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This class closely follows the third chapter of Callister

Radius ratio recap

The *Radius ratio* rule states that a coordination polyhedron is formed around each cation. The distance between the cation and the anion is the sum of the ionic radii ($r_A + r_C$). The number (coordination number CN) of anions around the cation is determined by the radius ratio r_A/r_C. Also see the in-class handout.

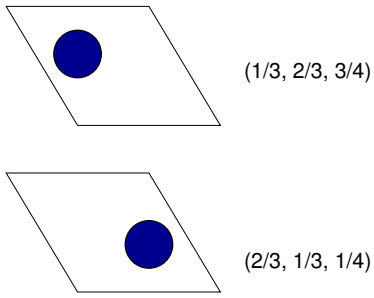
The crystal systems

See the in-class handout.

Some hexagonal structures

hcp – the structure of Mg The cell parameters are $a = 3.20$ Åand $c = 5.20$ Å.

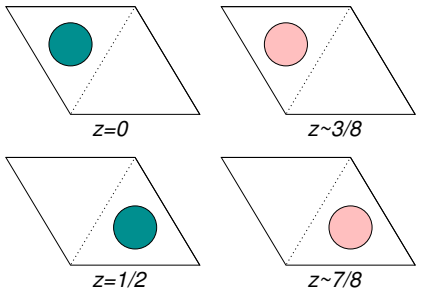
The cell comprises one Mg atoms at (2/3,1/3,1/4) and the other at (1/3,2/3,3/4).



Graphite The cell is $a = 2.4612$ Åand $c = 6.7090$ Å. The atoms are at (0,0,1/4), (0,0,3/4), (1/3,2/3,3/4) and (2/3,1/3,1/4).

Wurtzite, the other ZnS structure $a = 3.81$ Å $= 6.23$ Å

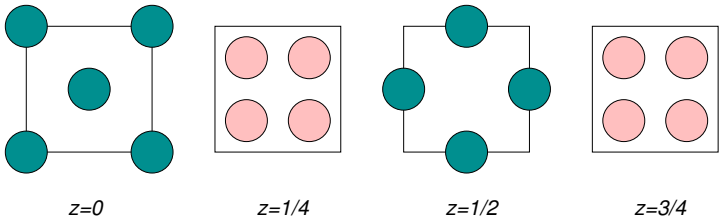
Atom	x	y	z
Zn	2/3	1/3	0
Zn	1/3	2/3	1/2
S	2/3	1/3	∼3/8
S	1/3	2/3	∼7/8



More complex cubic structures

Fluorite CaF_2 fcc $a = 5.45$ Å

Atom	x	y	z
Ca	0	0	0
F	1/4	1/4	1/4

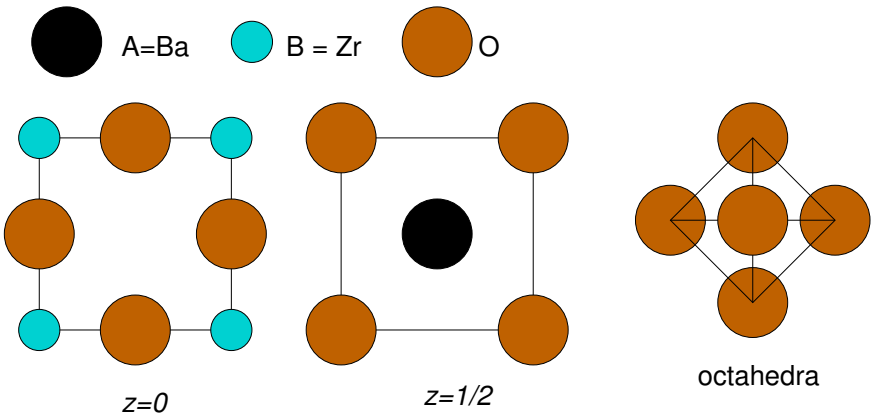


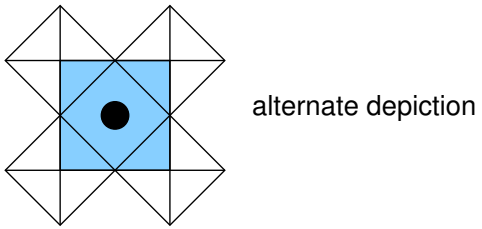
This structure type is also adopted by SrF_2, BaF_2, UO_2, ThO_2, Na_2O (the anti-type), ZrO_2 at high temperatures ...

ZrO_2 can be stabilized in the fluorite structure through doping with Ca^{2+} or Y^{3+} – these are *stabilized* zirconias and have many structural and electrochemical applications.

Perovskite ABO_3 $BaZrO_3$ (A = Ba, B = Zr):
Simple Cubic $a = 4.194$ Å

Atom	x	y	z
Ba	1/2	1/2	1/2
Zr	0	0	0
O	1/2	0	0





Miller indices

See the in-class handout.