SUMMARY

- Various statements of the Bragg condition:

$$2d \sin\theta = n\lambda \ ; \qquad \Delta\mathbf{k} = \mathbf{G} \ ; \qquad 2\mathbf{k}\cdot\mathbf{G} = \mathbf{G}^2 \ .$$

- Laue conditions:

$$\mathbf{a}_1\cdot\Delta\mathbf{k} = 2\pi v_1 \ ; \qquad \mathbf{a}_2\cdot\Delta\mathbf{k} = 2\pi v_2 \ ; \qquad \mathbf{a}_3\cdot\Delta\mathbf{k} = 2\pi v_3 \ .$$

- The primitive translation vectors of the reciprocal lattice are

$$\mathbf{b}_1 = 2\pi\frac{\mathbf{a}_2\times\mathbf{a}_3}{\mathbf{a}_1\cdot\mathbf{a}_2\times\mathbf{a}_3} \ ; \qquad \mathbf{b}_2 = 2\pi\frac{\mathbf{a}_3\times\mathbf{a}_1}{\mathbf{a}_1\cdot\mathbf{a}_2\times\mathbf{a}_3} \ ; \qquad \mathbf{b}_3 = 2\pi\frac{\mathbf{a}_1\times\mathbf{a}_2}{\mathbf{a}_1\cdot\mathbf{a}_2\times\mathbf{a}_3} \ .$$

  Here $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ are the primitive translation vectors of the crystal lattice.

- A reciprocal lattice vector has the form

$$\mathbf{G} = v_1\mathbf{b}_1 + v_2\mathbf{b}_2 + v_3\mathbf{b}_3 \ ,$$

  where v_1, v_2, v_3 are integers or zero.

- The scattered amplitude in the direction $\mathbf{k}' = \mathbf{k} + \Delta\mathbf{k} = \mathbf{k} + \mathbf{G}$ is proportional to the geometrical structure factor:

$$S_\mathbf{G} \equiv \sum f_j \exp(-i\mathbf{r}_j\cdot\mathbf{G}) = \sum f_j \exp[-i2\pi(x_j v_1 + y_j v_2 + z_j v_3)] \ ,$$

  where j runs over the s atoms of the basis, and f_j is the atomic form factor (49) of the jth atom of the basis. The expression on the right-hand side is written for a reflection $(v_1 v_2 v_3)$, for which $\mathbf{G} = v_1\mathbf{b}_1 + v_2\mathbf{b}_2 + v_3\mathbf{b}_3$.

- Any function invariant under a lattice translation $\mathbf{T}$ may be expanded in a Fourier series of the form

$$n(\mathbf{r}) = \sum_\mathbf{G} n_\mathbf{G} \exp(i\mathbf{G}\cdot\mathbf{r}) \ .$$

- The first Brillouin zone is the Wigner-Seitz primitive cell of the reciprocal lattice. Only waves whose wavevector $\mathbf{k}$ drawn from the origin terminates on a surface of the Brillouin zone can be diffracted by the crystal.

Crystal lattice	*First Brillouin zone*
Simple cubic	Cube
Body-centered cubic	Rhombic dodecahedron (Fig. 13)
Face-centered cubic	Truncated octahedron (Fig. 15)

Problems

1. ***Interplanar separation.*** Consider a plane hkl in a crystal lattice. (a) Prove that the reciprocal lattice vector $\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$ is perpendicular to this plane. (b) Prove that the distance between two adjacent parallel planes of the lattice is $d(hkl) = 2\pi/|\mathbf{G}|$. (c) Show for a simple cubic lattice that $d^2 = a^2/(h^2 + k^2 + l^2)$.

2. ***Hexagonal space lattice.*** The primitive translation vectors of the hexagonal space lattice may be taken as

$$\mathbf{a}_1 = (3^{1/2}a/2)\hat{\mathbf{x}} + (a/2)\hat{\mathbf{y}} \ ; \qquad \mathbf{a}_2 = -(3^{1/2}a/2)\hat{\mathbf{x}} + (a/2)\hat{\mathbf{y}} \ ; \qquad \mathbf{a}_3 = c\hat{\mathbf{z}} \ .$$

(a) Show that the volume of the primitive cell is $(3^{1/2}/2)a^2c$.
(b) Show that the primitive translations of the reciprocal lattice are

$$\mathbf{b}_1 = (2\pi/3^{1/2}a)\hat{\mathbf{x}} + (2\pi/a)\hat{\mathbf{y}} \ ; \qquad \mathbf{b}_2 = -(2\pi/3^{1/2}a)\hat{\mathbf{x}} + (2\pi/a)\hat{\mathbf{y}} \ ; \qquad \mathbf{b}_3 = (2\pi/c)\hat{\mathbf{z}} \ ,$$

so that the lattice is its own reciprocal, but with a rotation of axes.
(c) Describe and sketch the first Brillouin zone of the hexagonal space lattice.

3. ***Volume of Brillouin zone.*** Show that the volume of the first Brillouin zone is $(2\pi)^3/V_c$, where V_c is the volume of a crystal primitive cell. Hint: The volume of a Brillouin zone is equal to the volume of the primitive parallelepiped in Fourier space. Recall the vector identity $(\mathbf{c} \times \mathbf{a}) \times (\mathbf{a} \times \mathbf{b}) = (\mathbf{c} \cdot \mathbf{a} \times \mathbf{b})\mathbf{a}$.

4. ***Width of diffraction maximum.*** We suppose that in a linear crystal there are identical point scattering centers at every lattice point $\boldsymbol{\rho}_m = m\mathbf{a}$, where m is an integer. By analogy with (20), the total scattered radiation amplitude will be proportional to $F = \Sigma \exp[-im\mathbf{a} \cdot \Delta\mathbf{k}]$. The sum over M lattice points is

$$F = \frac{1 - \exp[-iM(\mathbf{a} \cdot \Delta\mathbf{k}]}{1 - \exp[-i(\mathbf{a} \cdot \Delta\mathbf{k})]} \ ,$$

by the use of the series

$$\sum_{m=0}^{M-1} x^m = \frac{1 - x^M}{1 - x} \ .$$

(a) The scattered intensity is proportional to $|F|^2$. Show that

$$|F|^2 \equiv F^*F = \frac{\sin^2 \frac{1}{2} M(\mathbf{a} \cdot \Delta\mathbf{k})}{\sin^2 \frac{1}{2} (\mathbf{a} \cdot \Delta\mathbf{k})} \ .$$

(b) We know that a diffraction maximum appears when $\mathbf{a} \cdot \Delta\mathbf{k} = 2\pi h$, where h is an integer. We change $\Delta\mathbf{k}$ slightly and define ϵ in $\mathbf{a} \cdot \Delta\mathbf{k} = 2\pi h + \epsilon$ such that ϵ gives the position of the first zero in $\sin \frac{1}{2} M(\mathbf{a} \cdot \Delta\mathbf{k})$. Show that $\epsilon = 2\pi/M$, so that the width of the diffraction maximum is proportional to $1/M$ and can be extremely narrow for macroscopic values of M. The same result holds true for a three-dimensional crystal.

5. ***Structure factor of diamond.*** The crystal structure of diamond is described in Chapter 1. The basis consists of eight atoms if the cell is taken as the conventional cube. (a) Find the structure factor S of this basis. (b) Find the zeros of S and show that the allowed reflections of the diamond structure satisfy $v_1 + v_2 + v_3 = 4n$, where all indices are even and n is any integer, or else all indices are odd (Fig. 18). (Notice that h, k, l may be written for v_1, v_2, v_3 and this is often done.)

6. ***Form factor of atomic hydrogen.*** For the hydrogen atom in its ground state, the number density is $n(r) = (\pi a_0^3)^{-1} \exp(-2r/a_0)$, where a_0 is the Bohr radius. Show that the form factor is $f_G = 16/(4 + G^2a_0^2)^2$.

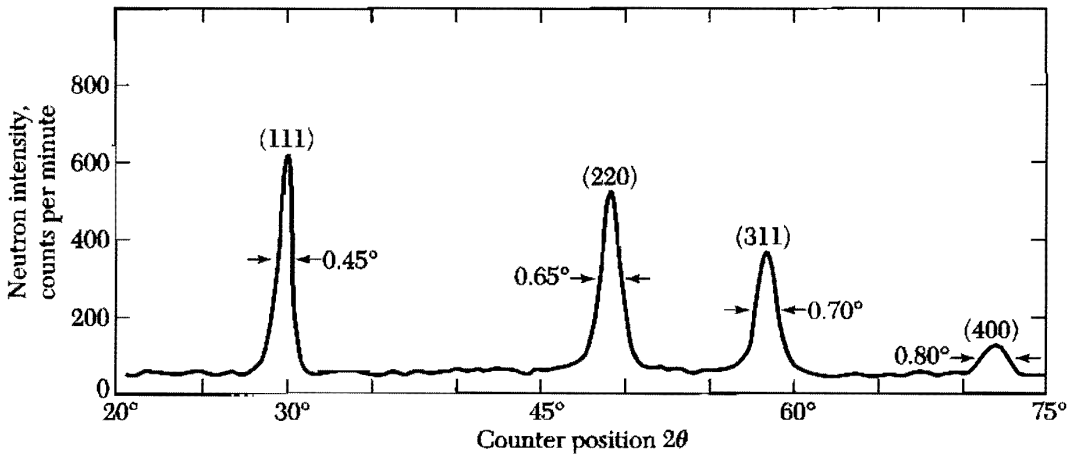

Figure 18 Neutron diffraction pattern for powdered diamond. (After G. Bacon.)

7. ***Diatomic line.*** Consider a line of atoms $ABAB \ldots AB$, with an A—B bond length of $\frac{1}{2}a$. The form factors are f_A, f_B for atoms A, B, respectively. The incident beam of x-rays is perpendicular to the line of atoms. (a) Show that the interference condition is $n\lambda = a \cos \theta$, where θ is the angle between the diffracted beam and the line of atoms. (b) Show that the intensity of the diffracted beam is proportional to $|f_A - f_B|^2$ for n odd, and to $|f_A + f_B|^2$ for n even. (c) Explain what happens if $f_A = f_B$.

The kinetic energy of the incident neutron is $p^2/2M_n$, where M_n is the mass of the neutron. The momentum $\mathbf{p}$ is given by $\hbar\mathbf{k}$, where $\mathbf{k}$ is the wavevector of the neutron. Thus $\hbar^2k^2/2M_n$ is the kinetic energy of the incident neutron. If $\mathbf{k}'$ is the wavevector of the scattered neutron, the energy of the scattered neutron is $\hbar^2k'^2/2M_n$. The statement of conservation of energy is

$$\frac{\hbar^2k^2}{2M_n} = \frac{\hbar^2k'^2}{2M_n} \pm \hbar\omega \ , \tag{34}$$

where $\hbar\omega$ is the energy of the phonon created (+) or absorbed (−) in the process.

To determine the dispersion relation using (33) and (34) it is necessary in the experiment to find the energy gain or loss of the scattered neutrons as a function of the scattering direction $\mathbf{k} - \mathbf{k}'$. Results for germanium and KBr are given in Fig. 8; results for sodium are given in Fig. 11. A spectrometer used for phonon studies is shown in Fig. 12.

SUMMARY

- The quantum unit of a crystal vibration is a phonon. If the angular frequency is ω, the energy of the phonon is $\hbar\omega$.
- When a phonon of wavevector $\mathbf{K}$ is created by the inelastic scattering of a photon or neutron from wavevector $\mathbf{k}$ to $\mathbf{k}'$, the wavevector selection rule that governs the process is

  $$\mathbf{k} = \mathbf{k}' + \mathbf{K} + \mathbf{G} \ ,$$

  where $\mathbf{G}$ is a reciprocal lattice vector.
- All elastic waves can be described by wavevectors that lie within the first Brillouin zone in reciprocal space.
- If there are p atoms in the primitive cell, the phonon dispersion relation will have 3 acoustical phonon branches and $3p - 3$ optical phonon branches.

Problems

1. ***Monatomic linear lattice.*** Consider a longitudinal wave

   $$u_s = u\cos(\omega t - sKa)$$

   which propagates in a monatomic linear lattice of atoms of mass M, spacing a, and nearest-neighbor interaction C.
   (a) Show that the total energy of the wave is

   $$E = \tfrac{1}{2}M\sum_s (du_s/dt)^2 + \tfrac{1}{2}C\sum_s (u_s - u_{s+1})^2 \ .$$

   where s runs over all atoms.

(b) By substitution of u_s in this expression, show that the time-average total energy per atom is

$$\tfrac{1}{4}M\omega^2u^2 + \tfrac{1}{2}C(1 - \cos Ka)u^2 = \tfrac{1}{2}M\omega^2u^2 \ ,$$

where in the last step we have used the dispersion relation (9) for this problem.

2. ***Continuum wave equation.*** Show that for long wavelengths the equation of motion (2) reduces to the continuum elastic wave equation

$$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2} \ ,$$

where v is the velocity of sound.

3. ***Basis of two unlike atoms.*** For the problem treated by (18) to (26), find the amplitude ratios u/v for the two branches at $K_{max} = \pi/a$. Show that at this value of K the two lattices act as if decoupled: one lattice remains at rest while the other lattice moves.

4. ***Kohn anomaly.*** We suppose that the interplanar force constant C_p between planes s and $s + p$ is of the form

$$C_p = A \frac{\sin pk_0a}{pa} \ ,$$

where A and k_0 are constants and p runs over all integers. Such a form is expected in metals. Use this and Eq. (16a) to find an expression for ω^2 and also for $\partial\omega^2/\partial K$. Prove that $\partial\omega^2/\partial K$ is infinite when $K = k_0$. Thus a plot of ω^2 versus K or of ω versus K has a vertical tangent at k_0: there is a kink at k_0 in the phonon dispersion relation $\omega(K)$.

5. ***Diatomic chain.*** Consider the normal modes of a linear chain in which the force constants between nearest-neighbor atoms are alternately C and $10C$. Let the masses be equal, and let the nearest-neighbor separation be $a/2$. Find $\omega(K)$ at $K = 0$ and $K = \pi/a$. Sketch in the dispersion relation by eye. This problem simulates a crystal of diatomic molecules such as H_2.

6. ***Atomic vibrations in a metal.*** Consider point ions of mass M and charge e immersed in a uniform sea of conduction electrons. The ions are imagined to be in stable equilibrium when at regular lattice points. If one ion is displaced a small distance r from its equilibrium position, the restoring force is largely due to the electric charge within the sphere of radius r centered at the equilibrium position. Take the number density of ions (or of conduction electrons) as $3/4\pi R^3$, which defines R. (a) Show that the frequency of a single ion set into oscillation is $\omega = (e^2/MR^3)^{1/2}$. (b) Estimate the value of this frequency for sodium, roughly. (c) From (a), (b), and some common sense, estimate the order of magnitude of the velocity of sound in the metal.

*7. ***Soft phonon modes.*** Consider a line of ions of equal mass but alternating in charge, with $e_p = e(-1)^p$ as the charge on the pth ion. The interatomic potential is

*This problem is rather difficult.