Solid State Theory
Solution 2

Problem 2.1 Packing fractions

The formula which gives the filling fraction for the general lattice is

$$f = \frac{V_s * N_{sites}}{V_{uc}}, \tag{1}$$

where V_s is given by the volume of a ball whose radius is the half of the shortest nearest neighbour distance, V_{uc} is the volume of the unit cell, and N_{sites} is the number of lattice points in the unit cell.
Using the same notation as in the lecture, the nearest neighbour distance is $\frac{1}{2}\,a$, $\frac{\sqrt{2}}{2}\,a$, and $\frac{\sqrt{3}}{4}\,a$ for the hcp, fcp, and diamond lattices, respectively (for illustrations see pg. 3 of the notes on lecture 3). The number of sites in a unit cell is 2 (hcp), 4 (fcp), and 8 (diamond) [1], and the volume of the unit cell is a^3 for the cubic lattices. For the hexagonal lattice, notice that $c = \sqrt{\frac{2}{3}}2a$ and the area of the base parallelogram is $\frac{\sqrt{3}}{2}a^2$, giving $\sqrt{2}a^3$ as the volume of the unit cell. Therefore, the filling fractions are

$$\frac{\pi}{\sqrt{18}}, \quad \frac{\pi}{\sqrt{18}}, \quad \frac{\sqrt{3}\pi}{16},$$

for the hcp, fcp, and diamond lattices respectively. Notice that the filling fractions of the two cubic close packed lattices are the same since changing the stacking order from ABC and ABA does not change the volume fraction.

Problem 2.2 Angle between the bonds in the diamond lattice

The nearest neighbour (n.n.) distance in a diamond lattice is $\frac{\sqrt{3}}{4}$. On the other hand, the next nearest neighbour (n.n.n.) distance is the same as the n.n. of the fcc lattice ($\frac{\sqrt{2}}{2}$). Therefore, the angle between two bonds joining a site of the diamond lattice is the same as the obtuse angle in the isosceles triangle in Fig.1, which is

$$cos^{-1}(-1/3) \approx \ 109.4\,\text{degrees}.$$

Notice that for each site in the diamond lattice their nearest neighbours form a perfect tetrahedron.[2]

[1] While counting the number of sites in a unit cell, one needs take into account whether the sites are lying on the corners, edges, or faces. Such sites can be considered to be shared equally by all cells they touch. For instance, for a 3D cubic lattice, each site situated at the corners are counted as $\frac{1}{8}$ sites, each site on the edges as $\frac{1}{4}$ sites, and each site on the faces are counted as $\frac{1}{2}$ sites. It is not necessary to compute the partial volume of a sphere contained in one cell because any part cut off by the cell boundary must be compensated by another sphere related to the first by a lattice translation.

[2] For an interactive viewing of the various 3D lattices : http://www.dawgsdk.org/crystal/en/library/diamond

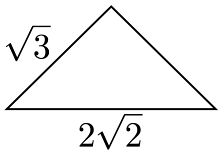

Figure 1: The triangle defined by three nearest neighbours in the diamond lattice

Problem 2.3 Anisotropy of the hexagonal lattice

The result follows from the fact that the 2D resistivity tensor is a symmetric two-tensor, which defines a quadratic form. A generic real symmetric matrix ρ, defines the quadratic form

$$q_A(\mathbf{x}) = \mathbf{x}^T \cdot \rho \cdot \mathbf{x}.$$

The symmetries of the matrix ρ are defined by the unitary matrices U that satisfy

$$U^{-1}\rho U = \rho.$$

Therefore, we have

$$q(\mathbf{x}) = \mathbf{x}^T \cdot \rho \cdot \mathbf{x} = \mathbf{x}^T \cdot (U^{-1}\rho U) \cdot \mathbf{x} = (U\mathbf{x})^T \cdot \rho \cdot (U\mathbf{x}). \tag{2}$$

Now notice that in two dimensions $q_A(x) = 1$ is an equation which describes an ellipse in the $x - y$ plane for positive definite ρ. [3] Since Eq. 2, describes a rotation of this ellipse, the only allowed non-trivial symmetries of a generic ρ are reflections ($\mathbf{x} \to -\mathbf{x}$ and $\mathbf{y} \to -\mathbf{y}$). If the crystal symmetry imposes any further symmetry on ρ, it can only be in the trivial representation of this symmetry group (i.e. the matrix ρ is proportional to identity and the ellipse a circle). As a result, any 2D lattice that has rotational symmetries higher than C_2 has an isotropic linear response.

[3] When ρ is negative definite the solutions describe an imaginary ellipse, and if it is indefinite the solutions describe a hyperbola. But the argument is also valid for these cases.