University of Anbar
College of Science
Department of Physics

فيزياء المواد

Physics of Materials

المرحلة الثالثة

الكورس الاول

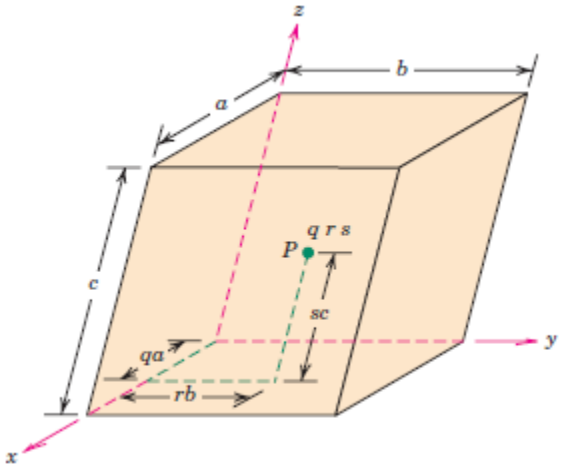
اعداد
م.د. قيس عبدالله عباس

3.1 Crystallographic Points, Directions, and Planes

When dealing نتعامل مع with crystalline materials, it often becomes necessary يصبح ضروري to specify a particular point نقاط معينة within a unit cell. a crystallographic direction الاتجاهات البلورية , or some crystallographic plane المستوي البلوري of atoms.

3.1.1 Point Coordinates الاحداثي النقطي

The position موقع of any point located موجودة within a unit cell may be specified in terms of its coordinates as fractional multiples of the unit cell edge lengths طول الحافة (i.e., in terms of a, b, and c). To illustrate, consider the unit cell and the point P situated يقع there in as shown in Figure



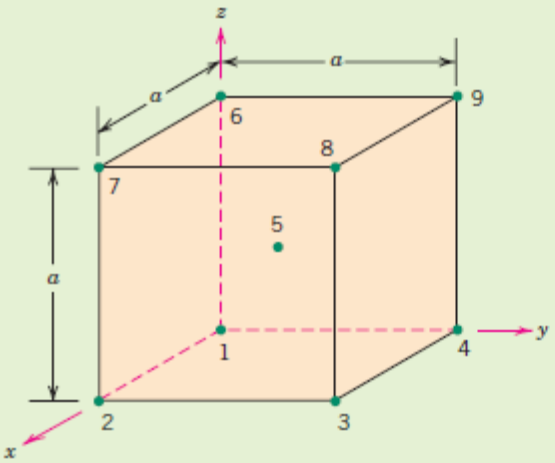
We specify نحدد the position of **P** in terms of the generalized coordinates **q, r**, and **s** where **q** is some fractional length of **a** along the **x** axis, **r** is some fractional length of **b** along the **y** axis, and similarly for **s**. Thus, the position of **P** is designated حددت using coordinates **q r s** with values that are less than or equal to unity.

Specification of Point Coordinates

Specify point coordinates for all atom positions for a BCC unit cell.

Solution

For the BCC unit cell of Figure , atom position coordinates correspond to the locations of the centers of all atoms in the unit cell—that is, the eight corner atoms and single center atom. These positions are noted (and also numbered) in the following figure.

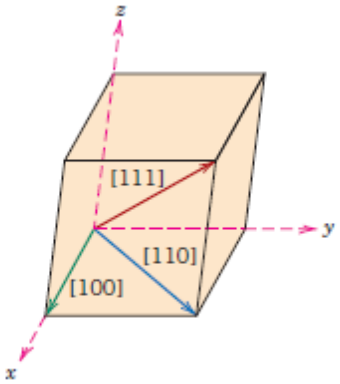


Point coordinates for position number 1 are 0 0 0; this position is located at the origin of the coordinate system, and, therefore, the fractional unit cell edge lengths along the x, y, and z axes are, respectively, $0a$, $0a$, and $0a$. Furthermore, for position number 2, because it lies one unit cell edge length along the x axis, its fractional edge lengths are a, $0a$, and $0a$, respectively, which yield point coordinates of 1 0 0. The following table presents fractional unit cell lengths along the x, y, and z axes, and their corresponding point coordinates for each of the nine points in the preceding figure.

Point Number	*Fractional Lengths*			*Point Coordinates*
	x axis	*y axis*	*z axis*	
1	0	0	0	0 0 0
2	1	0	0	1 0 0
3	1	1	0	1 1 0
4	0	1	0	0 1 0
5	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$
6	0	0	1	0 0 1
7	1	0	1	1 0 1
8	1	1	1	1 1 1
9	0	1	1	0 1 1

3.1.2 Crystallographic Directions

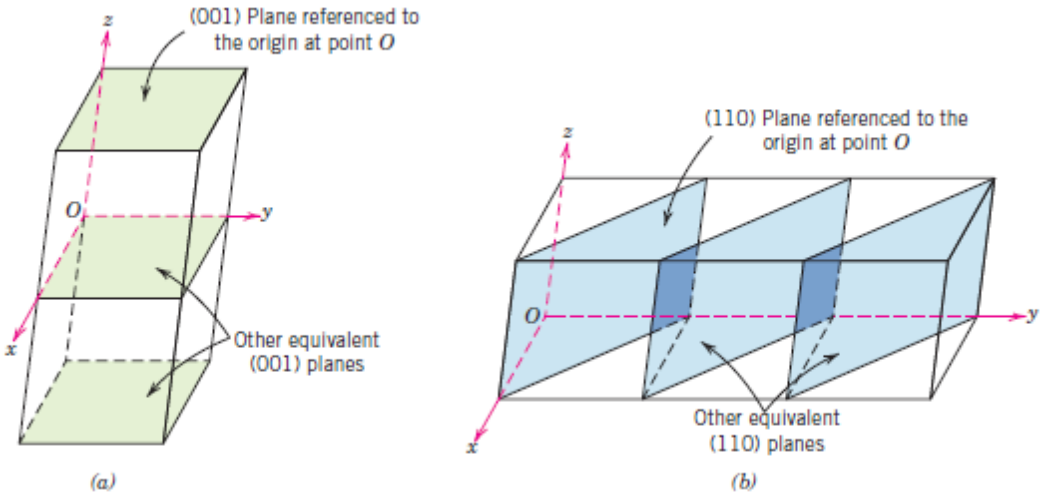
A crystallographic direction is defined as a line between two points, or a vector.



The [100], [110], and [111] directions within a unit cell.

3.1.3 Crystallographic Planes

crystallographic planes are specified by three Miller indices as (hkl). Any two planes parallel to each other are equivalent and have identical indices. The orientations of planes for a crystal structure are represented in a similar manner. the unit cell is the basis, with the three-axis coordinate system.



3.2 Crystalline and Non-crystalline Materials

3.2.1 Single Crystals:

is a crystalline material, when the periodic and repeated arrangement of atoms is perfect or extends throughout the entirety of the specimen without interruption. All unit cells interlock in the same way and have the same orientation.

هي مادة بلورية ، عندما يكون الترتيب الدوري والمتكرر للذرات مثاليًا أو يمتد في جميع أنحاء العينة بأكملها دون انقطاع. تتشابك جميع خلايا الوحدة بنفس الطريقة ولها نفس الاتجاه.

3.2.2. Polycrystalline Materials:

Most crystalline materials are composed of a collection of many small crystals or grains

تتكون معظم المواد البلورية من مجموعة من العديد من البلورات أو الحبوب الصغيرة

3.2.3 Noncrystalline:

materials that lack a systematic and regular arrangement of atoms or ions over relatively large distances (on an atomic scale). Sometimes the term amorphous is also used to describe these materials.

المواد التي تفتقر إلى ترتيب منظم ومنتظم للذرات أو الأيونات على مسافات كبيرة نسبيًا (على مقياس ذري). في بعض الأحيان يستخدم المصطلح غير متبلور أيضًا لوصف هذه المواد

3.2.4 Anisotropy:

The physical properties of single crystals of some substances depend on the crystallographic direction in which measurements are taken. For example, the elastic modulus, the electrical conductivity, and the index of refraction may have different values in the [100] and [111] directions. This directionality of properties is anisotropy.

تعتمد الخواص الفيزيائية للبلورات المفردة لبعض المواد على الاتجاه البلوري الذي تؤخذ فيه القياسات. على سبيل المثال ، قد يكون لمعامل المرونة والتوصيل الكهربائي ومعامل الانكسار قيم مختلفة في الاتجاهين [100] و [111]. اتجاه الخصائص هذا هو تباين الخواص.

3.3 X-Ray Diffraction and Bragg's Law

X-rays are a form of electromagnetic radiation اشعاع كهرو مغناطيسي that have high energies طاقات and short wavelengths طول موجي قصير . wavelengths on the order بمرتبة of the atomic spacings المسافات الذرية for solids. When a beam شعاع of x-rays impinges يصطدم on a solid material, a portion جزء of this beam will be scattered يستطار in all directions بجميع الاتجاهات by the electrons associated with each atom or ion that lies within the beam's path.

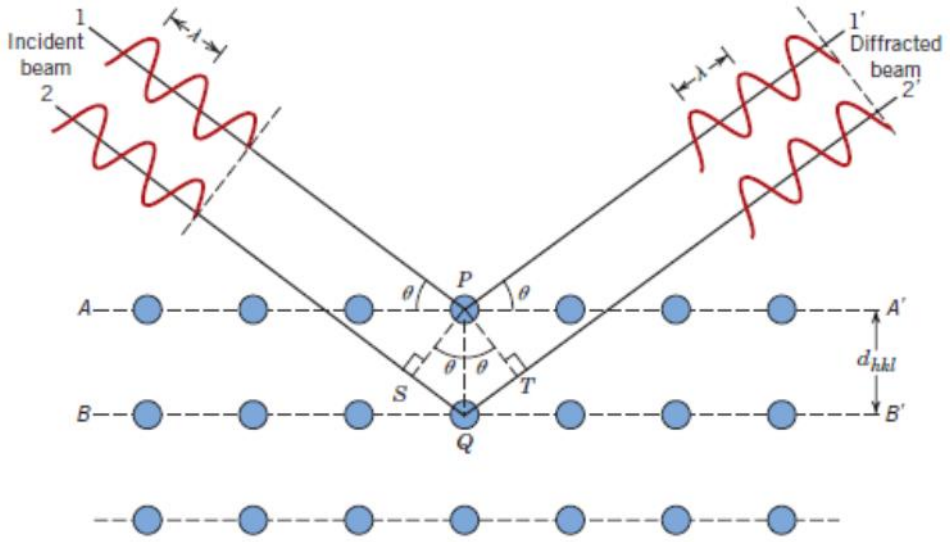


Figure 3.1

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.

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

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

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

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, . . .).

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 [redacted] $a = 0.2866$ 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 [redacted] $n = 1$, because this is a first-order reflection:

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

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

The diffraction angle is 2θ, or

$$2\theta = (2)(62.13^\circ) = 124.26^\circ$$

References

1- Fundamentals of Materials Science and Engineering, William D. Callister, Jr. David G. Rethwisch
2- Materials _Science_ and _Engineering_9th . William D. Callister, Jr. David G. Rethwisch