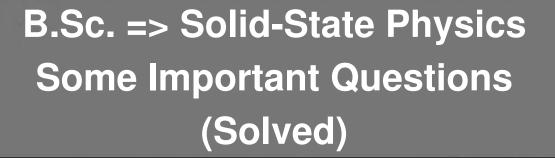
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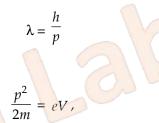
SOME IMPORTANT PROBLEMS

Problem 1. A beam of electrons with kinetic energy 1 keV is diffracted as it passes through a polycrystalline metal foil. The metal has a cubic crystal structure with a spacing of 1 Å. Given m, q, h, c,

(a) Calculate the wavelength of the electrons,

(b) Calculate the Bragg angle for the first order diffraction maximum. (Wisconsin)

Solution: (a) The electron wavelength is



V being the accelerating voltage of the electrons. Thus

$$\lambda = \frac{h}{(2meVP)^{1/2}} \approx \frac{12.25}{V^{1/2}} = \frac{12.25}{\sqrt{1000}} = 0.39 \text{ Å}.$$

(b) The condition for Bragg reflection

$$2d\sin\theta = n\lambda$$

gives for the first order diffraction maximum

$$\sin\theta = \frac{\lambda}{2d} = \frac{0.39}{2 \times 1} = 0.195$$

as n = 1, d = 1 Å. Hence

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$\theta = 11.18^{\circ}.$

Problem 2. Derive the reciprocal lattice of fcc structure is a bcc structure. [Important]

Solution:. Let b_1 , b_2 , b_3 be the reciprocal vectors of lattice vectors a_1 , a_2 , a_3 .

$$\vec{b}_1 = 2\pi \cdot \frac{\vec{a}_2 \times \vec{a}_3}{V} \qquad \dots (1)$$

$$\vec{b}_2 = 2\pi \cdot \frac{\vec{a}_3 \times \vec{a}_1}{V} \qquad \dots (2)$$

$$\vec{b}_3 = 2 \cdot \frac{\vec{a}_1 \times \vec{a}_2}{V} \qquad \dots (3)$$

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with $V = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$ as introduced above.

The primitive vectors are those vectors, the whole lattice structure can be made by repeating these vectors. The primitive vectors for an fcc structures are

$$\vec{a}_1 = \frac{a}{2} \cdot (\hat{y} + \hat{z}) \qquad \dots (4)$$

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$$\vec{a}_2 = \frac{a}{2} \cdot (\hat{x} + \hat{z}) \qquad \dots (5)$$

$$\vec{a}_3 = \frac{a}{2} \cdot (\hat{x} + \hat{y}) \qquad \dots (6)$$

Here \hat{x} , \hat{y} and \hat{z} denote the unit vectors in x, y, and z direction. If the origin of the coordinate system is chosen to be at one of the vertices, these vectors point to the lattice points at the neighboured faces.

Now we apply eqs. (1)-(3) and obtain:

$$\vec{b}_{1} = \frac{8\pi}{a^{3}} \cdot \vec{a}_{2} \times \vec{a}_{3} = \frac{4\pi}{a} \cdot \left(-\frac{\hat{x}}{2} + \frac{\hat{y}}{2} + \frac{\hat{z}}{2} \right) \qquad \dots (7)$$
$$\vec{b}_{2} = \frac{8\pi}{a^{3}} \cdot \vec{a}_{3} \times \vec{a}_{1} = \frac{4\pi}{a} \cdot \left(\frac{\hat{x}}{2} - \frac{\hat{y}}{2} + \frac{\hat{z}^{2}}{2} \right) \qquad \dots (8)$$
$$\vec{b}_{3} = \frac{8\pi}{a^{3}} \cdot \vec{a}_{1} \times \vec{a}_{2} = \frac{4\pi}{a} \cdot \left(\frac{\hat{x}}{2} + \frac{\hat{y}}{2} + \frac{\hat{z}}{2} \right) \qquad \dots (9)$$

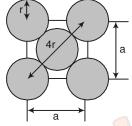
which turn out to be primitive translation vectors of the fcc structure. Thus, the reciprocal lattice of a fcc lattice with edge length a is a bcc lattice with edge length $\frac{4\pi}{a}$. Accordingly, the reciprocal-lattice of a bcc lattice is a fcc lattice.

Problem 3. The reciprocal lattice of a simple cubic is also a simple cubic.

Solution: $\vec{a} = a \cdot \vec{x}$ $\vec{b} = a \cdot \vec{y}$ Simple cubic $\vec{c} = a \cdot \vec{z}$ $\vec{a^*} = 2\pi \frac{b \times c}{a \cdot (b \times c)} = \frac{2\pi}{a} \vec{x}$

$$\overline{b^*} = 2\pi \frac{c \times a}{a \cdot (b \times c)} = \frac{2\pi}{a} \overline{y}$$
 Simple cubic
$$\overline{c^*} = 2\pi \frac{a \times b}{a \cdot (b \times c)} = \frac{2\pi}{a} \overline{z}$$

Problem 4. What is the packing fraction of fcc structure? Solution:



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Fig. When the lattice points are inflated gradually, at some point they start to touch each other along the diagonals of the faces of the cube. One can now interpret them as close packed spheres with a radius defined

geometrically by
$$4\pi = \sqrt{2a} \Leftrightarrow r = \frac{\sqrt{2}}{4}a$$

The packing density ρ is the ratio of the volume filled by the spherical atoms within a unit cell to the total volume V_{uc} of the unit cell. Overall there

are *n* = 4 atoms per unit cell with a volume of $V_{sph} = \frac{4}{3}\pi r^3$ each. Thus for the packing density one obtains.

$$\rho = \frac{n \cdot V_{sph}}{V_{uc}} = \frac{4 \cdot \frac{4}{3} \pi r \cdot \left(\frac{\sqrt{2}}{4}\right)^3 a^3}{4a^3}$$
$$= \frac{\sqrt{2}\pi}{6} \approx 74\% \qquad \dots(2)$$

Problem 5. What is Cooper pair?

Solution: A Cooper pair is two (a pair) of electrons that attract each other and thereby make having the Cooper pair lower in total energy than the electrons separately. Since a pair of electrons have an integral value of angular momentum, the Cooper pairs are bosons. As bosons, any number of Cooper pairs can exist, which means macroscopic superconductivity can exist.

Problem 6. How do Cooper pairs interact with the lattice to cause superconductivity?

Solution: In what are called low-Tc superconductivity, essentially those discovered prior to the cuprites two electrons form a Cooper pair indirectly. One electron electrically attracts nearby nuclei, which lowers the Coulomb potential energy. The second electron of the pair encounters this lower potential energy and for that reason a pair of electrons has a lower total energy that the two separate electrons. If we think of the two electrons forming a Cooper pair as doing so by having a "glue" exchanging a boson that causes their energy to lower-then the boson is a lattice vibration, a phonon. Starting with the coparties many superconductors have been discovered in which the pairing that lattice vibrations, and the glue, the exchange boson, is a mignon (which is a unit of magnetic excitation energy).

Problem 7. Give packing fraction of simple cubic and BCC structure? Solution: Atomic Packing Factor for Simple Cubic:

no, of atoms = 1

volume of one atom = $\frac{4}{3}\pi r^3$

volume of unit cell (cubic) = a^3

when, (a = 2r)

Filling Factor =
$$\frac{1 \times \frac{4\pi r^3}{3}}{a^3} = \frac{\frac{4\pi r^3}{3}}{(2r)^3} = \frac{\frac{4\pi r^3}{3}}{8r^3} = \frac{\pi}{6} = 52\%$$

Atomic Filling Factor for BCC:

no of atoms = 2

volume of low atoms $= 2 \times \frac{4\pi r^3}{3}$ Support by Donating volume of unit cell (cubic) $= a^3$ alllabexperiments.com when $r = \frac{a\sqrt{3}}{4}$ Filling Factor $= \frac{2 \times \frac{4\pi r^3}{3}}{a^3}$

$$=\frac{\frac{8\pi r^3}{3}}{\left(\frac{4r}{\sqrt{3}}\right)^3}=\frac{\frac{8\pi r^3}{3}}{\frac{64}{3\sqrt{3}}r^3}=\frac{\sqrt{3\pi}}{8}=68\%$$

Problem 8. Draw the following places in the cubic crystal? (001) - 3, (010) - 2, (100) - 1, (a) - (100) b - (010) c - (001) Solution: (a) - (100)

$$x = \frac{1}{1} = 1$$
$$y = \frac{1}{0} = \infty$$
$$z = \frac{1}{0} = \infty$$

Then miller indices are $(1\infty\infty)$

(b) – (010)

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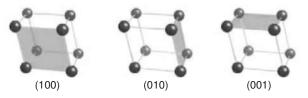
$$x = \frac{1}{0} = \infty$$
$$y = \frac{1}{1} = 1$$
$$z = \frac{1}{0} = \infty$$

Then miller indices are $(\infty 1 \infty)$

(c) – (001)

$$x = \frac{1}{0} = \infty$$
$$y = \frac{1}{0} = \infty$$
$$z = \frac{1}{1} = 1$$

then miller indices are $(\infty \infty 1)$



Problem 9. Draw 110 and 101 planes in a cubic lattice. Solution: 1 – (101)

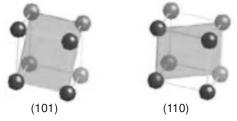
$$x = \frac{1}{1} = 1$$
$$y = \frac{1}{0} = \infty$$
$$z = \frac{1}{1} = 1$$

then miller indices are $(1 \ge 1)$

2 - (110)

Support by Donating $x = \frac{1}{1} = 1$ alllabexperiments.com $y = \frac{1}{1} = 1$ $z = \frac{1}{0} = \infty$

then miller indices are (11∞)



Problem 10. If BCS theory works for low-temperature superconductors why is insufficient for these high-temperature superconductors?

Solution: I do not know full answer. Part of the answer is that the highexchange bosons that are magnetic rather than phonon (lattice vibration). Another part of the answer lies in the idea of a mean field theory. Any mean field theory assume that the volume corresponds to one object- in the case of superconductivity one Cooper pair-also contains the effect of many other objects. For low- T_c BCS superconductors, this definitely works. For example, the coherence length is a rough measure of the 'size' of one Cooper pair. For any mean field theory to work, the volume corresponding to the size of one Cooper pair should contain many other Cooper pairs so that the interaction can be taken as the average of many pairs. In lead, the number of pairs in the volume of one Cooper pair is about 10⁴. In a typical coprate, the number of pairs is about one. So a mean field theory such as BCS is unlikely to work for the cuprates.

Problem 11. Define with diagram - diamagnetic, paramagnetic and ferromagnetic?

Solution: Diamagnetic: Atoms or ions with a closed shell of electrons, all of the electrons are paired.

Paramagnetic: Atoms or ions with unpaired electrons, where the moment of an atom with unpaired electrons is given by the spin, *S* and orbital angular, *L* and total momentum, *J*, quantum.

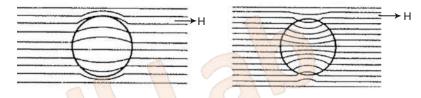


Figure: Diamagnetic materials: reduce the density of the lines of force (flux density).

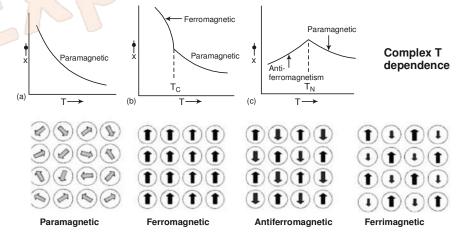
Figure: Paramagnetic materials: increase the density of the lines of force (flux density).

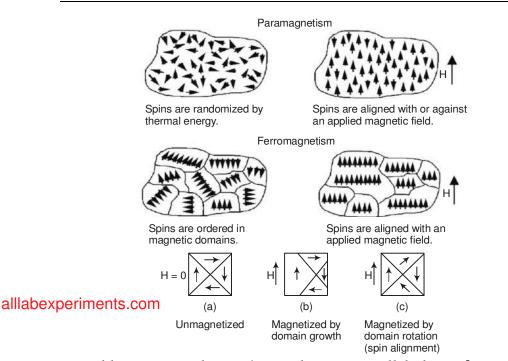
Ferromagnetism: magnetic moments of atoms align to produce a strong magnetic effect

• For ferromagnetism, the Curie Law becomes $\lambda = C/(T - T_c)$, where T_c is the Curie Temperature.

Antiferromagnetism: magnetic moments of atom align anti-parallel to produce a strong magnetic effect.

• For antiferromagnetism, the Curie Law becomes $l = C/(T + T_N)$, where T_N is the Neel temperature.





Problem 12. Interplaner Distance between parallel planes. [Important]

Solution: The space lattice consist from many crystal planes which separated by interplaner smallest distance. The distance can be calculated by using x-ray diffraction, by using the law below:

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

1

Where d_{hkl} = interplaner spacing between parallel closest planes with Miller indices h, k, and l.

Q.13. Angles between crystal planes.

Ans. The crystal consist many from plance which constant with them in vairty angles. The angle between crystal planes can be calculated by using the following equation.

$$\cos \theta = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\sqrt{(h_1^2 + k_1^2 + l_1^2)} \times \sqrt{(h_2^2 + k_2^2 + l_2^2)}}$$

Example:

Find the angle between planes $(1\overline{1}1)$ & (111)?

$$\cos \theta = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\sqrt{(h_1^2 + k_1^2 + l_1^2)} \times \sqrt{(h_2^2 + k_2^2 + l_2^2)}}$$

$$\cos \theta = \frac{1 + (-1) + 1}{\sqrt{1 + 1} + 1}$$
$$\cos \theta = \frac{1}{3}$$
$$\cos \theta = 0.333$$
$$\cos^{-1} 0.333 = \theta$$
$$\theta = 70.32^{\circ}$$

Problem 14. Find the interplaner distance for plane (220), which have FCC Crystal and radius of atom (1.141*A*)?

Solution: The crystal is FCC then

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$$a = \frac{4r}{\sqrt{2}}$$

$$a = \frac{4(1.414)}{\sqrt{2}} = \frac{4(1.414)}{1.414} = 4 \mathring{A}$$

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

$$d_{hkl} = \frac{4}{\sqrt{4 + 4 + 0}} = 1.414 \,\mathring{A}$$

Problem 15. Explain the magnetic hysteresis curve in detail.

Solution: Magnetic behavior of different ferromagnetic substance is demonstrated by hysteresis curves, a plot of magnetic flux density (*B*) against applied magnetic field (*H*).

Starting with a nonmagnetic sample (domains randomly aligned) *B* and *H* are zero, but as the field is increased the flux density also increases.

Upon reaching the maximum value of magnetization all the spins are aligned in the sample, but when the applied field is reduced the flux density does not follow the initial curve, because of the difficulty of reversing processes where domains have grown through crystal imperfections.

A sufficiently large magnetic field in the reverse direction must be applied before the magnetization process can be reversed.

The magnetization where H is zero, but B is not zero is known as the remnant magnetization.

The field that needs to be applied in the reverse direction to reduce magnetization to zero is the coercive force.

