TFY4245/FY8917 Solid State Physics, Advanced Course

Problemset 1

NTNU

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SUGGESTED SOLUTION

Problem 1

(a) One possible unit cell is a rhombohedral prism with rhombus ABCD serving as the base.

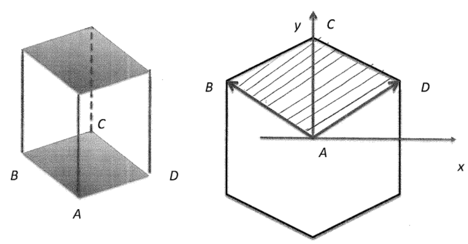

Figure 1: Possible unit cell. Figure taken from `https://www.phys.ufl.edu/~maslov/`.

The basis vectors are

$$\begin{aligned} \boldsymbol{a}_1 &= \frac{a}{2}(\sqrt{3}\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}}), \\ \boldsymbol{a}_2 &= \frac{a}{2}(-\sqrt{3}\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}}), \\ \boldsymbol{a}_3 &= c\hat{\boldsymbol{z}}. \end{aligned} \tag{1}$$

(b) The volume of the unit cell:

$$V = |(\boldsymbol{a}_1 \times \boldsymbol{a}_2) \cdot \boldsymbol{a}_3| = \sqrt{3}a^2c/2. \tag{2}$$

(c) Basis vectors of the reciprocal lattice:

$$\begin{aligned} \boldsymbol{b}_1 &= \frac{2\pi}{V}(\boldsymbol{a}_2 \times \boldsymbol{a}_3) = \frac{2\pi}{a}(\frac{\sqrt{3}3}{\hat{\boldsymbol{x}}} + \hat{\boldsymbol{y}}), \\ \boldsymbol{b}_2 &= \frac{2\pi}{V}(\boldsymbol{a}_3 \times \boldsymbol{a}_1) = \frac{2\pi}{a}(-\frac{\sqrt{3}}{3}\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}}), \\ \boldsymbol{b}_3 &= \frac{2\pi}{V}(\boldsymbol{a}_1 \times \boldsymbol{a}_2) = \frac{2\pi}{c}\hat{\boldsymbol{z}}. \end{aligned} \tag{3}$$

The reciprocal unit cell is a prism with a base built on the vectors $\boldsymbol{b}_1, \boldsymbol{b}_2$.

(d) Even though graphene has two sublattices conventionally denoted A and B (inequivalent atoms in terms of the surroundings that they see), all atoms are still identical carbon atoms. Thus, performing an inversion operation around the center of each 'tile' in the system leaves it invariant. Thus, graphene has inversion symmetry.

Problem 2

(a) A sphere at the corner of the fcc unit cell shares volume with 8 unit cells. Therefore, the number of spheres at the corner is 1/8. There are 8 corners in the fcc unit cell. A sphere at the face is shared by two unit cells, i.e. the number is 1/2 per unit cell. There are 6 faces in the fcc unit cell. The total number of spheres is then $1/8 \times 8 + 1/2 \times 6 = 4$.

(b) Same reasoning provides $1/8 \times 8 + 1 = 2$.

(c) Same reasoning provides $1/8 \times 8 + 1/2 \times 6 + 4 = 8$. This can also be seen from the fact that the diamond unit cell consists of four bcc unit cells. Thus, the number of atoms is four times the bcc value.

Problem 3

(a) GaAs has a zincblende structure and has 4 Ga atoms per unit cell. The density is therefore $4/(5.65 \times 10^{-8})^3 = 2.22 \times 10^{22}$ [atoms/cm^3].

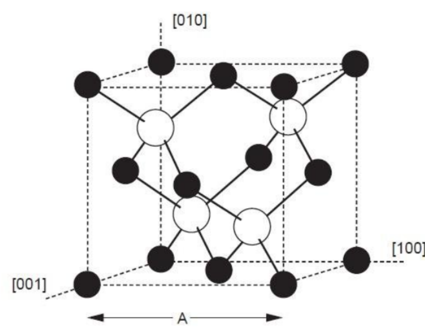

Figure 2: GaAs unit cell (As atoms in white). The lattice constant a is denoted A in the figure. Figure taken from `https://www.researchgate.net/figure/Unit-cube-of-GaAs-crystal-lattice-Nayak-et-al-2006_fig1_262049410`.

(b) Ge has a diamond structure with 8 Ge atoms per unit cell, as we saw in Problem 2(c). Thus, the density is $8/(5.65 \times 10^{-8})^3 = 4.44 \times 10^{22}$ [atoms/cm^3].