University of Anbar

College of Science

Department of Physics

فيزياء الحالة الصلبة

Solid state Physics

المرحلة الرابعة

الكورس الاول

صلبة 1

Syllabus of this course مفردات الكورس

1- crystal structure
2- x-ray diffraction
3- lattice vibration
4- thermal properties in solids
5- free electron model

3. X-Ray Diffraction In Crystals

It can determine بالامكان تحديد the structure التركيب of a crystal by studying بدراسة the diffraction pattern طيف الانكسار of a beam شعاع of radiation الاشعاع incidentالساقط on the crystal. By measuring the directions of the diffraction and the corresponding تبعا الى intensities الشدات , can obtain information concerning the crystal structure responsible for the diffraction.

Three types of radiation ثلاث انواع من الاشعاع are used: x-rays, neutrons, and electron. The treatment المعالجة of these three types is quite similar متشابه جدا; therefore, we shall examine in detail only the x-ray case.

3.1 Generation توليد and Absorption امتصاص Of X-Rays

X-rays are electromagnetic waves موجات كهرومغناطيسية whose wavelengths اطوال موجية are in about of 1 $\dot{A}$. Therefore, their wavelength is so shortقصير . they have the same physical properties as other electromagnetic waves, such as optical waves الموجات البصرية . The wavelength of an x-ray is thus of the same order نفس المرتبة of magnitude المقدار as the lattice constants ثوابت الشبيكة of crystals and this which makes هذا يجعل x-rays useful مفيدة in the analysis في تحليل of crystal structures. The energy of an x-ray photon is given by the **Einstein** relation علاقة انيشتاين $E=h\nu$, where h is Planck's constant ثابت بلانك and ν is the frequency التردد,

Substituting بتعويض القيم h=6.6 x 10^{-27} erg-s and $\lambda=1\dot{A}$, $\boldsymbol{\nu=c/\lambda}$ therefore, E= 10^4 eV, which is a typical value القيمة المثالية.

The basic experimental arrangement الترتيب العملي for generating توليد an x-ray beam is showed in Fig 3.1

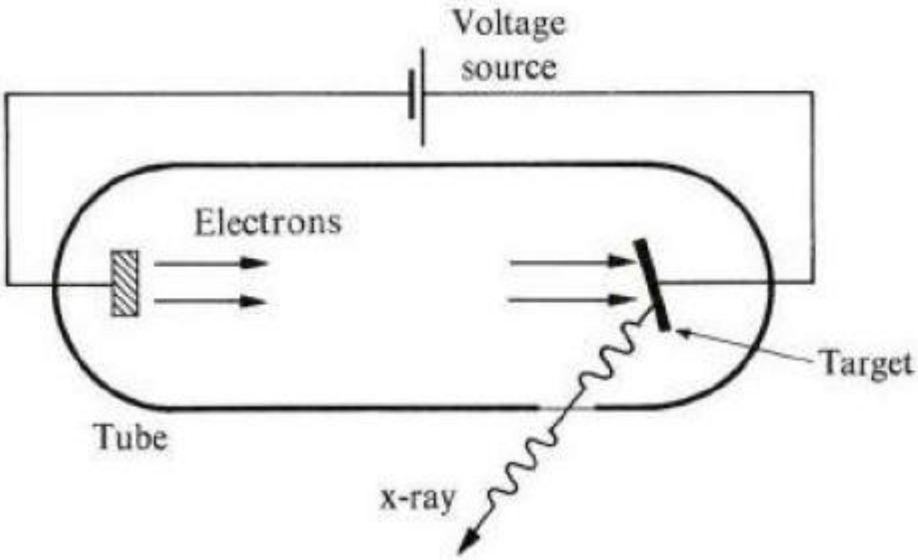


Figure 3.1 Generation of X-ray

Electrons emitted الالكترونات المنبعثة from the cathode of a vacuum tube انبوب فراغي are accelerated والمعجلة by a large potential بجهد عالي acting across the tube.

The electrons thus acquire تمتلك high kinetic energy طاقة حركية عالية, and when they impinge تصطدم on a metallic target هدف معدني, forming تشكل the anode الانود at the end of the tube, the x-rays are emitted تنبعث from the target, The emitted radiation الاشعاع المنبعث has يمتلك a wide عريض continuous مستمر spectrumطيف, on which is superimposed متراكب a series سلسلة of discrete lines خطوط منفصلة, The continuous spectrum is due to نتيجة emission انبعاث of radiation by the incident electrons الالكترونات الساقطة as they are deflected تنحرف by the nuclear charges شحنات النواة in the target, while the discrete lines are due to the emission by atoms in the target after they are excited تتهيج by the incident electrons.

The maximum frequency of the continuous spectrum v_o is related له علاقة to the accelerating potential جهد التعجيل by $eV = hv_o$, since the maximum energy of a photon cannot exceedيتجاوز the kinetic energy of the incident electron. The corresponding wavelength λ_o , is given by

$$\lambda_0 = \frac{12.3}{V}\,\text{Å}, \tag{3.1}$$

When an x-ray beam passes through a material medium it is partially absorbed. The intensity of the beam is attenuated according to the relation

$$I = I_0 e^{-\alpha x} \tag{3.2}$$

where $\boldsymbol{I_o}$, is the initial intensity at the surface of the medium and **x** the distance travelled. The parameter **α** is known as the absorption coefficient.

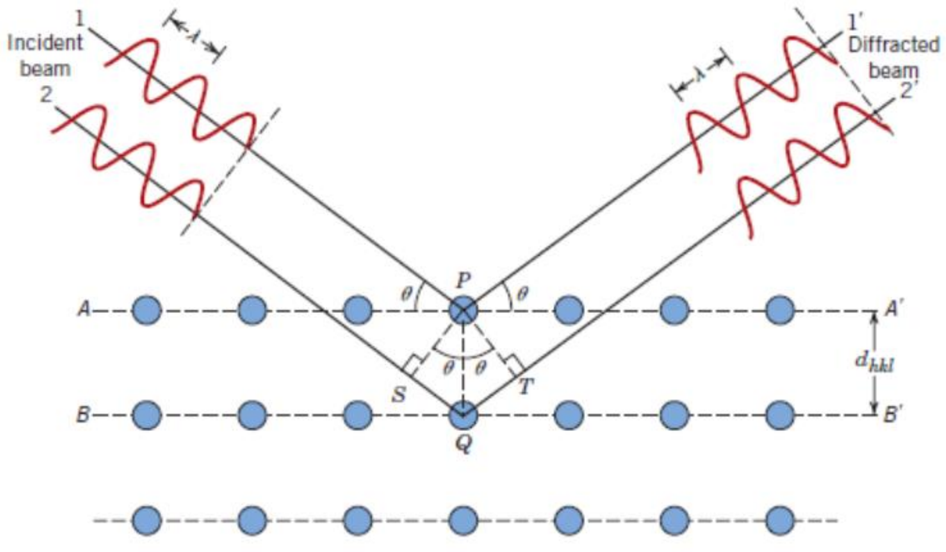
3.2 Bragg's Law قانون براك

When a monochromatic أحادي اللون x-ray beam is incident on the surface of a crystal, it is reflected. However, the reflection takes place only when the angle of incidence has certain values. These values depend on the wavelength and the lattice constants of the crystal,

The model is illustrated in Fig 3.2(a), where the crystal is represented by a set of parallel planes, corresponding to the atomic planes. The incident beam is reflected partially at each of these planes, which act as mirrors, and the reflected rays are then collected at a distant detector. the interference تداخل is constructive بناء only if the difference between the paths of any two consecutive rays is an integral multiple of the wavelength,

$$\text{Path difference} = n\lambda, \qquad n = 1, 2, 3, \ldots,$$

where , **λ**, is the wavelength and **n** a positive integer. The path difference Δ between rays 1 and 2 in the figure 3.2



Consider لنفرض the two parallel planes مستويين متوازية of atoms $A - A'$ and $B - B'$ in Figure 3.1, which have the same لها نفس h, k, and l Miller indices معاملات ميلير and are separated مفصولة by the interplanar spacing بمسافة بينية d_{hkl}.
Now assume لنفترض that a parallel متوازي, monochromatic احادي اللون and coherent متماسك beam of x-rays of wavelength λ is incident يسقط on these two planes at an angle θ. Two rays in this beam, labelled المرقمة 1 and 2, are scattered by atoms P and Q. Constructive interference تداخل بناء of the scattered rays $1'$ and $2'$ occurs also at an angle θ to the planes, if the path length difference between $1 - P - 1'$ and 2–Q–$2'$ (i.e., $\overline{SQ} + \overline{QT}$) is equal to a whole number, n, of wavelengths.

$$n\lambda = \overline{SQ} + \overline{QT}$$

$$n\lambda = d_{hkl} \sin\theta + d_{hkl} \sin\theta$$

$$= 2d_{hkl} \sin\theta$$

$$2d \sin\theta = n\lambda. \qquad 3.5$$

Equation is known as Bragg's law قانون براك; also, n is the order of reflection مرتبة الانعكاس, which may be any integer عدد صحيح (1, 2, 3, . . .).

where θ is the angle between the incident beam and the reflecting planes

This is the Bragg's law. The angles determined by this equation, for a given d and λ, are the only angles at which reflection takes place.

The magnitude مقدار of the distance between two adjacent and parallel planes of atoms (i.e., the interplanar spacing d_{hkl}) is a function of the Miller indices معاملات ميلير (h, k, and l) as well as the lattice parameter(a). For example, for crystal structures that have cubic symmetry مكعب متناظر او متماثل,

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

where **a** is the lattice parameter (unit cell edge length).

EXAMPLE 3.1

Interplanar Spacing and Diffraction Angle Computations

For BCC iron, compute (a) the interplanar spacing and (b) the diffraction angle for the (220) set of planes. The lattice parameter for Fe is 0.2866 nm. Also, assume that monochromatic radiation having a wavelength of 0.1790 nm is used, and the order of reflection is 1.

Solution

(a) The value of the interplanar spacing d_{hkl} is determined using $a = 0.2866$ nm, and $h = 2$, $k = 2$, and $l = 0$, because we are considering the (220) planes. Therefore,

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

$$= \frac{0.2866 \text{ nm}}{\sqrt{(2)^2 + (2)^2 + (0)^2}} = 0.1013 \text{ nm}$$

(b) The value of θ may now be computed using $n = 1$, because this is a first-order reflection:

$$\sin\theta = \frac{n\lambda}{2d_{hkl}} = \frac{(1)(0.1790 \text{ nm})}{(2)(0.1013 \text{ nm})} = 0.884$$

$$\theta = \sin^{-1}(0.884) = 62.13°$$

The diffraction angle is 2θ, or

$$2\theta = (2)(62.13°) = 124.26°$$

3.3 The Reciprocal Lattice الشبيكة المقلوبة

Starting with a lattice which has basis vectors المتجهات الاساسية are a, b, and c, which are the primitive translational vectors المتجهات الانتقالية of a space lattice in real space, then we define the fundamental vectors of the reciprocal lattice by a*, b*, and c* according to the relations

$$\mathbf{a}^* = \frac{2\pi \mathbf{b}\times\mathbf{c}}{\mathbf{a}\cdot\mathbf{b}\times\mathbf{c}}$$
$$\mathbf{b}^* = \frac{2\pi \mathbf{c}\times\mathbf{a}}{\mathbf{a}\cdot\mathbf{b}\times\mathbf{c}}$$
$$\mathbf{c}^* = \frac{2\pi \mathbf{a}\times\mathbf{b}}{\mathbf{a}\cdot\mathbf{b}\times\mathbf{c}} \qquad 3.6$$

A fundamental reciprocal vector such as a* is not necessarily ليس بالضرورة parallel متوازي to **a** of the direct lattice, but is required مطلوب to be perpendicular عمودي to both b and c. We can write zeros for the various dot products الضرب العددي

$$\mathbf{a}^*\cdot\mathbf{b} = \mathbf{a}^*\cdot\mathbf{c} = \mathbf{b}^*\cdot\mathbf{a} = \mathbf{b}^*\cdot\mathbf{c} = \mathbf{c}^*\cdot\mathbf{a} = \mathbf{c}^*\cdot\mathbf{b} = 0 \qquad 3.7$$

whereas

$$\mathbf{a}^*\cdot\mathbf{a} = \mathbf{b}^*\cdot\mathbf{b} = \mathbf{c}^*\cdot\mathbf{c} = 2\pi \qquad 3.8$$

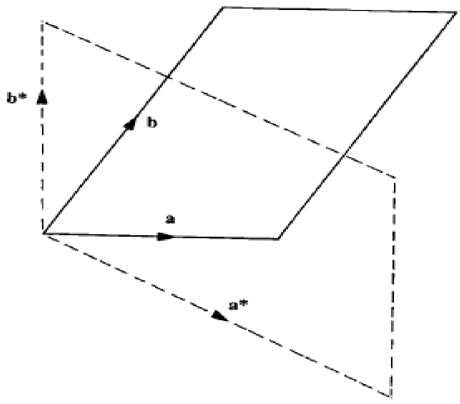


Figure 3.3 The fundamental vectors of the reciprocal lattice for a two-dimensional oblique منحرف "real" lattice. Note that a* is perpendicular to b and b* is perpendicular to a; also, that a* • a equals b* • b

The inverse معكوس of the transformation defined in Equation 3.6 , We can easily confirm that

$$a = \frac{2\pi b^{*} \times c^{*}}{a^{*}.b^{*} \times c^{*}}$$

$$b = \frac{2\pi c^{*} \times a^{*}}{a^{*}.b^{*} \times c^{*}} \qquad 3.9$$

$$c = \frac{2\pi a^{*} \times b^{*}}{a^{*}.b^{*} \times c^{*}}$$

3.4 Reciprocal Lattice Vectors

The translations lattice vector in the real lattice

$$\mathbf{T} = n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c} \qquad \mathbf{3.10}$$

These translation vector connect pairs of points in the crystal lattice which have identical atomic environments. So also, in reciprocal space is there set of translations that we call reciprocal lattice vectors.

$$G_{hkl} = ha^* + kb^* + lc^* \qquad (3.11)$$

a simple expression for the spacing *d* between (hkl) planes, was possible for a cubic lattice. In terms of the reciprocal lattice vector G_{hkl}.

$$d_{hkl} = \frac{a \cdot G_{hkl}}{h\,|G_{hkl}|} \qquad (3.12)$$

But from Equations 3.8 and 3.11, $a \cdot G_{hkl}$ is just $2\pi h$.

Therefore, the spacing of (hkl) planes in real space is connected متصل with the h, k, 1 reciprocal lattice vector length by

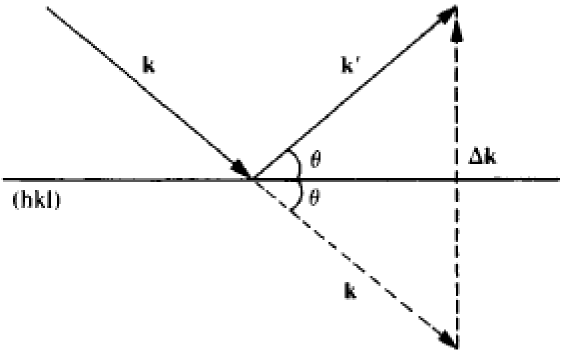
$$d_{hkl} = \frac{2\pi}{|G_{hkl}|} \qquad (3.13)$$

3.5 The Diffraction Condition

The reciprocal lattice permits تجيز an interesting مفيد perspective انطباع of the Bragg condition شرط براك for the reflection. Instead of بالاضافة الى considering يعتبر just the wavelength of the radiation which interacts يتفاعل with the atoms of a set of planes.

the initial بدائي and final نهائي wave-vectors k, k' of a reflected wave-particle. Provided يجهز that scattering استطارة is elastic مرنة, there is no change in magnitude of wave-vector

$$|\mathbf{k}| = |\mathbf{k}'| = (2\pi/\lambda) \qquad (3.14)$$



The change Δk in k is in the direction perpendicular عمودي to the (hkl) planes, the direction we have just been associating المرافق with G_{hkl}, or with the unit vector n.

$$\begin{aligned}\Delta\mathbf{k} = (\mathbf{k}' - \mathbf{k}) &= 2\sin\theta|\mathbf{k}|\mathbf{n} \\ &= \left[\frac{4\pi \sin\theta}{\lambda}\right]\mathbf{n} \\ &= \left[\frac{4\pi \sin\theta}{\lambda|\mathbf{G}_{hkl}|}\right]\mathbf{G}_{hkl} \\ &= \left[\frac{2d_{hkl}\sin\theta}{\lambda}\right]\mathbf{G}_{hkl}\end{aligned} \quad \mathbf{3.15}$$

When the combination التراكب of λ, θ and d_{hkl} is appropriate مناسب for satisfaction قناعة او رضا of the Bragg condition,

$$\Delta\mathbf{k} = \mathbf{G}_{hkl} \quad \mathbf{3.16}$$

$$\mathbf{k'-k= G_{hkl}}$$

the vector relation between the initial and final wave-vectors of a Bragg-reflected wave-particle can be written as

$$\mathbf{k}' = \mathbf{G}_{hkl} + \mathbf{k} \qquad \mathbf{3.17}$$

When each side كل جانب of this equation is squared يتربع and the quantity الكمية $|k|^2 = |k'|^2$ is subtracted from each side, the Bragg condition appears يظهر in the form بالصيغة

$$\mathbf{k}'^2 = (\boldsymbol{G}_{hkl} + \boldsymbol{k})^2$$

$$\boldsymbol{k}^2 = \boldsymbol{G}_{hkl}{}^2 + 2\boldsymbol{G}_{hkl}\,\boldsymbol{k} + \boldsymbol{k}^2$$

$$\boldsymbol{k}^2 - \boldsymbol{k}^2 = \boldsymbol{G}_{hkl}{}^2 + 2\boldsymbol{G}_{hkl}\,\boldsymbol{k}$$

$$\boldsymbol{G}_{hkl}{}^2 + 2\boldsymbol{G}_{hkl}\,\boldsymbol{k} = \mathbf{0} \qquad \mathbf{3.18}$$

$$\left.\begin{aligned} \mathbf{a}\cdot\Delta\mathbf{k} &= 2\pi\mathrm{h} \\ \mathbf{b}\cdot\Delta\mathbf{k} &= 2\pi\mathrm{k} \\ \mathbf{c}\cdot\Delta\mathbf{k} &= 2\pi\mathrm{l} \end{aligned}\right\} \qquad \mathbf{3.19}$$

Equations 3.19 are the **Laue equations**, which provide one useful avenue وسيلة مفيدة for discussions of crystal symmetry التماثل and structure.

References

1- **Charles Kittel - Introduction to Solid State Physics-Wiley (2005)**
2- **J. S. Blakemore - Solid State Physics-Cambridge University Press (1985)**

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