Exercise 1 Lattice planes, Miller indices and the reciprocal lattice

(a) Consider a generic crystallographic plane (hkl) in a crystal lattice. Prove that:

(i) the reciprocal lattice vector $\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$ is perpendicular to the given plane.

Hint: recall that the Miller indices of a plane represent the reciprocal of the intercepts of that plane with the basis vectors.

(ii) the distance between two adjacent parallel planes of the lattice is $d(hkl) = 2\pi/G$, where G here indicates the norm of the vector $\mathbf{G}$.

(b) Show that the density of lattice points per unit area in a lattice plane is d/V, where V is the primitive cell volume and d is the spacing between neighboring planes in the family to which the given plane belongs.

(c) Prove that the lattice planes with the greatest densities of points are the $\{111\}$ planes in the face–centered cubic and the $\{110\}$ planes in a body–centered cubic Bravais lattice.

Hint: use the relation between families of lattice planes and vectors of the reciprocal lattice.

Solution to Exercise 1

1. (a) To prove that the reciprocal lattice vector $\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$ is perpendicular to the plane (hkl), it suffices to show that $\mathbf{G}$ is perpendicular to two non–parallel vectors in this plane. For the plane (hkl), it intercepts axis $\mathbf{a}_1$, $\mathbf{a}_3$ and $\mathbf{a}_3$ at a ratio $\frac{1}{h} : \frac{1}{k} : \frac{1}{l}$, thus the two vectors in the plane can be chosen as $\mathbf{v}_1 = \left(\frac{1}{h}\mathbf{a}_1 - \frac{1}{k}\mathbf{a}_2\right)$ and $\mathbf{v}_2 = \left(\frac{1}{h}\mathbf{a}_1 - \frac{1}{l}\mathbf{a}_3\right)$. Clearly, these vectors are not parallel to each other. From direct calculation:

$$\mathbf{G} \cdot \mathbf{v}_1 = (h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3) \cdot (\frac{1}{h}\mathbf{a}_1 - \frac{1}{k}\mathbf{a}_2) = 0,$$

$$\mathbf{G} \cdot \mathbf{v}_2 = (h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3) \cdot (\frac{1}{h}\mathbf{a}_1 - \frac{1}{l}\mathbf{a}_3) = 0.$$

Since $\mathbf{G}$ is perpendicular to those two vectors, it is also perpendicular to the given plane.

(b) Among the indices (hkl), at least one of them is non zero; without loss of generality, we can choose $h \neq 0$. Since, by definition, this family of planes divide vector $\mathbf{a}_1$ into h parts with equal length, then the vector $\mathbf{R}_1 = 0$ ends on one plane, and $\mathbf{R}_2 = \frac{1}{h}\mathbf{a}_1$ ends on an adjacent plane. Therefore, the projection of $\mathbf{R}_2 - \mathbf{R}_1$ on the direction perpendicular to this family of planes will be the distance between two neighboring planes. From (a) we know that $\mathbf{G}$ is perpendicular to these planes, hence

$$d(hkl) = \left|\frac{1}{h}\mathbf{a}_1 \cdot \frac{\mathbf{G}}{G}\right| = \left|\frac{1}{h}\mathbf{a}_1 \cdot \frac{h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3}{G}\right| = \frac{2\pi}{G}.$$

2. Within each plane, the lattice is a two–dimensional lattice. Let the area of the primitive cell for this 2D lattice be A, then since V is volume of primitive cell for 3D lattice, it follows that $A \cdot d = V$. Since every primitive cell contains exactly one lattice point, the number density of lattice points on this plane ρ is
$$\rho = 1/A = d/V.$$

3. Once the type of a lattice is given, the volume of primitive cell V is fixed. Thus from part (b), the larger the interplane distance d is, the greater the density of points ρ is. From the result of (a–ii), the largest d corresponds to the family of planes for which the length of a reciprocal lattice vector $\mathbf{G}$ perpendicular to them is minimized. Thus, if we could find out a $\mathbf{G}_0$ in reciprocal space with least length, then the real space lattice planes perpendicular to this $\mathbf{G}_0$ will have largest density of lattice points. Let's discuss separately the two cases:

   (a) For the FCC the primitive basis is
   $$\mathbf{a}_1 = \frac{a}{2}(\mathbf{y}+\mathbf{z}), \quad \mathbf{a}_2 = \frac{a}{2}(\mathbf{x}+\mathbf{z}), \quad \mathbf{a}_3 = \frac{a}{2}(\mathbf{x}+\mathbf{y})$$
   and then the reciprocal lattice has
   $$\mathbf{b}_1 = \frac{4\pi}{a}\frac{1}{2}(\mathbf{y}+\mathbf{z}-\mathbf{x}), \quad \mathbf{b}_2 = \frac{4\pi}{a}\frac{1}{2}(\mathbf{x}+\mathbf{z}-\mathbf{y}), \quad \mathbf{b}_3 = \frac{4\pi}{a}\frac{1}{2}(\mathbf{x}+\mathbf{y}-\mathbf{z}).$$
   It's easy to see that the reciprocal lattice of FCC is a BCC lattice with a cubic cell length of $4\pi/a$. Since in a BCC the shortest vector is the one from the corner of the cube to the point at the center, we can take
   $$\mathbf{G}_0 = \mathbf{b}_1 = \frac{2\pi}{a}(\mathbf{y}+\mathbf{z}-\mathbf{x}).$$
   In real space, the family of lattice planes perpendicular to this $\mathbf{G}_0$ is the $\{111\}$, therefore the lattice planes with the greatest density of points in a FCC lattice are the $\{111\}$ planes.

   (b) BCC lattice: we know that the reciprocal lattice of a BCC is a FCC lattice. Thus we can follow the same argument described for the FCC lattice, just exchanging the $\mathbf{a}$ and $\mathbf{b}$ vectors (with the appropriate pre–factors). Since in a FCC lattice the shortest vector is the one from the corner of the cube to the face center, we can take as $\mathbf{G}_0$
   $$\mathbf{G}_0 = \mathbf{b}_1 = \frac{2\pi}{a}(\mathbf{y}+\mathbf{z}).$$
   In the real space, the lattice planes perpendicular to this $\mathbf{G}_0$ belong to the family of $\{110\}$, hence the lattice planes with the greatest density of points are the $\{110\}$ planes in a BCC lattice.

Exercise 2 Average distance between kinks on a step

Consider a step with the edge along the [100] direction, on the (100) surface of a simple cubic crystal. At finite temperature the step edge fluctuates (this is called *roughening transition*) as a result of the formation of kinks. We can consider the edge line as made up of N segments of length equal to the lattice parameter ($L = Na$). On each of these segments we may find a positive kink (i.e. an atom that sticks from the step), a negative kink (a missing atom on the step) or no kink at all.

Cont.

(a) Assuming that the temperature is low enough so that only kinks of atomic size occur (i.e. only single atoms stick on the kink), show that the average distance λ_0 between kinks is

$$\lambda_0 = a\frac{1+2\gamma}{2\gamma} \qquad \text{with} \quad \gamma = \exp(-\epsilon\beta)$$

where a is the lattice parameter, ϵ is the formation energy of a kink and $\beta = 1/k_BT$ (where T is the temperature). *Hints:*

- *Write down the "constraints" on the number of positive and negative kinks per unit length of step (call them n_+ and n_-, for example). Take also into account that in a segment of the step no kink is also possible!*
- *By minimizing the free energy F, one can prove the following relation: $n_+n_-/n_0^2 = \gamma^2$.*

(b) Are you able to sketch a rough plot of the result as a function of temperature (with ϵ fixed)? Does it make sense from a physical point of view?

Solution to Exercise 2

1. There are two constraints on the number density of positive/negative kinks:

$$n_+ + n_- + n_0 = 1/a,$$

i.e. the total number on kinks per unit length must be equal to the linear density of atoms on the step. And

$$n_+ - n_- = 0,$$

in order to conserve the average orientation of the step line. We can determine the values of n_+, n_- and n_0 by solving the two above equations together with the relation coming from the minimization of the free energy. Thus, we need to solve the system

$$\begin{cases} n_+ + n_- + n_0 = 1/a \\ n_+ - n_- = 0 \\ n_+n_-/n_0^2 = \gamma^2 \end{cases}$$

We obtain

$$n_+ = n_- = \frac{1}{a(2+e^{\epsilon\beta})}, \quad n_0 = \frac{1e^{\epsilon\beta}}{a(2+e^{\epsilon\beta})}.$$

The average distance between two kinks can be defined as the reciprocal of the total number of kinks per unit length, namely

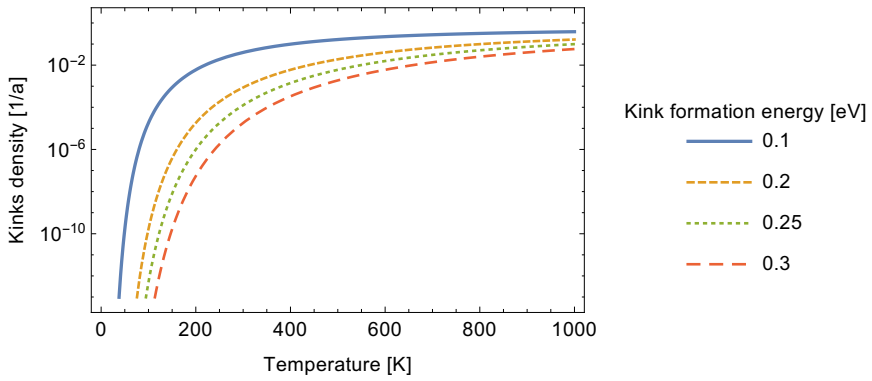
$$\lambda_0 = \frac{1}{n_+ + n_-}.$$

With the expression above for $n_\pm$ and recalling that $n = N/L = 1/a$, we get

$$\lambda_0 = \frac{1}{\frac{2(1/a)}{2+\exp\epsilon\beta}} = a\frac{2+e^{\epsilon\beta}}{2} = a\frac{1+2\gamma}{2\gamma} = \frac{a}{2}(2+\exp\epsilon\beta).$$

Cont.

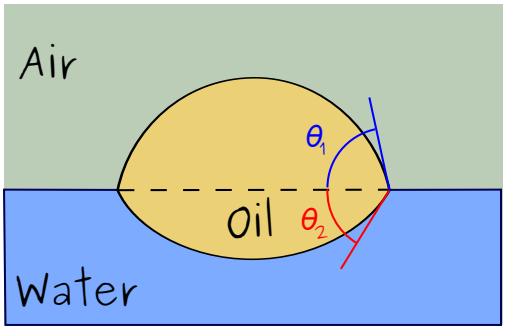
2. The figure below is the plot of the function $1/\lambda_0$ (log scale), the average number of kinks per unit length, with respect to the temperature. With an increase in temperature the kink density increases exponentially, while with a decrease it falls off.



Exercise 3 Generalized Young equation for soft matter

Consider an oil droplet in water. This case is similar to a liquid drop on top of a surface of soft matter. Since the oil superficial tension is comparable with water superficial tension (or with elastic constant of soft matter in that direction), the oil droplet creates a curved meniscus inside water (as shown in figure below).

(a) Determine the form of generalized Young equation relying only on geometrical considerations.



Solution to Exercise 3

1. We know that at every point the sum of the surface tension vectors must be zero. Then, we get:

$$\gamma_{WA} = \gamma_{OA}\cos\theta_1 + \gamma_{WO}\cos\theta_2.$$

The End.