Workshop 1: Answers

1. Tennis balls and argon atoms

The packing fraction is the fraction of space which is occupied by spheres. The best possible packing fraction is $f = \pi/(3\sqrt{2}) \approx 74\%$ (although in random packing 63% is more realistic).

The *usable* volume is $f \times V_C$ where V_C is the volume of the cuboid. The volume of a sphere is $V_S = (4/3)\pi r^3$. Hence $N = fV_C/V_S \approx 155k$.

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Very similar physical picture to the above, but much much smaller.

Density is mass per volume $\rho = nm$ where n is the number density and, in the FCC, there are 4 atoms per conventional unit cell i.e. $n = 4/a^3$ where a is the length of the conventional unit cell.

Hence, $a = (4m/\rho)^{1/3} \approx 547\,\mathrm{pm}$.

Draw one face of the FCC and a triangle, or recall: $a^2 + a^2 = (4r)^2 \implies r = a/(2\sqrt{2}) \approx 193\,\mathrm{pm}$.

2. X-ray diffraction

Amplitude of the diffracted electric field is non-zero when the difference in wavevector is a reciprocal lattice vector. We describe the lattice with simple cubic vectors, and reciprocal lattice vectors correspond to h, k, l being integers.

The additional requirement, arising from interference between the 2 (BCC) or 4 (FCC) points in the conventional unit cell, is captured by the GSF.

One approach to this problem is to find the ratio squared of orders to the first observed order, and compare that with the value of $h^2 + k^2 + l^2$. i.e. $(0.333/0.289)^2 = 1.33 = 4/3$ and $(0.471/0.289)^2 = 2.66 = 8/3$. These ratios correspond to the first few non-zero orders for the FCC. Hence, we identify the structure as FCC.

We can then pick an order and calculate the lattice constant. e.g. $a = \frac{\lambda}{2\times 0.289} \times \sqrt{3} = 3.0\,\mathrm{A}$.