
Elements of X-RAY DIFFRACTION

SECOND EDITION

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X-ray diffraction technique had its x-rays, the manne x-ray diffraction v however, other us structure determin stress measurement cle size, to the de orientations in a j

The purpose of edge of the subject involved, and the majority of these ever, little or no n tion of nonmetall depend on the m metallurgists, che who use x-ray di already mentioned

Members of t cerned with the d rotating-crystal m of such structures

This is a boo reference book fo given beyond tho example, the thec in detail, but the development, and described, becaus x-ray diffraction i

The book is c ods, and applicati based on, the con of a substance is

3. The reflection of visible light by a good mirror is almost 100 percent efficient. The intensity of a diffracted x-ray beam is extremely small compared to that of the incident beam.

Despite these differences, we often speak of "reflecting planes" and "reflected beams" when we really mean diffracting planes and diffracted beams. This is common usage and, from now on, we will frequently use these terms without quotation marks but with the tacit understanding that we really mean diffraction and not reflection.*

To sum up, diffraction is essentially a scattering phenomenon in which a large number of atoms cooperate. Since the atoms are arranged periodically on a lattice, the rays scattered by them have definite phase relations between them; these phase relations are such that destructive interference occurs in most directions of scattering, but in a few directions constructive interference takes place and diffracted beams are formed. The two essentials are a wave motion capable of interference (x-rays) and a set of periodically arranged scattering centers (the atoms of a crystal).

3-3 THE BRAGG LAW

Two geometrical facts are worth remembering: (1) The incident beam, the normal to the reflecting plane, and the diffracted beam are always coplanar. (2) The angle between the diffracted beam and the transmitted beam is always 2θ . This is known as the diffraction angle, and it is this angle, rather than θ , which is usually measured experimentally.

As previously stated, diffraction in general occurs only when the wavelength of the wave motion is of the same order of magnitude as the repeat distance between scattering centers. This requirement follows from the Bragg law. Since $\sin \theta$ cannot exceed unity, we may write

$$\frac{n\lambda}{2d'} = \sin \theta < 1. \quad (3-2)$$

Therefore, $n\lambda$ must be less than $2d'$. For diffraction, the smallest value of n is 1. ($n = 0$ corresponds to the beam diffracted in the same direction as the transmitted beam. It cannot be observed.) Therefore the condition for diffraction at any observable angle 2θ is

$$\lambda < 2d'. \quad (3-3)$$

For most sets of crystal planes d' is of the order of 3 Å or less, which means that λ cannot exceed about 6 Å. A crystal could not possibly diffract ultraviolet radiation, for example, of wavelength about 500 Å. On the other hand, if λ is very small, the diffraction angles are too small to be conveniently measured.

* For the sake of completeness, it should be mentioned that x-rays *can* be totally reflected by a solid surface, just as visible light is by a mirror, but only at very small angles of incidence (below about one degree).

The Bragg law

Since the coefficient of a first-order reflection is the same as the previous space group and write the Bragg law

This form will be

This usage is shown in (a). Scattered by adjacent real plane of atoms. Fig. 3-3(b), where of the (200) set of between rays scattered so that this reflection 300, 400, etc., reflection orders from the (1 of spacing d' may planes of spacing definition of Miller to the (hkl) planes

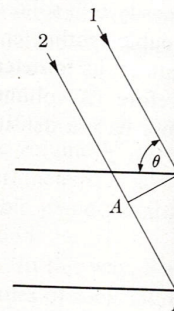


Fig. 3-3 Equivalence reflection.

* This means the reflecting plane hkl , with plane (hkl) .

The Bragg law may be written in the form

$$\lambda = 2 \frac{d'}{n} \sin \theta. \quad (3-4)$$

Since the coefficient of λ is now unity, we can consider a reflection of any order as a first-order reflection from planes, real or fictitious, spaced at a distance $1/n$ of the previous spacing. This turns out to be a real convenience, so we set $d = d'/n$ and write the Bragg law in the form

$$\lambda = 2d \sin \theta. \quad (3-5)$$

This form will be used throughout this book.

This usage is illustrated by Fig. 3-3. Consider the second-order 100 reflection* shown in (a). Since it is second-order, the path difference ABC between rays scattered by adjacent (100) planes must be two whole wavelengths. If there is no real plane of atoms between the (100) planes, we can always imagine one as in Fig. 3-3(b), where the dotted plane midway between the (100) planes forms part of the (200) set of planes. For the same reflection as in (a), the path difference DEF between rays scattered by adjacent (200) planes is now only one whole wavelength, so that this reflection can properly be called a first-order 200 reflection. Similarly, 300, 400, etc., reflections are equivalent to reflections of the third, fourth, etc., orders from the (100) planes. In general, an n th-order reflection from (hkl) planes of spacing d' may be considered as a first-order reflection from the $(nh \ nk \ nl)$ planes of spacing $d = d'/n$. Note that this convention is in accord with the definition of Miller indices since $(nh \ nk \ nl)$ are the Miller indices of planes parallel to the (hkl) planes but with $1/n$ th the spacing of the latter.

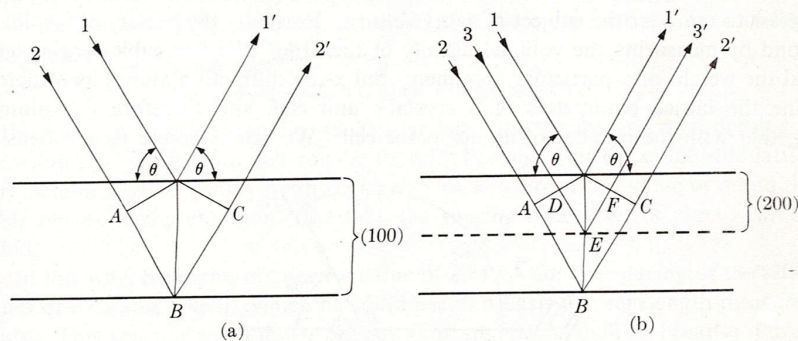


Fig. 3-3 Equivalence of (a) a second-order 100 reflection and (b) a first-order 200 reflection.

* This means the reflection from the (100) planes. Conventionally, the Miller indices of a reflecting plane hkl , written without parentheses, stand for the reflected beam from the plane (hkl) .