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"Crystal Structure Analysis"
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Updated Jan. 28, 2020

Chapter 1 Bragg's law

First of all, let us study the Bragg's law. It is a fundamental law, but many students, professional engineers or scientists do not really understand the theory.

1－1 What is the Bragg's law?

Bragg's law means that the diffraction can occur only when the following equation is satisfied.

$$n\lambda = 2d\sin\theta \,, \tag{1.1}$$

where

n is a positive integer,
λ is the wavelength of the X-ray,
d is the distance between the lattice plane,
θ is the incident glancing angle (supplement of the incident angle).

One may think: "isn't θ the "incident angle ?"..., but the "incident angle" is defined as the angle between the normal direction of a reflection plane and the incident ray (or more generally quantum beam), in a traditional theory of optics.

The Bragg's law is often expressed in another way :

$$\lambda = 2d\sin\theta \,, \tag{1.2}$$

and this expression may be more popular than that of Eq. (1.1). Be sure that the left side of Eq. (1.2) does not include " n ".

Why can there be different expressions ? Do you think one of those equations should be wrong ? Actually, both of them are correct. The definition of d in Eq. (1.2) is different from the definition of d in Eq. (1.1), and it is equivalent with (d / n) for the definition of d in Eq. (1.2). In the following sections in this chapter, the expression by Eq. (1.1) will be used, because it looks easier to be understood.

1－2 Illustrate the Bragg's law

It is not a bad idea just to memorize the Bragg's equation, because it is often used on analysis of diffraction data. But such memory will easily be volatilized, if you do not use the equation for a while. And it is likely that you might forget the meanings of the symbols, even if you do remember the equation. It is recommended to draw illustrations several times, and to remember how the Bragg's is derived.

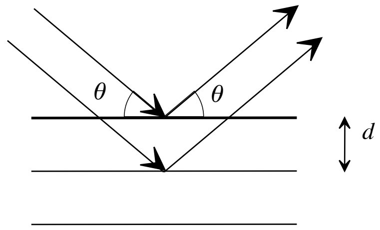

Fig. 1.1　Illustration to derive the Bragg's law

1－3　Difference in path length

The most significant point of the Bragg's law can be explained by the constructive interference, which occurs when the **path difference** of traveling waves matches with the **integral multiplication of the wave length**. See the figure below.

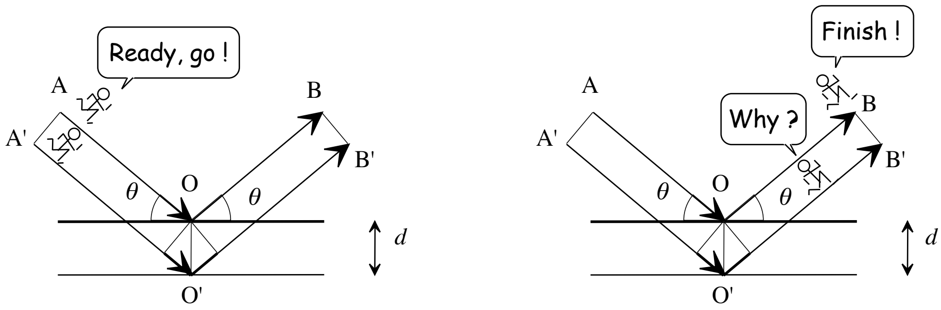

Fig. 1.2　It will take additional length when you move along the path A'O'B' as compared with the path AOB. How long is the additional length (path difference) ?

Note that the path difference corresponds to the length of the two segments drawn as heavier lines. Then look at the figure below.

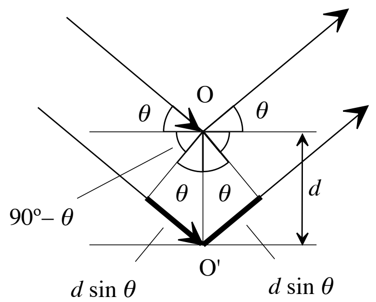

Fig. 1.3　Relations among path length, d and θ

The length of one segment should be " $d \sin \theta$ ", because the segment is the opposite side to "the corner with the angle θ " in a right triangle with the oblique side of length d ".

You may feel as if most part of the Eq. (1.1) have already been explained by the above relation ..., but actually, it can explain only small part of what the Bragg's law means !

1－4 Symmetric reflection

The Bragg's law implies that the incident and reflected glancing angles are both equal to θ. Why should the angles of incident and reflected beams be coincided ? Of course, the reflection by a mirror should be symmetric, but we are talking about the diffraction of X-ray by a lattice plane ! The lattice plane should be something like planar arrangement of atoms ... Can you imagine existence of smooth surface like a mirror in the arrangement of atoms ?

What will occur on the asymmetric reflection shown in the figure below, for example ?

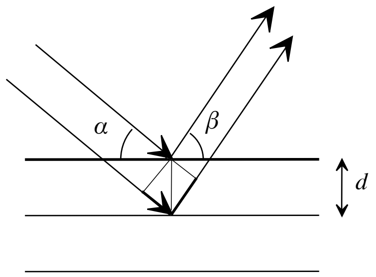

Fig. 1.4 What will occur on the reflection with the incident (glancing) angle of α and reflected (glancing) angle of β ?

The path difference should be " d (sin α + sin β) ", because it is the sum of the two segments, the lengths of which are " d sin α " and " d sin β ", as shown in the figure below.

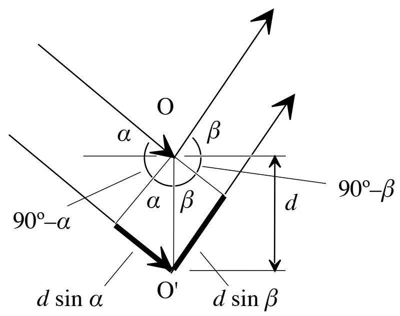

Fig. 1.5 Path difference for the incident (glancing) angle of α and reflected (glancing) angle of β should be " d (sin α + sin β) ".

Don't you think diffraction may occur, if the value of " d (sin α + sin β) " matches to the integral multiplication of the wave length ?

Actually, diffraction does never occur in such a case ... What is this trick ?? The path difference in the asymmetric reflection appears to be " d (sin α + sin β) ", because the reflection point O' on the second lattice plane is located right below the reflection point O of the first lattice plane, in Fig. 1.4 or Fig. 1.5. But the path difference should be " $d\left[\sin(\alpha+\phi)+\sin(\beta-\phi)\right]/\cos\phi$ ", if the reflection point O' is located at the point displaced by such distance given by " $d\tan\phi$ ", as shown in the Figs. 1.6 & 1.7 below.

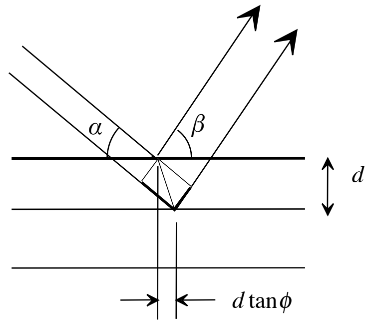

Fig. 1.6 How about displace the reflection point for asymmetric reflection ?

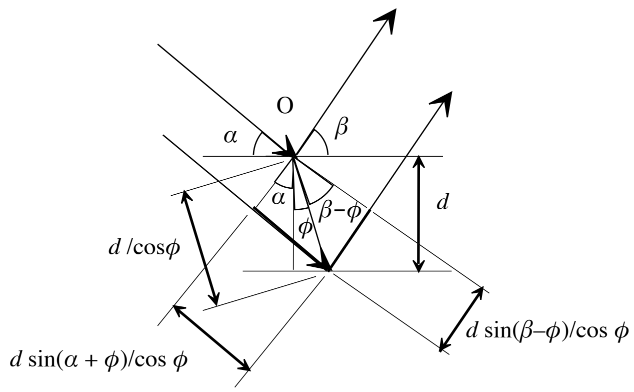

Fig. 1.7 Path difference should be " $d\,[\sin(\alpha+\phi)+\sin(\beta-\phi)]\,/\cos\phi$ " for asymmetric reflection.

Both constructive and destructive interferences, depending on the location of the reflection point (different value of ϕ) can occur in the case of asymmetric reflection. There may be a special arrangement of atoms that leads only constructive interference, but it will be just a "symmetric Bragg reflection" for different lattice planes.

On the other hand, the path difference should always be "$2\,d\sin\theta$" for symmetric reflection, no matter where the reflection point is located on a lattice plane. You can confirm this relation by the fact that the following equation holds for arbitrary ϕ,

$$\frac{\sin(\theta-\phi)+\sin(\theta+\phi)}{\cos\phi}=2\sin\theta\ ,$$

which can easily be derived by applying trigonometric addition formulas. In conclusion, we can say that diffraction occurs only when the reflection is symmetric about the lattice plane.

1–5 Bragg's condition

The Bragg's law does not only mean the constructive interference on Eq. (1.1), but it has a much more strict meaning to forbid any reflections not satisfying Eq. (1.1). How can this strict condition be derived ?

So far, we have considered only two lattice planes, the top one and the 2nd one, but we must consider the 3rd, 4th, ..., and much more lattice planes to explain such a strict condition.

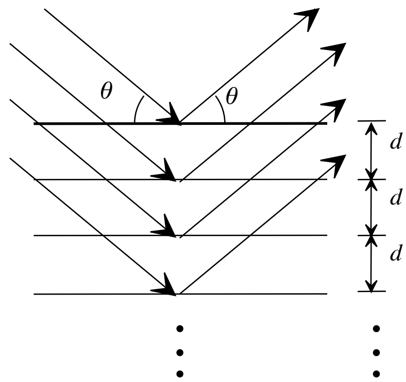

Fig. 1.8 We must take many lattice planes into consideration to understand the Bragg's law.

The path difference is " $2\,d \sin\theta$ " for the reflection from the 2nd lattice plane, as shown in Sec. 1-3, and it should be " $4\,d \sin\theta$ " for the 3rd plane, " $6\,d \sin\theta$ " for the 4th, ..., and " $2\,(j-1)\,d \sin\theta$ " for the j-th lattice plane.

All the reflections from any lattice planes (1st, 2nd, 3rd, ... planes) will always be interfered constructively, if the relation:

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

is only satisfied. Then, how about the case:

$$(n + 1/2)\,\lambda = 2\,d \sin\theta$$

is satisfied ? The reflection from the 1st and 2nd planes will be canceled, and the reflection from the 3rd and 4rh will also be canceled, and so on. Most of the reflections will vanish except the last one for the odd number of planes.

Similarly, when the following relation:

$$(n + 1/3)\,\lambda = 2\,d \sin\theta$$

is satisfied, the sum of the reflections from the 1st, 2nd and 3rd planes will be canceled.

In general, when the following relation:

$$(l\,/\,m)\,\lambda = 2\,d \sin\theta$$

where $(\,l\,/\,m\,)$ is an irreducible fraction,

is satisfied, the sum of the reflections from the 1st to the m-th planes are canceled, and the sum from $(m + 1)$ to $(2m)$ will be canceled, and so on. In conclusion, when the value of $(\,2\,d \sin\theta\,)\,/\,\lambda$ is not an integer, there will always be a combination of planes which cancels the amplitude of the reflected waves.

Therefore, **diffraction will never occur, if Eq. (1.1) is not satisfied**, in case of **infinitely large number of lattice planes**. (In other words, diffraction may be observed, even if the situation is slightly deviated from the condition defined by Eq. (1.1), in case of finite number of lattice planes, which will be discussed in Chap. 6).

1－6　Difference of observation from theory

Let us confirm that the Bragg's law can certainly be applied to diffraction intensity data observed with a realistic instrument, in this section.

In a realistic diffraction measurement, the sample is irradiated by x-ray emitted from a generator, and the intensity of the diffracted beam is measured with a detector. The distance between the generator and the sample, and also the distance between the sample and the detector are several ten cm, 20 cm = 200 mm, for example. We may apply the Bragg's law, if we can treat the distance "infinitely long". Are you sure that this assumption should be ?

Since tinterference of X-rays, no matter constructive or destructive, can occur only when they are emitted from the identical point on the radiation source and also detected at the same point on the detector, the path difference should be expressed somehow shown in the figure below. Let us calculate the deviation of the realistic situation from that assumed in the theory.

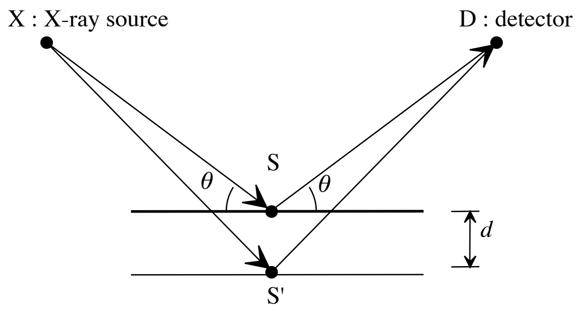

Fig. 1.9　Exercise: evaluate the difference in length of the path XS'D and XSD, and compare it with the value of 2 d sin θ, assuming XS = SD = R = 200 mm, d = 0.2 nm, θ = 21°

As interatomic distance is usually 0.1 nm to 0.3 nm, it is assumed that the distance of lattice plances is 0.2 nm, in this exercise. The angle to satisfy the Bragg's equation for n = 1, the interplanar distance d = 0.2 nm and the wavelength λ = 0.15 nm will be θ = 21°.

The length to be evaluated is given by 2 (R' - R) = 2 (XS' - XS) in the figure below.

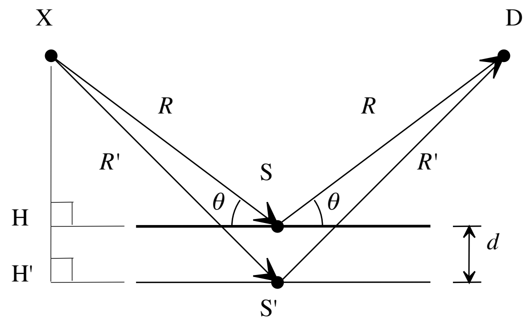

Fig. 1.10　Let H and H' be the feet of the perpendicular lines from X to the two lattice planes.

Following relations are derived from Fig. 1.10,

$$\mathrm{XH} = R \sin\theta\ ,$$
$$\mathrm{XH'} = \mathrm{XH} + \mathrm{HH'} = R \sin\theta + d,$$
$$\mathrm{SH} = \mathrm{S'H'} = R \cos\theta\ ,$$

then

$$R'-R=\overline{\mathrm{XS'}}-\overline{\mathrm{XS}}=\sqrt{\overline{\mathrm{XH}}^2+\overline{\mathrm{S'H'}}^2}-\overline{\mathrm{XS}}$$
$$=\sqrt{(R\sin\theta+d)^2+(R\cos\theta)^2}-R$$
$$=\sqrt{R^2+2Rd\sin\theta+d^2}-R$$

It should be noted that the formula

$$\sqrt{R^2+\delta}-R \quad (\delta << R^2)$$

is not suitable for calculation, even if you can use a calculator or a computer. It is well known to use the formula on the right side of the following equation,

$$\sqrt{R^2+\delta}-R=\frac{\delta}{\sqrt{R^2+\delta}+R}.$$

Then, it should be calculated applying the following transformation,

$$R'-R=\sqrt{R^2+2Rd\sin\theta+d^2}-R$$
$$=\frac{2Rd\sin\theta+d^2}{\sqrt{R^2+2Rd\sin\theta+d^2}+R}$$

$$R=0.2 \qquad [\mathrm{m}]$$
$$2Rd\sin\theta+d^2=(2R\sin\theta+d)d$$
$$=(2\times0.2\times\sin21^\circ+0.2\times10^{-9})\times0.2\times10^{-9}$$
$$=2.866943600362402\times10^{-11} \qquad [\mathrm{m}^2]$$

for the exercise here, and we will have

$$2(R'-R)=\frac{2\times2.866943600362402\times10^{-11}}{\sqrt{0.2^2+2.866943600362402\times10^{-11}}+0.2}$$
$$=1.433471799924345\times10^{-10} \qquad [\mathrm{m}]$$

On the other hand, we have

$$
\begin{aligned}
&2d\sin\theta = 2\times 0.2\times 10^{-9}\times \sin 21^\circ \\
&= 1.433471798181201\times 10^{-10} \qquad [\mathrm{m}],
\end{aligned}
$$

so it is found that the two values are coincided up to the significant figures of 9. If required, we can evaluate the difference of the two values by calculating

$$
\begin{aligned}
&2(R'-R) - 2d\sin\theta \\
&= 2\sqrt{R^2 + 2Rd\sin\theta + d^2} - 2R - 2d\sin\theta \\
&= \frac{2\left[\left(R^2 + 2Rd\sin\theta + d^2\right) - \left(R + d\sin\theta\right)^2\right]}{\sqrt{R^2 + 2Rd\sin\theta + d^2} + R + d\sin\theta} \\
&= \frac{2d^2\cos^2\theta}{\sqrt{R^2 + 2Rd\sin\theta + d^2} + R + d\sin\theta} \\
&= 1.743144824852707\times 10^{-19} \qquad [\mathrm{m}]
\end{aligned}
$$

In conclusion, we can expect the deviation of the observation from the Bragg’s law to be extremely small and negligible. But it also shows that a kind of approximation is necessary for the Bragg’s law to be applied to realistic data. It is recommended to calculate the difference by yourself, applying the values for the dimension of the instrument you use for the experiment, and examine if it is certainly negligible on application of the Bragg’s law.