1)\)) 1 pt

ii) Hint: Move the plane to a parallel location if it intercepts the origin. Or move the origin put origin where \((0,1,0)\) used to be

intercepts \[
\begin{array}{ccc}
  x & y & z \\
  \frac{1}{2} & -1 & 1
\end{array}
\]

reciprocal (plane \((2\ 1\ 1)\)) 1 pt

iii) Move origin again

intercepts \[
\begin{array}{ccc}
  x & y & z \\
  1 & -1 & \infty
\end{array}
\]

reciprocal (plane \((1\ 1\ 0)\)) 1 pt
a) Cubic unit cell

\[(111)\]

\[h = \frac{1}{A}\]
\[k = \frac{1}{B}\]
\[l = \frac{1}{C}\]

\[A = \frac{1}{h}\]
\[B = \frac{1}{k}\]
\[C = \frac{1}{l}\]

\[A = \frac{1}{1} = 1\]  \[B = \frac{1}{1} = 1\]  \[C = \frac{1}{1} = 1\]

b) \((201)\)

\[A = \frac{1}{2}\]
\[B = \infty\]
\[C = \frac{1}{1} = 1\]
Problem 6 [3]

Identify the crystallographic directions shown in the unit cell below.  
1 pt each

A) \((0, 1/2, 1) - (2/3, 0, 1) = (-2/3, 1/2, 0) \) ----- [430]

B) \((1, 0, 2/3 ) - (1/3, 1, 0) = (2/3, -1, 2/3) \) ----- [232]

C) \((2/3, 0, 0) - (1/3, 1, 1) = (1/3, -1, -1) \) ----- [133]
Problem 8 [2]

The planar density (PD) is the number of atoms per unit area measured in reciprocal area (e.g. m^-2 or radius ^ -2), where PD = \( \frac{\text{number of atoms centered on a plane}}{\text{area of plane}} \). For the FCC unit cell, calculate PD for the (100), (110), or (111) plane in terms of the atom radius \( r \)

\[
\text{1 pt Natoms, 1 pt Aplane}
\]

\[
\begin{align*}
\text{(100) } & \quad \text{PD} = \frac{\text{Natoms}}{A\text{plane}}; \\
& \quad a = 2\sqrt{2} \times r; \\
\end{align*}
\]

\[
\begin{align*}
\text{(110) } & \quad \text{Natoms} = 1 + 4 \times 1/4; \\
& \quad A\text{plane} = a^2; \\
& \quad \text{PD}[\text{Natoms, Aplane}] = \frac{1}{4 \times r^2} \\
& \quad 1/4. \\
\end{align*}
\]

\[
\begin{align*}
\text{(111) } & \quad 0.25
\end{align*}
\]
(110)

\[ \text{Natoms} = 4 \times \frac{1}{4} + 2 \times \frac{1}{2}; \]
\[ l_{110} = 4 \times r; \text{(*the length of the unit cell along the [110] direction*)} \]
\[ \text{Aplane} = a \times l_{110}; \]
\[ \text{PD[Natoms, Aplane]} \]
\[ \frac{1}{4 \sqrt{2} \ r^2} \]
\[ 1/(4 \text{Sqrt}[2.]) \]
\[ 0.176777 \]

(111)

\[ \text{Natoms} = 3 \times \frac{1}{2} + 3 \times \frac{1}{6}; \]
\[ \text{Aplane} = \sqrt{3}/4 \times (4 \times r)^2; \text{(*area of equilateral triangle*)} \]
\[ \text{PD[Natoms, Aplane]} \]
\[ \frac{1}{2 \sqrt{3} \ r^2} \]
\[ 1/(2 \text{Sqrt}[3.]) \]
\[ 0.288675 \]