1. Maximum impurity radius $r$ of FCC octahedral site

\[ Z = \frac{1}{2} \text{ in FCC} \]

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

\[ \sqrt{2}2R + \sqrt{2}2r = 4R \]
\[ \sqrt{2}R + \sqrt{2}r = 2R \]
\[ r = \frac{2R - \sqrt{2}R}{\sqrt{2}} \]
\[ \frac{r}{R} = \frac{2 - \sqrt{2}}{\sqrt{2}} = 0.41 \]

2. Maximum impurity radius $r$ of BCC tetrahedral site @ $\frac{1}{2}$, $\frac{1}{4}$

\[ Z = 0 = 1 \text{ in BCC} \]

\[ a = \frac{4R}{\sqrt{3}} \]

\[ (R + r)^2 = \left(\frac{a}{4}\right)^2 + \left(\frac{a}{2}\right)^2 \]

\[ (R + r)^2 = \frac{R^2}{(\sqrt{3})^2} + \left(\frac{2R}{\sqrt{3}}\right)^2 \]

\[ R^2 + 2Rr + r^2 = \frac{R^2}{3} + \frac{4R^2}{3} = \frac{5R^2}{3} \]

\[ -\frac{2R^2}{3} + 2Rr + r^2 = 0 \]

use quadratic formula

\[ r = -2R \pm \sqrt{4R^2 + \frac{8R^2}{3}} \]
\[ = -2R \pm R \sqrt{\frac{20}{3}} \]
\[ = \frac{2}{2} \]

\[ r = 0.29R \]

\[ \frac{r}{R} = 0.29 \]

\[ \frac{R}{R} = 0.29 \]

[3]
2. Consider a sample of AISI 5160 steel which has the following composition.

<table>
<thead>
<tr>
<th>Site</th>
<th>Reasoning</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>similar size, BCC</td>
</tr>
<tr>
<td>Mn</td>
<td>similar size, BCC</td>
</tr>
<tr>
<td>Cr</td>
<td>small, different crystal structure, different electronegativity</td>
</tr>
<tr>
<td>C</td>
<td>small, different electronegativity</td>
</tr>
<tr>
<td>P</td>
<td></td>
</tr>
</tbody>
</table>

```
In[1]:= atoms = {"Fe", "Mn", "Cr", "C", "P"};
weights = {97.6, 1, 0.7, 0.66, 0.04};
molarmasses = {55.847, 54.938, 51.996, 12.011, 30.974};
atomicradiuspm = {126, 127, 128, 70, 100};
crystalstructures = {"BCC", "BCC", "BCC", "diamond, graphite", "BCC"};
electronegativity = {1.83, 1.55, 1.66, 2.55, 2.19};
site = {"", "sub", "sub", "interstitial", "int"};
reasoning = {"", "similar size, BCC", "similar size, BCC",
  "small, different crystal structure, different electronegativity",
  "small, different electronegativity"};

atomicpcts = weights / molarmasses / Total[weights / molarmasses] * 100;

Total[atomicpcts]
100.
```
In[14]:= Grid[Transpose[Prepend[Transpose[{Atoms, Weights, MolarMasses, AtomicRadiusPm, CrystalStructures, Electronegativity, Sites, Reasoning, AtomicPcts}], {"atom", "wt\%", "molar mass (amu)", "atomic radius (pm)", "crystal structure", "electronegativity (pauling)", "site", "reasoning", "atomic \%"}], Frame -> All, ItemSize -> 6]]

<table>
<thead>
<tr>
<th>atom</th>
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<th>Mn</th>
<th>Cr</th>
<th>C</th>
<th>P</th>
</tr>
</thead>
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<tr>
<td>wt%</td>
<td>97.6</td>
<td>1</td>
<td>0.7</td>
<td>0.66</td>
<td>0.04</td>
</tr>
<tr>
<td>molar mass (amu)</td>
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<tr>
<td>crystal structure</td>
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<td>BCC</td>
<td>BCC</td>
<td>diamond, graphite</td>
<td>BCC</td>
</tr>
<tr>
<td>electronegativity (pauling)</td>
<td>1.83</td>
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<td>1.66</td>
<td>2.55</td>
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<td>reasoning</td>
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<td>small, different electronegativity</td>
<td></td>
</tr>
<tr>
<td>atomic %</td>
<td>95.2109</td>
<td>0.991662</td>
<td>0.73344</td>
<td>2.99365</td>
<td>0.0703557</td>
</tr>
</tbody>
</table>

BCC has 12 interstitial sites per 2 substitutional

latticeatoms = Total[atomicpcts[[1 ;; 3]]]
substatoms = Total[atomicpcts[[4 ;; 5]]]
96.936
3.06401

let's say we have 100 atoms: 97 of them will be lattice atoms and 3 will be substitutional atoms
latticeatoms * 6
581.616

that leaves us with 582 tetrahedral interstitial sites

substatoms / (latticeatoms * 6)
0.0052681

0.526 % of sites are filled
edge dislocation line $\perp \mathbf{b}$ \cite{1}

Screw dislocation line $\parallel \mathbf{b}$ \cite{1}
4. Consider the following high-angle annular dark-field scanning transmission electron microscopy (HAADF STEM) image of a low-angle grain boundary in strontium titanate.

(a) How many dislocation cores are in this image? 2 [1 pt]

(b) Use a Burger's circuit and the resulting Burger's vector to classify each dislocation as either an edge, screw, or point dislocation (point dislocations have a Burgers vector of 0). Both edge [2]
a) twin boundary — A special kind of grain boundary across which there is a specific mirror lattice symmetry.

b) twin — the region of material between twin boundaries

b) Applied mechanical shear forces (observed in BCC and HCP)

- Annealing heat treatments following deformation (typically FCC)

5

6

a) ... ABC A BC B AC BA ...

b) ... ABC A BC BCA B C ...

FCC HCP FCC

This defect is a twin boundary.

We can tell because the stacking sequence is mirrored on either side of the boundary.

Stacking fault between the 2 lines.