MATRL 218/CHEM 227: Class V — Structures 1
CCP and HCP, voids, radius ratio rules, the structures of elements α-Po, Fe, Cu, Mg, Si (diamond), C (graphite)

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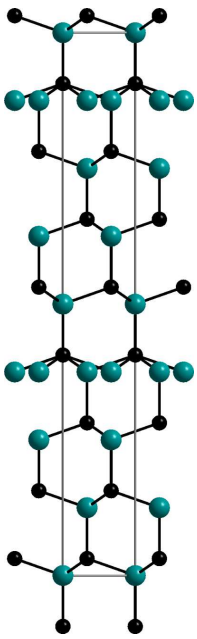
The simplest crystal structures, including of most elements, can be considered as formed from the close packings of spheres. Studying the close-packing of spheres throws light on the kind of criteria that are important for stabilizing some structures over others.

- Close packing of spheres — ccp and hcp; the different stackings (see handout)
- The sizes of tetrahedral and octahedral voids and the notion of radius ratio (see handout)
- The structure of SiC — Polytypism

  SiC has a binary tetrahedral structure in which the Si and C layers are stacked alternately, each C atom layer occupying half the tetrahedral voids between successive close-packed Si layers. The structure can be considered as being formed between identical interpenetrating close-packings.

  Whilst in a simple hcp structure, the packing of layers could be written ABABAB . . . , in SiC, one could write for the simplest *polytype* the packing as AaBbAaBbAaBb . . . , where the first (upper case) letter refers to Si, and the second (lower case) letter refers to C.

  However, SiC in particular, can show horrendously complicated packing sequences, and some of the polytypes have cell parameters as large as a 1000 Å in the stacking (C) direction. The structure below shows the so-called $8H$ form, the 8 standing for the number of repeats and the H signifying that the resulting structure falls into a hexagonal (rather than cubic or rhombohedral) space group:



  The (larger) Si atoms are olive and the C, black. The stacking sequence is AaBbCcAaBbAaCcBbAaBbCcAaBb

- The structures of the elements:
  - α-Po at 283 K:
    SG = $Pm\bar{3}m$ (No. 221) a = 3.295 Å

Atom	x	y	z
Po	0	0	0

  - α-Fe (bcc-Fe):
    SG = $Im\bar{3}m$ (No. 229) a = 2.86 Å

Atom	x	y	z
Fe	0	0	0

  - Cu:

    SG = $Fm\bar{3}m$ (No. 225) a = 3.60 Å

Atom	x	y	z
Cu	0	0	0

  - Mg:

    SG = $P6_3/mmc$ (No. 194) a = 3.20 Å c = 5.20 Å

Atom	x	y	z
Mg	1/3	2/3	1/4

  - Si:

    SG = $Fd\bar{3}m$ (No. 227) a = 5.43042 Å

Atom	x	y	z
Si	0	0	0

  - C (graphite):

    SG = $P6_3/mmc$ (No. 194) a = 2.4612 Å c = 6.7090 Å

Atom	x	y	z
C	0	0	1/4
C	1/3	2/3	1/4