Crystal structures

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The simplest crystal structures, including of most elements, can be considered as formed from the close packings of spheres. Studying the close-packing of spheres throws light on the kind of criteria that are important for stabilizing some structures over others.

- Close packing of spheres — ccp and hcp
- The sizes of tetrahedral and octahedral voids and the notion of radius ratio (see handout)
- The structures of the elements:
  - α-Po at 283 K:
    SG = \( Pm\bar{3}m \) (No. 221) \( a = 3.295 \ \text{Å} \)
    
    \[
    \begin{array}{cc}
    \text{Atom} & x \ y \ z \\
    \hline
    \text{Po} & 0 \ 0 \ 0 \\
    \end{array}
    \]
  - α-Fe (bcc-Fe):
    SG = \( Im\bar{3}m \) (No. 229) \( a = 2.86 \ \text{Å} \)
    
    \[
    \begin{array}{cc}
    \text{Atom} & x \ y \ z \\
    \hline
    \text{Fe} & 0 \ 0 \ 0 \\
    \end{array}
    \]
  - Cu:
    SG = \( Fm\bar{3}m \) (No. 225) \( a = 3.60 \ \text{Å} \)
    
    \[
    \begin{array}{cc}
    \text{Atom} & x \ y \ z \\
    \hline
    \text{Cu} & 0 \ 0 \ 0 \\
    \end{array}
    \]
  - Mg:
    SG = \( P6_3/mmc \) (No. 194) \( a = 3.20 \ \text{Å} \ c = 5.20 \ \text{Å} \)
    
    \[
    \begin{array}{cc}
    \text{Atom} & x \ y \ z \\
    \hline
    \text{Mg} & 1/3 \ 2/3 \ 3/4 \\
    \end{array}
    \]
  - Si:
    SG = \( Fd\bar{5}m \) (No. 227) \( a = 5.43042 \ \text{Å} \)
    
    \[
    \begin{array}{cc}
    \text{Atom} & x \ y \ z \\
    \hline
    \text{Si} & 0 \ 0 \ 0 \\
    \end{array}
    \]
  - C (graphite):
    SG = \( P6_3/mmc \) (No. 194) \( a = 2.4612 \ \text{Å} \ c = 6.7090 \ \text{Å} \)
    
    \[
    \begin{array}{cc}
    \text{Atom} & x \ y \ z \\
    \hline
    \text{C} & 0 \ 0 \ 1/4 \\
    \text{C} & 2/3 \ 1/3 \ 1/4 \\
    \end{array}
    \]
- AB crystal structures (NaCl, CsCl, ZnS (wurtzite), ZnS (zinc blende) NiAs)

**NaCl:** SG = $Fm\bar{3}m$ (No. 225) $a = 5.63 \text{ Å}$

| Atom | $x$  | $y$  | $z$  |
|------|------|------|------|
| Na   | 0    | 0    | 0    |
| Cl   | 1/2  | 1/2  | 1/2  |

**CsCl:** SG = $Pm\bar{3}m$ (No. 229) $a = 4.11 \text{ Å}$

| Atom | $x$  | $y$  | $z$  |
|------|------|------|------|
| Cs   | 1/2  | 1/2  | 1/2  |
| Cl   | 0    | 0    | 0    |

**ZnS (wurtzite):** SG = $P6_3mc$ (No. 186) $a = 3.83 \text{ Å} = 6.23 \text{ Å}$

| Atom | $x$  | $y$  | $z$  |
|------|------|------|------|
| Zn   | 2/3  | 1/3  | 0    |
| S    | 2/3  | 1/3  | $\sim 3/8$ |
**ZnS (zinc blende):** SG = $F\overline{4}3m$ (No. 216) $a = 5.41 \, \text{Å}$

| Atom | $x$ | $y$ | $z$  |
|------|-----|-----|------|
| Zn   | 0   | 0   | 0    |
| S    | 1/4 | 1/4 | 1/4  |

**NiAs:** SG = $P6_3/mmc$ (No. 194) $a = 3.60 \, \text{Å} \ c = 5.01$

| Atom | $x$ | $y$ | $z$  |
|------|-----|-----|------|
| Ni   | 0   | 0   | 0    |
| As   | 2/3 | 1/3 | 1/4  |

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### Diagrams

**ZnS**

- Zn at $z=0$
- S at $z=1/4$, $z=1/2$, $z=3/4$

**NiAs**

- Ni at $z=0$
- As at $z=1/4$, $z=1/2$, $z=3/4$