Chapter 1

Introduction

1.8 Exercise Problems

1.1 Find the distance d between nearest lattice points along the $\langle 1\,0\,0\rangle$, $\langle 1\,1\,0\rangle$, $\langle 1\,1\,1\rangle$, $\langle 1\,1\,2\rangle$ and $\langle 1\,2\,3\rangle$ lines for the simple cubic lattice with lattice constant a. Rank the line directions in increasing order of d.

Solution

	$\langle 1\,0\,0\rangle$	$\langle 1\,1\,0\rangle$	$\langle 1\,1\,1\rangle$	$\langle 1\,1\,2\rangle$	$\langle 1\,2\,3\rangle$
d	a	$\sqrt{2}\,a \approx 1.41\,a$	$\sqrt{3}\,a \approx 1.73\,a$	$\sqrt{6}\,a \approx 2.45\,a$	$\sqrt{14}\,a \approx 3.74\,a$

$$d_{\langle 1\,0\,0\rangle} < d_{\langle 1\,1\,0\rangle} < d_{\langle 1\,1\,1\rangle} < d_{\langle 1\,1\,2\rangle} < d_{\langle 1\,2\,3\rangle}$$

1.2 Repeat the analysis in 1.1 for the FCC lattice.

Solution
Note that $\frac{1}{2}[1\,1\,0]$ is a lattice vector in the FCC lattice. $\frac{1}{2}[1\,1\,2] = \frac{1}{2}[1\,1\,0] + [0\,0\,1]$ and $\frac{1}{2}[1\,2\,3] = \frac{1}{2}[1\,0\,1] + [0\,1\,1]$ are also lattice vectors in the FCC lattice.

	$\langle 1\,0\,0\rangle$	$\frac{1}{2}\langle 1\,1\,0\rangle$	$\langle 1\,1\,1\rangle$	$\frac{1}{2}\langle 1\,1\,2\rangle$	$\frac{1}{2}\langle 1\,2\,3\rangle$
d	a	$\frac{\sqrt{2}}{2}\,a \approx 0.71\,a$	$\sqrt{3}\,a \approx 1.73\,a$	$\frac{\sqrt{6}}{2}\,a \approx 1.22\,a$	$\frac{\sqrt{14}}{2}\,a \approx 1.87\,a$

$$d_{\frac{1}{2}\langle 1\,1\,0\rangle} < d_{\langle 1\,0\,0\rangle} < d_{\frac{1}{2}\langle 1\,1\,2\rangle} < d_{\langle 1\,1\,1\rangle} < d_{\frac{1}{2}\langle 1\,2\,3\rangle}$$

1.3 Repeat the analysis in 1.1 for the BCC lattice.

Solution
Note that $\frac{1}{2}[1\,1\,1]$ is a lattice vector in the BCC lattice.

	$\langle 1\,0\,0\rangle$	$\langle 1\,1\,0\rangle$	$\frac{1}{2}\langle 1\,1\,1\rangle$	$\langle 1\,1\,2\rangle$	$\langle 1\,2\,3\rangle$
d	a	$\sqrt{2}\,a \approx 1.41\,a$	$\frac{\sqrt{3}}{2}\,a \approx 0.87\,a$	$\sqrt{6}\,a \approx 2.45\,a$	$\sqrt{14}\,a \approx 3.74\,a$

$$d_{\frac{1}{2}\langle 1\,1\,1\rangle} < d_{\langle 1\,0\,0\rangle} < d_{\langle 1\,1\,0\rangle} < d_{\langle 1\,1\,2\rangle} < d_{\langle 1\,2\,3\rangle}$$

1.4 Find the distance h between nearest parallel planes of lattice points perpendicular to directions of the type $\langle 1\,0\,0\rangle$, $\langle 1\,1\,0\rangle$, $\langle 1\,1\,1\rangle$, $\langle 1\,1\,2\rangle$ and $\langle 1\,2\,3\rangle$ for the simple cubic lattice with lattice constant a. Rank the directions in decreasing order of h.

Solution
A plane perpendicular to the $[u\,v\,w]$ direction is described by the equation

$$u\,x + v\,y + w\,z = n\,a$$

where x, y, and z are coordinates of an arbitrary point on the plane and n is a constant. If the plane must pass through some lattice points in a simple cubic lattice, and for the five types of directions in this problem, we can show that the possible values of n are all the integers, $n = \cdots, -2, -1, 0, 1, 2, \cdots$. The case of $n = 0$ corresponds to the plane that passes through the origin. This means that, for each of the five directions in this problem, the next plane that is closest to the $n = 0$ plane is the $(h\,k\,l)$ plane, where $h = u$, $k = v$, $l = w$. The interplanar distance equals the distance from the origin to the $(h\,k\,l)$ plane, which is

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{a}{\sqrt{u^2 + v^2 + w^2}}$$

direction	$[1\,0\,0]$	$[1\,1\,0]$	$[1\,1\,1]$	$[1\,1\,2]$	$[1\,2\,3]$
plane	$(1\,0\,0)$	$(1\,1\,0)$	$(1\,1\,1)$	$(1\,1\,2)$	$(1\,2\,3)$
h	a	$\frac{1}{\sqrt{2}}\,a \approx 0.71\,a$	$\frac{1}{\sqrt{3}}\,a \approx 0.58\,a$	$\frac{1}{\sqrt{6}}\,a \approx 0.41\,a$	$\frac{1}{\sqrt{14}}\,a \approx 0.27\,a$

$$h_{(1\,0\,0)} > h_{(1\,1\,0)} > h_{(1\,1\,1)} > h_{(1\,1\,2)} > h_{(1\,2\,3)}$$

1.5 Repeat the analysis in 1.4 for the FCC lattice.

Solution
A plane perpendicular to the $[u\,v\,w]$ direction is described by the equation

$$u\,x + v\,y + w\,z = n\,a$$

where x, y, and z are coordinates of an arbitrary point on the plane and n is a constant. If the plane must pass through some lattice points in an FCC lattice, we can show that when $[u\,v\,w]$ is $[1\,0\,0]$, $[1\,1\,0]$, $[1\,1\,2]$ or $[1\,2\,3]$, the possible values of n include all integers and half-integers, $n = 0, \pm\frac{1}{2}, \pm 1, \pm\frac{3}{2}, \pm 2, \cdots$. In this case, the plane closest to the plane of $n = 0$ is the $(h\,k\,l)$ plane where $h = 2u$, $k = 2v$, $l = 2w$. The interplanar distance is

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{a}{2\sqrt{u^2 + v^2 + w^2}}$$

However, when $[u\,v\,w]$ is $[1\,1\,1]$, it can be shown that the possible values of n are all integers (no half-integers), $n = 0, \pm 1, \pm 2, \cdots$. In this case, the plane closest to the plane of $n = 0$ is the $(h\,k\,l)$ plane where $h = u$, $k = v$, $l = w$, i.e. the $(1\,1\,1)$ plane. The interplanar distance is

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{a}{\sqrt{u^2 + v^2 + w^2}}$$

direction	[1 0 0]	[1 1 0]	[1 1 1]	[1 1 2]	[1 2 3]
plane	(2 0 0)	(2 2 0)	(1 1 1)	(2 2 4)	(2 4 6)
h	$\frac{1}{2}a$	$\frac{1}{2\sqrt{2}}\,a \approx 0.35\,a$	$\frac{1}{\sqrt{3}}\,a \approx 0.58\,a$	$\frac{1}{2\sqrt{6}}\,a \approx 0.20\,a$	$\frac{1}{2\sqrt{14}}\,a \approx 0.13\,a$

$$h_{(1\,1\,1)} > h_{(2\,0\,0)} > h_{(2\,2\,0)} > h_{(2\,2\,4)} > h_{(2\,4\,6)}$$

Notice that $\{1\,1\,1\}$ planes are the most widely spaced planes in an FCC lattice.

1.6 Repeat the analysis in 1.4 for the BCC lattice.

Solution
A plane perpendicular to the $[u\,v\,w]$ direction is described by the equation

$$u\,x + v\,y + w\,z = n\,a$$

where x, y, and z are coordinates of an arbitrary point on the plane and n is a constant. If the plane must pass through some lattice points in a BCC lattice, we can show that when $[u\,v\,w]$ is $[1\,0\,0]$ or $[1\,1\,1]$, the possible values of n include all integers and half-integers, $n = 0, \pm\frac{1}{2}, \pm1, \pm\frac{3}{2}, \pm2, \cdots$. In this case, the plane closest to the plane of $n = 0$ is the $(h\,k\,l)$ plane where $h = 2u$, $k = 2v$, $l = 2w$. The interplanar distance is

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{a}{2\sqrt{u^2 + v^2 + w^2}}$$

However, when $[u\,v\,w]$ is $[1\,1\,0]$, $[1\,1\,2]$, or $[1\,2\,3]$, it can be shown that the possible values of n are all integers (no half-integers), $n = 0, \pm1, \pm2, \cdots$. In this case, the plane closest to the plane of $n = 0$ is the $(h\,k\,l)$ plane where $h = u$, $k = v$, $l = w$, i.e. the $(1\,1\,1)$ plane. The interplanar distance is

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{a}{\sqrt{u^2 + v^2 + w^2}}$$

direction	[1 0 0]	[1 1 0]	[1 1 1]	[1 1 2]	[1 2 3]
plane	(2 0 0)	(1 1 0)	(2 2 2)	(1 1 2)	(1 2 3)
h	$\frac{1}{2}a$	$\frac{1}{\sqrt{2}}\,a \approx 0.71\,a$	$\frac{1}{2\sqrt{3}}\,a \approx 0.29\,a$	$\frac{1}{\sqrt{6}}\,a \approx 0.41\,a$	$\frac{1}{\sqrt{14}}\,a \approx 0.27\,a$

$$h_{(1\,1\,0)} > h_{(2\,0\,0)} > h_{(1\,1\,2)} > h_{(2\,2\,2)} > h_{(1\,2\,3)}$$

Notice that $\{1\,1\,0\}$ planes are the most widely spaced planes in a BCC lattice.

1.7 Consider an atom in a simple cubic crystal and located at the origin. Find the distance between this atom and its first, second and third nearest neighbors in terms of the lattice constant a. Express the vectors from this atom to its first, second and third nearest neighbors in Miller indices. How many first, second and third nearest neighbors does this atom have?

Solution

- 6 first nearest neighbors: $\{1\,0\,0\}$. Distance: a.

- 12 second nearest neighbors: $\{1\,1\,0\}$. Distance: $\sqrt{2}\,a \approx 1.41\,a$.
- 8 third nearest neighbors: $\{1\,1\,1\}$. Distance: $\sqrt{3}\,a \approx 1.73\,a$.

1.8 Repeat the analysis in 1.7 for a FCC crystal with lattice constant a.

Solution

- 12 first nearest neighbors: $\frac{1}{2}\{1\,1\,0\}$. Distance: $\frac{\sqrt{2}}{2}a \approx 0.71\,a$.
- 6 second nearest neighbors: $\{1\,0\,0\}$. Distance: a.
- 24 third nearest neighbors: $\frac{1}{2}\{1\,1\,2\}$. Distance: $\frac{\sqrt{6}}{2}\,a \approx 1.22\,a$.

1.9 Repeat the analysis in 1.7 for a BCC crystal with lattice constant a.

Solution

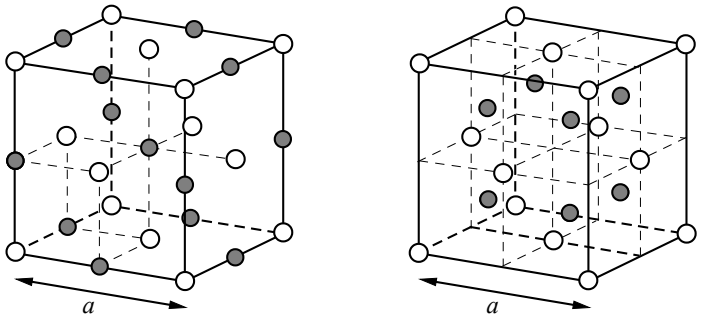
- 8 first nearest neighbors: $\frac{1}{2}\{1\,1\,1\}$. Distance: $\frac{\sqrt{3}}{2}\,a \approx 0.87\,a$.
- 6 second nearest neighbors: $\{1\,0\,0\}$. Distance: a.
- 12 third nearest neighbors: $\{1\,1\,0\}$. Distance: $\sqrt{2}\,a \approx 1.41\,a$.

1.10 The NaCl (table salt) crystal has a cubic structure. Its unit cell is shown in Fig. 1.14(a). The Na atoms (white spheres) form an FCC sub-lattice. The Cl atoms (gray spheres) also form an FCC sub-lattice that is offset from the Na sub-lattice by $a/2$ in the $[1\,0\,0]$ direction. Identify the lattice and basis for the crystal structure of NaCl. Express the average atomic volume in terms of the lattice constant a. The NaCl structure is also called the B1 structure, which is also the crystal structure of AgCl, MgO and CaO.

Solution

- Lattice: FCC.
- Two-atom basis: Na at $[0\,0\,0]$ and Cl at $[\frac{1}{2}\,0\,0]$.
- Average atomic volume: $\Omega_{\text{avg}} = a^3/8$.

1.11 The CaF_2 (fluorite) crystal has a cubic structure. Its unit cell is shown in Fig. 1.14(b). The Ca atoms (white spheres) form an FCC sub-lattice. To specify the position of F atoms, imagine that the unit cell cube is divided into 8 smaller cubes of equal sizes. The F atoms are located at the centers of these smaller cubes. Identify the lattice and basis for the crystal structure of CaF_2.



(a) (b)

Figure 1.14: (a) The unit cell of the B1 (NaCl) crystal structure. (b) The unit cell of the C1 (CaF_2) crystal structure.

Express the average atomic volume in terms of the lattice constant a. The CaF_2 structure is also called the C1 structure, which is also the crystal structure of $NiSi_2$ and cubic ZrO_2.

Solution

- Lattice: FCC.
- Three-atom basis: Ca at [0 0 0], F at $[\frac{1}{4}\ \frac{1}{4}\ \frac{1}{4}]$, and F at $[\frac{3}{4}\ \frac{3}{4}\ \frac{3}{4}]$.
- Average atomic volume: $\Omega_{\text{avg}} = a^3/12$.

1.12 List three useful defect-controlled properties of crystalline solids that impact your daily life. For each property, identify whether the controlling defect is a point, line, or planar defect.

Solution
For example,

- Light-emitting diodes (LEDs) generate light by passing currents through a p-n junction, which are formed by doping. Dopant are solute atoms, i.e. point defects.
- The body of a car is manufactured by deforming metal plates plastically into the desired shape. The plastic deformation of metals require motion of dislocations, i.e. line defects.
- Computer hard disks store information in magnetic domains of the disk material. The magnetization of the domain switches by the motion of magnetic domain boundaries, which are planar defects. Reducing the grain size has led to improvement of storage density. The grain boundaries are planar defects.

Chapter 2

Stress, Strain and Isotropic Elasticity

2.7 Exercise Problems

2.1 A strip of metal is subjected to a uniform tension stress $\sigma_{yy} = \sigma$, as shown in Fig. 2.16.

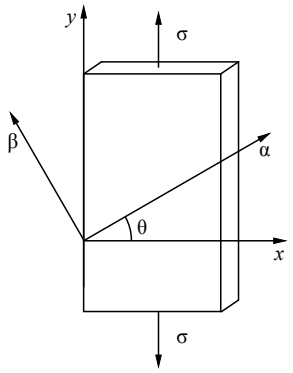


Figure 2.16: A strip of metal subjected to tensile stress.

(a) Calculate the shear stress $\sigma_{\alpha\beta}$ acting on a plane that is 45° to the horizontal axis.

(b) Write a general expression for the shear stress $\sigma_{\alpha\beta}$ on a plane making an arbitrary angle θ with the horizontal axis.

(c) Show that $\sigma_{\alpha\beta}$ is maximum at $\theta = 45°$.

(d) Calculate the hydrostatic pressure p in the strip.

Solution
(a) $\sigma_{\alpha\beta} = (\cos 45°)(\sin 45°)\,\sigma_{yy} = \frac{1}{2}\,\sigma$.

(b) $\sigma_{\alpha\beta} = (\cos\theta)(\sin\theta)\,\sigma_{yy} = \frac{1}{2}\sin(2\theta)\,\sigma$.

(c) Maximum of $\sin(2\theta)$ occurs at $\theta = 45°$ where $\sin(2\theta) = \sin 90° = 1$. Therefore, maximum of $\sigma_{\alpha\beta}$ occurs at $\theta = 45°$ where $\sigma_{\alpha\beta} = \frac{1}{2}\,\sigma$.

(d) $p = -\frac{1}{3}(\sigma_{xx} + \sigma_{yy} + \sigma_{zz}) = -\frac{1}{3}\,\sigma$.

2.2 An FCC single crystal thin film with the orientation shown in Fig. 2.17 is subjected to an equal-biaxial tensile stress σ. Plastic deformation of this crystal will occur by slip on the $(1\,\bar{1}\,1)$ plane (shaded) and along the $[0\,1\,1]$ direction as shown. Write an expression for the shear stress acting on the slip plane in the slip direction.

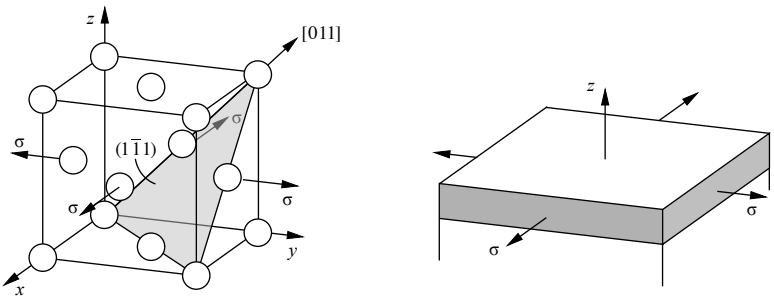


Figure 2.17: An FCC single crystal thin film under biaxial tension.

Solution
In $(x\,y\,z)$ coordinate system,

$$\sigma_{xx} = \sigma_{yy} = \sigma\,, \quad \sigma_{zz} = 0$$

Choose a new coordinate system $(x'\,y'\,z')$ in which the x'-, y'-, and z'-axes are along the $[0\,1\,1]$, $[1\,\bar{1}\,1]$, and $[2\,1\,\bar{1}]$ directions respectively. The stress component in question is $\sigma_{x'y'}$.

$$\begin{aligned}\sigma_{x'y'} &= Q_{1k}\,Q_{2l}\,\sigma_{kl} \\ &= Q_{11}\,Q_{21}\,\sigma_{xx} + Q_{12}\,Q_{22}\,\sigma_{yy}\end{aligned}$$

where $Q_{ik} = (\hat{e}'_i \cdot \hat{e}_k)$.

$$\begin{aligned}Q_{11} &= \frac{1}{\sqrt{2}}[0\,1\,1]\cdot[1\,0\,0] = 0 \\ Q_{21} &= \frac{1}{\sqrt{3}}[1\,\bar{1}\,1]\cdot[1\,0\,0] = \frac{1}{\sqrt{3}} \\ Q_{12} &= \frac{1}{\sqrt{2}}[0\,1\,1]\cdot[0\,1\,0] = \frac{1}{\sqrt{2}} \\ Q_{22} &= \frac{1}{\sqrt{3}}[1\,\bar{1}\,1]\cdot[0\,1\,0] = -\frac{1}{\sqrt{3}}\end{aligned}$$

Therefore,

$$\sigma_{x'y'} = \left(\frac{1}{\sqrt{2}}\right)\left(-\frac{1}{\sqrt{3}}\right)\sigma = -\frac{1}{\sqrt{6}}\,\sigma$$

2.3 A single crystal of BCC iron is pulled in uniaxial tension along a cube direction, $[1\,0\,0]$. We assume slip occurs on the $(\bar{2}\,1\,1)$ plane and in the $[1\,1\,1]$ direction as shown in Fig. 2.18(a). The