Problem Set 1

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1. Given two vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ from Fig. 10,

$$\mathbf{a}_1 = \frac{1}{2}a\left(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}\right)$$
$$\mathbf{a}_2 = \frac{1}{2}a\left(-\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}}\right),$$

the angles between these can be found using the inner product,

$$\mathbf{a}_1 \cdot \mathbf{a}_2 = \frac{a^2}{4}(-1+1-1) = -\frac{a^2}{4}$$
$$= a_1 a_2 \cos\theta.$$
$$\cos\theta = -\frac{a^2}{4}\left(\frac{2}{a\sqrt{3}}\right)^2 = \frac{1}{3}$$
$$\boxed{\theta \approx 70.53\,\mathrm{deg.}}$$

2. From Figure 11, the (100) plane intercepts the x and z axis at $\sqrt{2}a$. Normalizing this, the new plane is (100).

   For (001), it's similar but intercepts the y and z axis, leading to (011).

3. A single NaCl molecule will have a volume

$$23\,\mathrm{u} \times 1.660 \times 10^{-27}\,\mathrm{kg}\cdot\mathrm{u}^{-1} \times 1000\,\mathrm{g}\cdot\mathrm{kg}^{-1}/1.0\,\mathrm{g}\cdot\mathrm{cm}^{-3} = 3.82 \times 10^{-23}\,\mathrm{cm}^3$$
$$= a^3$$
$$\boxed{\implies a = 3.37\,\text{Å}.}$$

4. For simple cubic, the spheres will have radius $a/2$. Using a volume of a sphere,

$$V_{\mathrm{sph}} = \frac{4}{3}\pi\left(\frac{a}{2}\right)^3$$
$$= \frac{a^3}{6}\pi$$
$$\text{Packing fraction } P = \frac{V_{\mathrm{sph}}}{V_{\mathrm{cube}}}$$
$$= \frac{1}{6}\pi.$$

   For body-centered cubic, the spheres will have radius $\sqrt{3}a/4$ (from the listed nearest neighbor distance, halved to give radius) and there will be two full spheres. The volume is then

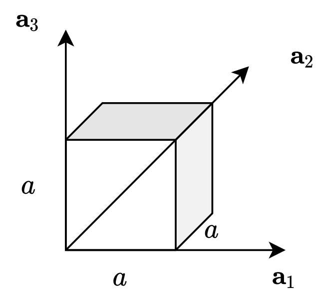
$$V_{\mathrm{sph}} = 2 \times \frac{4}{3}\pi\left(\sqrt{3}a/4\right)^3$$
$$= \frac{\pi\sqrt{3}}{8}a^3.$$
$$P = \frac{\pi\sqrt{3}}{8}.$$

For face-centered cubic, the spheres will have radius $a/2\sqrt{2}$ and now there are four full spheres enclosed.

$$\begin{aligned} V_{\text{sph}} &= 4 \times \frac{4}{3}\pi\left(\frac{a}{2\sqrt{2}}\right)^3 \\ &= \frac{\pi\sqrt{2}}{6}a^3. \\ P &= \frac{\pi\sqrt{2}}{6}. \end{aligned}$$

5. (a) ABC_3? I'm not entirely sure.
   (b) sc.
   (c) A primitive lattice translation vectors are just a in each direction,

$$\begin{aligned} \mathbf{a}_1 &= a\,\hat{\mathbf{x}} \\ \mathbf{a}_2 &= a\,\hat{\mathbf{y}} \\ \mathbf{a}_3 &= a\,\hat{\mathbf{z}}. \end{aligned}$$



   (d) For atom A, there is one atom per cell,

$$\mathbf{r}_1 = 0.$$

   For atom B, there is one atom per cell,

$$\mathbf{r}_5 = 0.5\mathbf{a}_1 + 0.5\mathbf{a}_2 + 0.5\mathbf{a}_3.$$

   For atom C, there are 3 atoms per cell,

$$\begin{aligned} \mathbf{r}_2 &= 0.5\mathbf{a}_1 + 0.5\mathbf{a}_2 \\ \mathbf{r}_3 &= 0.5\mathbf{a}_1 + 0.5\mathbf{a}_3 \\ \mathbf{r}_4 &= 0.5\mathbf{a}_2 + 0.5\mathbf{a}_4. \end{aligned}$$