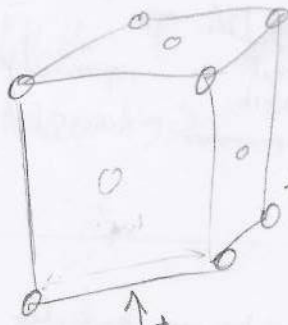
oblig 4

2). assume fcc-Si ($a = 5.43\,\text{Å}$)
"diamond cubic"

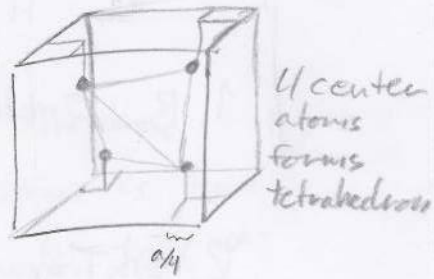


a) There are atoms at:

Corners ($8 \cdot 1/8$): 000 001 010 100 011 101 110 111

Faces ($6 \times 1/2$): 0 1/2 1/2, 1/2 0 1/2, 1/2 1/2 0, 1 1/2 1/2, 1/2 1 1/2, 1/2 1/2 1

Inside (4): 1/4 1/4 1/4, 3/4 3/4 1/4, 3/4 1/4 3/4, 1/4 3/4 3/4



Basis vectors:

$\vec{a} = (0\ 1/2\ 1/2)$ $\vec{b} = (1/2\ 1/2\ 0)$ $\vec{c} = (1/4\ 1/4\ 1/4)$

Summing any integer-scaled basis vectors (linear combination with integers as weights) gives the position of an atom. All atoms can be represented in this way.

$$\vec{x} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c} = 2n_1(0\ 1/4\ 1/4) + 2n_2(1/4\ 0\ 1/4) + n_3(1/4\ 1/4\ 1/4)$$

c) $N_a = 8 \cdot 1/8 + 6 \cdot 1/2 + 1 \cdot 4 = \underline{8}$ eight atoms / unit cell

each Si-atom has 14 electrons. $8 \cdot 14 = \underline{112} = N_e$

b) $N_a = 8 \cdot 1/8 + 6 \cdot 1/2 = 4$ $N_e = 4 \cdot 14 = 56$