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WIDTH OF THE DARWIN TABLE FOR FORBIDDEN REFLEXES

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In neutron and x-ray diffractometry the Bragg reflexes, for which form-factor $F(q) = 0$, where $q = 2k_B$ is the momentum transfer, and k_B is the Bragg wave vector, are called forbidden, because reflection for these q are absent. We want to show here that these reflexes, strictly speaking, are not forbidden. They are the same as nonforbidden ones with the only difference that the Darwin table width (DTW) for them is very narrow. We shall show it with the help of multiple wave Darwin (MWD) approach [1],[2] to the Dynamical Diffraction Theory (DDT) applied to a simple model of a crystal having two atoms in the elementary cell. As a result of such approach it will be shown that the reflection amplitude depends on two different form-factors: $F(q)$ and $G(q)$ and both of them give nearly the same contribution to DTW. If we denote the DTW of nonforbidden reflex by w, the DTW for forbidden one has a value of order $w_f \propto wu/k_B^2$, where u is optical potential of the crystal: $u = 4\pi N_0 b$, N_0 is the atomic density and b is coherent amplitude.

Our model is a semi-infinite crystal consisting of crystalline planes parallel to the entrance surface. The elementary cell of a plane is a square with the lattice parameter α being considerably smaller than the period s in the direction of the normal to the surface. The period consists of two identical planes separated by distance a along the normal. All the atoms of the crystal are motionless, nonabsorbing and have the same scattering amplitude b_s, which for a single atom, separated from the crystal, and surrounded by vacuum is representable in the form

$$b_s = b_0/(1 + ikb_0), \tag{1}$$

where b_0 is a real magnitude, called "scattering length", and k is the wave-number of the incident neutron. Such a representation of the amplitude automatically satisfies the requirements of optical theorem.

We consider the reflection of neutrons from this crystal when neutrons have wave number $k \ll 2\pi/\alpha$. For such neutrons we can neglect diffraction on a single crystalline plane and describe the scattering on a plane with the help of only two parameters: reflection r and transmission $t = 1 + r$ amplitudes.

Reflection amplitude r from a plane is equal to

$$r = -ip/(k_\perp + ip), \qquad p = 2\pi N_2 b, \tag{2}$$

where N_2 is two-dimensional density of atoms $N_2 = 1/\alpha^2$, and b is a somewhat renormalized amplitude b_0 (see (1)), which was calculated in [1]. The expression (2) can be obtained with the help of multiple wave scattering theory [1] or with one-dimensional Schrödinger equation, in which the crystalline plane is represented by a potential of the form $2p\delta(x)$ like in Kronnig-Penney potential. In the following we shall omit the subscript $\perp$.

Now we consider reflection r_{12} and transmission t_{12} amplitudes for the system of two planes separated by a distance a. From multiple wave scattering in MWD approach it follows that

$$r_{12} = r + t^2 e^{2ika} r/(1 - r^2 e^{2ika}) = r\frac{1 + (t^2 - r^2)\exp(2ika)}{1 - r^2\exp(2ika)},$$

and

$$t_{12} = t^2 \exp(ika)/[1 - r^2\exp(2ika)].$$

Substituting $t = 1 + r$ and r from (2) in these relations, we get

$$r_{12} = -2ipe^{ika}\frac{k\cos(ka) + p\sin(ka)}{k^2 + 2ipk + 2ip^2\sin(ka)\cos(ka) - 2p2\sin^2(ka)} \tag{3}$$

$$t_{12} = e^{ika}\frac{k^2}{k^2 + 2ipk + 2ip^2\sin(ka)\cos(ka) - 2p2\sin^2(ka)} \tag{4}$$

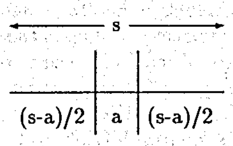

Figure 1: The single period of the model. It contains two planes at distance a and two vacuum gaps on both sides of them. The total width s is the length of the period.

Now we must define reflection from a period. To do that it is necessary to choose the form of the period. We choose it to be symmetrical as is shown in fig. 1.

The reflection amplitude from the period, ρ, is $\rho = \exp[ik(s-a)]r_{12}$, where the first factor appears because before and after reflection from two planes the wave is to propagate through the vacuum gap of the width $(s-a)/2$. Substitution of (3) in this formula leads to

$$\rho = -2ipe^{iks}\frac{k\cos(ka)+p\sin(ka)}{k^2+2ikp+2ip^2\sin(ka)\cos(ka)-2p^2\sin^2(ka)} \tag{5}$$

In the same way we get the transmission amplitude τ of the period

$$\tau = e^{ik(s-a)}t_{12} = e^{iks}\frac{k^2}{k^2+2ipk+2ip^2\sin(ka)\cos(ka)-2p^2\sin^2(ka)} \tag{6}$$

Reflection amplitude R from the semi-infinite crystal is defined by the expression [1]

$$R\frac{\sqrt{(1+\rho)^2-\tau^2}-\sqrt{(1-\rho)^2-\tau^2}}{\sqrt{(1+\rho)^2-\tau^2}+\sqrt{(1-\rho)^2-\tau^2}}.$$

After dividing numerator and denominator by

$$\sqrt{(1+\rho+\tau)(1-\rho+\tau)}$$

we get

$$R = \frac{\sqrt{(1-\tau+\rho)/(1+\tau-\rho)}-\sqrt{(1-\tau-\rho)/(1+\tau+\rho)}}{\sqrt{(1-\tau+\rho)/(1+\tau-\rho)}+\sqrt{(1-\tau-\rho)/(1+\tau+\rho)}} \tag{7}$$

From (5), and (6) it follows that $\tau \pm \rho$ can be represented in the form

$$\tau \pm \rho = e^{iks}\frac{k^2 \mp 2ip[k\cos(ka)+p\sin(ka)]}{k^2+2ikp+2p^2\sin^2(ka)+2ip^2\sin(ka)\cos(ka)} = \exp(iks - i\delta_\pm)$$

with $\delta_\pm = \mp\phi_1 - \phi_2$, and

$$\phi_1 = \arctan\left(\frac{2p[k\cos(ka)+p\sin(ka)]}{k^2}\right), \tag{8}$$

$$\phi_2 = \arctan\left(\frac{2pk+2p^2\sin(ka)\cos(ka)}{k^2-2p^2\sin^2(ka)}\right). \tag{9}$$

After substitution into (7) we get

$$R = \frac{\sqrt{\tan(ks/2+\phi_1/2-\phi_2/2)}-\sqrt{\tan(ks/2-\phi_1/2-\phi_2/2)}}{\sqrt{\tan(ks/2+\phi_1/2-\phi_2/2)}+\sqrt{\tan(ks/2-\phi_1/2-\phi_2/2)}} \tag{10}$$

If two tan have different sign, this expression becomes of the form $R = (a-ib)/(a+ib)$ with real a, and b. In that case $|R| = 1$, and we have total or Bragg reflection. It happens when

$$ks/2 - \phi_1/2 - \phi_2/2 \le n\pi/2 \le ks/2 + \phi_1/2 - \phi_2/2, \tag{11}$$

where n is integer. The magnitude ϕ_2 determines position of the Bragg peak, and ϕ_1 determines the width of the Darwin table.

Now, let us remind how form-factor of elementary cell is defined. Usually it is defined as

$$F(q) = \sum_j b_j \exp(iqr_j),$$

where b_j is scattering amplitude of an atom at point r_j, and q is momentum transfer. We use a slightly modified definition:

$$F(q) = \sum_j \beta_j \exp(iqr_j), \qquad \beta_j = b_j/\sum_l b_l.$$

In our model we have two atoms, so the form-factor is equal to

$$F(q) = \cos(qa/2),$$

if the origin is chosen in the middle between planes. For specular reflection we have $q = 2k$, so in our case $F(q) = \cos(ka)$.

In the expressions (8), and (9) besides $F(q)$ enters another form-factor, which is represented by $\sin(ka)$, and which we shall denote by $G(q)$. Thus the expressions (8), and (9) can be represented in the form

$$\phi_1 = \arctan\left(\frac{2pkF(2k)+2p^2F(0)G(2k)}{k^2}\right), \tag{12}$$

$$\phi_2 = \arctan\left(\frac{2pkF(0)+2p^2F(k)G(2k)}{k^2-2p^2G^2(2k)}\right). \tag{13}$$

where $F(0) = 1$ is introduced to get a form-factor for every entry of p.

It is supposed that it is $G(q)$, which is important for determination of the DTW for forbidden reflexes.

To get the width of the Darwin table it is necessary to find $2|\phi_1(k_c)|$, where k_c is the solution of the equation $(k_c - k_B)s = \phi_2(k_c)$. Let us suppose that $a = s/4$. The forbidden reflex should be at $k_B = 2\pi/s$, but because of small shift the center of the reflex is at $k_c = k_B + 2p/sk_B$. Substitution of this value into (8) gives

$$2\phi_1(k_c) = 2\frac{2p}{k_B}\left(-\frac{p}{2k_B}+\frac{p}{k_B}\right) = 2\frac{p^2}{k_B^2} \tag{14}$$

If we take into account, that $p = 2\pi N_2 b \equiv us/4$, where $u = 4\pi N_0 b$ is the optical potential of the medium, (we can also represent it in the form $u = uF(0)$, since $F(0) = 1$) and N_0 is the number of atoms in a unit volume, we obtain that the DTW in the considered case is equal to

$$|k - k_c| = \frac{\pi}{4}\frac{u}{k_B^3}, \quad \text{or} \quad |k^2 - k_c^2| = \frac{\pi}{2}\frac{u}{k_B^2}u \tag{15}$$

For nonforbidden reflex (for instance for $k \approx \pi/s$) we have

$$|k^2 - k_B^2| = 2uF(k_B) = \sqrt{2}u.$$

It follows from (14), that DTW is determined not only by the additional form-factor but also by the main form-factor which is zero only precisely at Bragg point, and is not zero at the shifted position. For instance, let us suppose, that there are no additional form-factor, i.e. we calculate ϕ_1 and ϕ_2 by perturbation theory and get:

$$\phi_1 = \arctan(2pF(2k)/k), \qquad \phi_2 = \arctan(2p/k).$$

Since for $p > 0$ the reflex takes place for $k > k_B$, and the phase $\phi_1 < 0$ for these k, the inequality (11) must be represented in the form:

$$ks/2 + \phi_1/2 - \phi_2/2 \leq n\pi/2 \leq ks/2 - \phi_1/2 - \phi_2/2, \tag{16}$$

or

$$2p\cos(ka) \leq k_b s - ks + 2p/k \leq -2p\cos(ka), \tag{17}$$

and we get the the same DTW as before. Of course the coincidence here is an accidental one.

It is also important to stress that the result obtained here was not possible to obtain in the framework of the Ewald theory, because there it is not the form-factor $F(2k)$, which enters the theory, but the pure number: $F(2k_B)$, and this number is identically zero for forbidden reflexes. To explain forbidden reflexes that are observed experimentally [3] in Ewald theory it is necessary to consider four wave approximation

Thus we proved that forbidden reflexes differ from unforbidden ones only by the width of the Darwin table. This width is provided by an additional form-factor and by the shift of the central point in the main form-factor that is zero at precisely the Bragg point. In practice the forbidden reflexes are sometimes observed (see for example [5]- [9]) but they are usually ascribed to double unforbidden ones.

The presented here considerations are also aplicable to x-ray diffraction. It is interesting to note, that because of very narrow width the forbidden reflexes can be used for measurements of small shifts of atoms under the action of external forces.

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