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# The Absorption Coefficient in the BJR Dynamical Theory of Electron Diffraction

By G. Jeschke and H. Niedrig

*I. Physikalisches Institut der Technischen Universität Berlin,* 1 *Berlin* 12, *Germany*

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The basic assumptions and limits of the BJR dynamical theory of electron diffraction are discussed. In the two-beam approximation the absorption coefficient derived in the BJR theory takes account of the thermal diffuse scattering and of the weakly excited beams, but neglects their dynamical interaction with the two strong beams. This seems to be a suitable approximation for real crystals with defects and grain boundaries as in polycrystalline foils. For thick perfect single crystals a better approximation may be obtained by removing the weak beam term from the absorption coefficient, leading to the results of Hall & Hirsch. In both cases the same simple expression for the temperature dependence of the two strong beams is obtained for anomalous transmission, being in good agreement with experiment.

## 1. Introduction

In a series of papers (Boersch, Jeschke & Raith, 1964; Glaeser & Niedrig, 1966; Albrecht & Niedrig, 1968) a dynamical theory of elastic electron scattering in crystals (BJR theory) including thermal diffuse scattering has been outlined, based on a phase grating approximation (defined below) using complex atomic scattering amplitudes for elastic scattering. Because this theory has been subject to critical discussions by some authors (Fukuhara, 1965; Cowley & Moodie, 1970) the basic assumptions and limits of the BJR theory will be discussed from a new angle, especially the physical meaning of the absorption coefficient derived in the two-beam formulation of the BJR theory, and its temperature dependence.

For simplicity we restrict all the following calculations to crystals of only one kind of atom and with a cubic primitive unit cell, but the calculation can easily be extended to other crystals.

In the usual treatment of the dynamical theory of electron diffraction in crystals (Bethe, 1928) the Fourier representation of the real periodic potential of the crystal is introduced into the Schrödinger equation. The wave function within the crystal is represented by a superposition of plane waves. The amplitudes of these plane waves are determined by the real Fourier coefficients of the potential. In the two-beam approximation of this treatment all weakly excited beams are set equal zero except the primary beam and one strongly reflected, consequently no absorption within the two-beam system arises. Any diminution of the number of electrons within the two-beam system, *e.g.* by weak beam effects or thermal diffuse scattering, must be considered by formally introducing an imaginary part of the potential (Molière, 1939) and by additional calculations (Yoshioka & Kainuma, 1962; Gjønnes, 1962, Hall & Hirsch 1965*a*,*b*; Kainuma & Yoshioka, 1966; Ohtsuki, 1966).

Other treatments of the dynamical theory deal with the successive scattering of the incident plane wave by the set of plane gratings of atoms within the crystal. This was done by Cowley & Moodie (1957) and Howie & Whelan (1961), and in a different way by Boersch, Jeschke & Raith (1964). In the calculation by Boersch, Jeschke & Raith each single layer of atoms in the crystal is regarded as a two-dimensional phase grating, which is derived by projecting the phase shift suffered by the electron wave passing through the atomic layer onto the plane formed by the centres of these atoms. In this treatment which we will call the 'phase grating approximation', the amplitudes of the scattered waves from every atomic plane are determined by complex atomic scattering amplitudes $f_g$. In the two-beam approximation this leads to an absorption within the two-beam system, contrary to the results of the Bethe treatment. As will be shown later, this absorption takes account of the maximum limit of absorption due to weak-beam effects in the case of very thin crystals or thick imperfect crystals and, for $T>0$, of the thermal diffuse scattering.

These different results indicate that the two-beam formulae derived from the Schrödinger equation (Bethe formulation) and from the phase grating treatment (BJR), although both are applied to a two-beam system, are not equivalent but represent two different approximations, the first completely neglecting elastic scattering absorption phenomena, the second yielding a maximum limit for the absorption due to elastic scattering. We will discuss the phase grating treatment for two different cases: (*a*) a thick perfect crystal,* (*b*) a thin perfect crystal and a thick crystal with imperfections. The results will be compared with those of Hall & Hirsch (1965*a*) derived from the Bethe formulation introducing additional scattering processes.

## 2. Scattering amplitudes and lattice potential

At first we will give some definitions of the quantities describing electron scattering in crystals.

The periodic potential in a crystal is real provided

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* Only this case has been considered in the paper by Fukuhara (1965). Cowley & Moodie (1970) also only consider a perfect crystal (thick and thin) in their paper.

that inelastic scattering is neglected. The Fourier coefficients $V_g$ of the real lattice potential of a primitive cubic crystal are exactly proportional to the atomic scattering amplitudes in the first Born approximation, $f^B_g$:

$$V_g \sim f^B_g \, . \tag{1}$$

$f^B_g$ is always real for atoms with spherical symmetry.

The amplitudes of the waves scattered by a single unit cell, *e.g.* the case of a cubic primitive crystal, are equal to the correct, generally complex scattering amplitudes $f_g$:

$$f_g = f'_g + if''_g \, . \tag{2}$$

Any calculation more accurate than the first Born approximation gives such complex atomic scattering amplitudes (Hoerni & Ibers, 1954; Raith, 1968) by use of the real atomic potential.

In a two-dimensional cross grating scattering problem the amplitudes of the scattered waves are given by the Fourier coefficients $q_g$ of the complex object function. These Fourier coefficients are related to the correct atomic scattering amplitudes $f_g$ by

$$q_g = i \frac{\lambda}{F_A} f_g \tag{3}$$

(Howie & Whelan, 1961; Boersch, Jeschke & Raith, 1964). In this description the primary beam ($g=0$) has the amplitude $(1+q_0)$; $\lambda$ is the electron wave length, and $F_A$ is the area per atom in the cross grating. As was stated by Boersch, Jeschke & Raith (1964, pages 439 and 451) there exists no linear relation similar to equation 1 between $f_g$ and the real Fourier coefficients, $V_g$, of the potential, except in the approximation of very weak phase objects (first Born approximation).†

## 3. Elastic scattering by a phase grating of atoms

A crystal can be regarded as a system of cross gratings with atoms at the lattice points. Neglecting inelastic scattering these atoms can be regarded as phase objects for the elastic scattering of electrons. Therefore the cross gratings are phase gratings.

As a consequence the incident intensity is preserved after scattering. Observing this intensity conservation for the scattering of one or two incident electron waves by a single phase grating the following relations can be derived:

$$-2 \,\mathrm{Re}\, q_0 = \frac{2\lambda}{F_A} f''_0 = \sum_h |q_h|^2 = \frac{1}{F_A} \sigma_{\mathrm{tot}} \tag{4}$$

and

$$-2 \,\mathrm{Re}\, q_g = \frac{2\lambda}{F_A} f''_g = \mathrm{Re} \sum_h q_h q^*_{h-g} \tag{5}$$

The sum has to be taken for all reflexions **h**. Equations 4 and 5 (similar equations are implicitly included in the calculations of Fukuhara, 1965) show that the imaginary part of the atomic scattering amplitude for elastic scattering is related to the amplitudes of all scattered waves. Equation (4) corresponds to the optical theorem (Feenberg, 1932); equation (5) is equivalent to a relation derived by Glauber & Schomaker (1953). $\sigma_{\mathrm{tot}}$ is the total elastic scattering cross-section.

Now we regard two incident beams with equal amplitudes $1/\sqrt{2}$ and opposite or equal sign. Again observing the intensity conservation and with the help of equations (3)–(5) we obtain for $T>0$ for the total scattered intensity by a single plane grating

$$I^{1,2}_g = \frac{2\lambda}{F_A} (f''_0 \mp f''_g \exp[-M_g]) = I^{1,2}_{g,\mathrm{TDS}} + I^{1,2}_{g,\mathrm{WB}} \, . \tag{6}$$

Equation (6) represents the total intensity elastically scattered by a single phase grating from an incident Bloch wave (index 1 or 2, see §4), consisting of two plane waves, into thermal diffuse background, $I^{1,2}_{g,\mathrm{TDS}}$, and into all Bragg reflected beams (mainly weak beams), $I^{1,2}_{g,\mathrm{WB}}$. The upper sign always belongs to Bloch wave 1. The two terms on the right side of equation 6 are given by

$$\begin{aligned} I^{1,2}_{g,\mathrm{TDS}} &= I_{0,\mathrm{TDS}} \mp \triangle I_{g,\mathrm{TDS}} \\ &= \sum_h \{|q_h|^2(1-\exp[-2M_h]) \mp \mathrm{Re}\, q_h q^*_{h-g} \\ &\quad \times (\exp[-M_g] - \exp[-(M_h + M_{h-g})]\} \end{aligned} \tag{7}$$

and

$$I^{1,2}_{g,\mathrm{WB}} = \tfrac{1}{2} \sum_h |q_h \exp(-M_h) \mp q_{h-g} \exp(-M_{h-g})|^2 . \tag{8}$$

The factors $\exp(-M)$ are the Debye–Waller-factors (Debye, 1914) describing the diminution of amplitudes of the scattered beams by thermal diffuse scattering (TDS).

The TDS term in equation (6) given by equation (7) is due to phonon scattering and will be incoherent to the two-beam system, whereas the weak beam term [equation (8)] is coherent. Therefore when regarding the successive scattering by the atomic layers in the crystal the TDS term will lead to an absorption, whereas the weak beam term causes absorption only for special cases discussed in the following section.

## 4. Dynamical two-beam case

The dynamical case of diffraction in crystals in the phase grating approximation can be derived by calculating the successive scattering of the electron waves by the set of plane gratings of atoms within the crystal.*

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† It is possible to construct a complex potential by using equation (1) for the complex quantities $f_g$. But this has only a formal meaning for the two-beam approximation calculated from the Schrödinger equation, and this has not been done by BJR (1964), although Fukuhara (1965) has said that it was; the remark of Fukuhara on this point is incorrect.

* As was stated by BJR (1964, p. 451) the description of the successive scattering by the plane gratings within a crystal in terms of the Fraunhofer treatment is only an approximation. But for $\lambda^2 \ll F_A$ the distribution of amplitudes behind a phase grating can be described by the complete system of all scattered plane waves and then also includes Fresnel diffraction phenomena (Jeschke, Raith & Zorn, 1966).

We regard a system of two strong beams* selected by the Bragg-equation for a suitable crystal orientation. For any crystal thickness this system can be divided into two Bloch waves (1 and 2) each consisting of two plane waves with equal amplitude and opposite (1) or equal (2) sign. Taking the Bloch waves to be independent,† we treat the weak beams and the thermal diffuse scattering from each plane grating as a perturbation diminishing the intensities of the Bloch waves. Applying equations (6)–(8) to each plane grating we easily obtain absorption coefficients

$$\mu_g^{1,2}=\mu_0\mp\varDelta\mu_g \tag{9}$$

for the intensities of the two Bloch waves ($\mu_0$: normal or mean absorption coefficient; $\mu_g^{1,2}$: anomalous absorption coefficient).

Calculating the two-beam case in this way we neglect the scattering from the weak beams into the strong beams. Strictly speaking we should also consider the incident weak beams previously scattered by the atomic planes above. This would reduce the weak-beam term in equations (6) and (8). By an *n*-beam calculation Goodman (1968) found an oscillatory behaviour of all intensities with crystal thickness while the average intensities of both strong and weak beams were found to be independent of crystal thickness. This means that the intensity of the weak beams is periodically scattered back into the two strong beams, and the weak beam term does not contribute to absorption for a thick perfect crystal.‡ We therefore can distinguish between two limiting cases:

(*a*) For thick perfect crystal plates we have to remove the weak-beam term from the absorption according to the above considerations in agreement with the treatment of Hall & Hirsch (1965*a*,*b*). The remaining TDS-term [equation (7)] leads to the following absorption coefficient (after replacing the sums by integrals, see *e.g.* Kainuma & Yoshioka, 1966):

$$\begin{aligned}\mu_{g,\mathrm{TDS}}^{1,2}&=\mu_{0,\,\mathrm{TDS}}\mp\varDelta\mu_{g,\,\mathrm{TDS}}\\&=2N_A\lambda\oint\{|f_s|^2(1-\exp[-2M_s])\\&\mp\mathrm{Re}\,f_sf_{s-g}^*(\exp[-M_g]-\exp[-(M_s+M_{s-g})])\}\\&\times\mathrm{d}\Omega\,.\end{aligned}\tag{10}$$

Here **g** is the reciprocal lattice vector due to the strong reflection $g$, $f_s$ and $f_{s-g}$ are the scattering amplitudes due to the scattering from the primary and the reflected beam into the direction corresponding to a scattering vector **S**. $N_A$ is the density of atoms. Equation (10) is equivalent to the result of Hall & Hirsch (1965*a*) which is an approximation of equation 10, replacing the complex values $f$ by the real values $f^B$ derived from the first Born approximation.

The effect of weak beams in this case will be restricted to, for example, an alteration of the extinction distance of the two-beam system, which may be taken into account by using the additional potentials of Bethe (1928) as was recently shown by Meyer-Ehmsen (1969).

(*b*) For small crystal depths less than one or two extinction distances for the strong beams the weak beams cannot fully build up. In this region of crystal thickness an effective absorption on the strong beams arises due to weak beams (Gjønnes, 1962; Hall & Hirsch, 1965*b*; Kainuma & Yoshioka, 1966).

A similar effect is to be expected in large crystals with sufficient lattice defects and grain boundaries causing incoherent multiple scattering. This affects the dynamical interaction between the weak beams and the strong beams and may result in an additional absorption for the two-beam system (Cowley, 1969). This was confirmed by *n*-beam calculations of Goodman (1968).

We can assume that in polycrystalline foils these effects will strongly influence the effective absorption (Albrecht & Niedrig, 1968). The upper limit of the weak beam contribution to absorption can easily be calculated from equation (8) neglecting completely the dynamical interaction between weak and strong beams. We therefore obtain for this case the following absorption coefficient from equation (6):

$$\mu_g^{1,2}=\mu_0\mp\varDelta\mu_g=2N_A\lambda(f_0''\mp f_g''\exp[-M_g])\,. \tag{11}$$

This absorption coefficient is identical with that used in the BJR theory for $T>0$ (Bostanjoglo & Niedrig, 1964; Glaeser & Niedrig, 1966; Albrecht & Niedrig, 1968). As was shown above [equation (6)] it includes both thermal diffuse scattering and a limiting value for the weak beam scattering.* The experimental absorption coefficient has values between those of equations (10) and (11.)

## 5. The temperature dependence in the case of anomalous transmission

In the preceding publications (Boersch, Bostanjoglo & Niedrig, 1964; Glaeser & Niedrig, 1966; Albrecht & Niedrig, 1967, 1968) the following temperature behaviour of dynamical diffraction intensities from polycrystalline foils was found experimentally:

$$I_g(T,D)\simeq I_g(O,D)\,.\,\exp(-b_gTD)\,. \tag{12}$$

The temperature coefficient $b_g$ can be derived theoretically from the absorption coefficient by

$$b_g=\frac{\delta\mu_g}{\delta T} \tag{13}$$

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* For simplicity we only consider the exact Bragg incidence.

† This same assumption was made by Hall & Hirsch (1965*a*,*b*).

‡ This differs from earlier opinions of the authors (BJR, 1964).

* The result is identical with that obtained from the Bethe formulation of the two-beam case by formally introducing a complex potential with the help of equation 1 for the complex value $f_g$. But such a derivation cannot be physically justified. On the other hand Cowley & Murray (1968) have shown that it is also possible to derive a complex periodic potential from a phase grating approximation describing the diffuse elastic scattering from a lattice with static disorder.

We will calculate this coefficient using the two limiting cases given above for fully developed anomalous transmission, *i.e.* for crystal thicknesses $D$, where the Bloch wave 2, because of its larger absorption coefficient [equations (10) and (11)], is small compared with Bloch wave 1. This case has been experimentally investigated by Boersch, Bostanjoglo & Niedrig (1964), Glaeser & Niedrig (1966), Albrecht & Niedrig (1968) and Jeschke, Niedrig & Ridder (1968). For simplicity we use the value of $M$ for $T > \Theta$ ( = Debye temperature) being proportional to $T$ (Debye, 1914):

$$M_g \simeq C_g T . \tag{14}$$

with

$$C_g = \frac{3h^2}{2kd_g^2 m\Theta^2} \tag{14$a$}$$

($h,k$: Planck's and Boltzmann's constant, $d_g$: lattice spacing found from reflexion $g,m$: atomic mass).

For the calculation based on thick perfect single crystals [case (*a*) §4] we use an approximation of equation (10), which can be derived similarly to a method given by Hall & Hirsch (1965*a*):

$$\mu^1_{g,\mathrm{TDS}} \simeq 2N_A\lambda(1-\exp[-M_g]) \operatorname{Re} \oint f_s f^*_{s-g} \mathrm{d}\Omega . \tag{15}$$

Equation (15) is a good approximation for materials of high atomic number. We can simplify equation (15) by a relation corresponding to equation 5 (Glauber & Schomaker, 1953)

$$2\lambda f''_g = \operatorname{Re} \oint f_s f^*_{s-g} \mathrm{d}\Omega \tag{16}$$

and obtain (Albrecht & Niedrig, 1968):

$$\mu^1_{g,\mathrm{TDS}} \simeq 2N_A\lambda f''_g(1-\exp[-M_g]) . \tag{17}$$

Calculating $b_g$ from (17) we get

$$b_{g,\mathrm{TDS}} = \frac{\delta\mu^1_{g,\mathrm{TDS}}}{\delta T} \simeq 2N_A\lambda f''_g\, C_g \,.\, \exp(-M_g) . \tag{18}$$

Using the case (*b*) (more suited to imperfect crystals) we obtain from equation (11):

$$b_g = \frac{\delta\mu^1_g}{\delta T} = 2N_A\lambda f''_g\, C_g \,.\, \exp(-M_g) \tag{19}$$

We see that both limiting cases lead to the same temperature coefficient, which is identical to that derived in previous publications (Niedrig *et al.*, 1964, 1966, 1968).† This is due to the fact that the temperature dependence of the weak beam term of Bloch wave 1 [equation (8)] is not very strong. However, this fact hinders the estimation of the weak beam contribution from measurements of the temperature dependence in the case of anomalous transmission.

The calculated temperature coefficient $b_g$ [equations (18) and (19)] is in good agreement with experiment (Albrecht & Niedrig, 1967, 1968; Boersch, Jeschke & Willasch, 1969). This indicates that the thermal diffuse scattering from the two strong beams (corresponding to the first two points of the list of Cowley & Moodie, 1969) is the main contribution to the temperature dependence. Other contributions, especially that of the inelastic scattering, seem to be small compared with the TDS (Boersch, 1947, 1948; Yoshioka, 1957; Whelan, 1965).*

For single crystals it is possible to measure the temperature dependence of $\mu_0$ and $\Delta\mu_g$ separately from each other. This has been done by Watanabe (1965), Goringe (1966), and Meyer (1966) and Meyer–Ehmsen (1969) respectively. The results indicate that for perfect single crystals of elements with low or medium atomic number (Al, Si, Cu, Ge) the weak-beam contribution in fact is small compared with TDS, corresponding to the limiting case (*a*).

An $n$-beam theory considering all these possible absorption phenomena certainly gives more information, but unfortunately can be evaluated only by the use of computers.† On the other hand the BJR theory and especially its application to the temperature dependence of anomalous transmission gives simple relations, which can easily and successfully be applied.

## 6. Conclusions

It has been shown that the absorption coefficient derived from the BJR dynamical theory of electron diffraction includes thermal diffuse scattering and a maximum limit of weak-beam scattering, neglecting the dynamical interaction between the weak beams and the two strong beams. This treatment has some significance for imperfect crystals. Removing the weak beam term from the absorption coefficient for the case of thick perfect-crystal plates the result of Hall & Hirsch for thermal diffuse scattering only is obtained as an approximation for $f \rightarrow f^B$. In the case of anomalous transmission it has been shown that both models lead to approximately the same temperature dependence of the absorption coefficient, which is in good agreement with experiment.

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† The identity becomes obvious using equation 14*a* and remembering that for the strong low order reflexions $M_g$ is small, so that $b_g$ approximately becomes independent of temperature.

* In very thick imperfect crystals incoherent elastic and inelastic multiple scattering exceeds the coherent elastic scattering within the two-beam system (Uyeda, 1968). For polycrystalline gold foils for example this results in a reduction of the temperature coefficient $b_g$ for crystal thicknesses > 1000–1500 Å (Boersch, Just & Niedrig, 1969).

† At high electron energies (> 300 keV) an $n$-beam calculation seems to be necessary in any case because of the breakdown of the two-beam approximation (Dupouy, Perrier, Uyeda, Ayroles & Mazel, 1965; Vingsbo, 1966; Sevely, 1969).

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# Lorentz and Orientation Factors in Fiber X-ray Diffraction Analysis

By R. J. Cella, Byungkook Lee* and R. E. Hughes

*Department of Chemistry, Cornell University, Ithaca, New York* 14850, *U.S.A.*

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The application of a general formulation of the Lorentz factor for any distribution of crystallite orientations to a uniaxial fiber structure reveals that current practice, which involves the use of a standard single-crystal rotation factor, is inadequate. An analysis is presented which eliminates the need for a detailed knowledge of the distribution function and which can be applied to measured peak intensities. The resulting expressions significantly improved the agreement between sets of experimental test data.

The Lorentz factor is applied to X-ray diffraction intensity data to account for the fact that not all sets of crystal planes have the same opportunity to diffract the incident beam. The form the factor takes depends not only on the kinematics of the diffraction system but also upon the nature of the crystalline sample. For single-crystal rotation techniques this geometric factor is a measure of the relative amount of time different sets of planes spend in the diffraction position or, alternatively, the relative amounts of time the corresponding reciprocal lattice points take in passing through the Ewald sphere. For stationary powder methods, it is simply the fractional number of reciprocal lattice points which lie on the surface of the Ewald sphere.

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* Present address: Department of Molecular Biology and Biophysics, Yale University, New Haven, Connecticut 06520, U.S.A.