

# Analysis of Formation of the Suppression Effect of Nuclear Reaction Inelastic Channels in the Presence of Hyperfine Splitting

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*Dedicated to Prof. Dr. G. Borrmann on his 65<sup>th</sup> birthday*

The analysis, carried out in the work, of the emergence of the effect of suppression of the nuclear reaction (ES) during resonance Bragg scattering of Mössbauer gamma-quanta from nuclei under conditions of a hyperfine splitting allows to clearly reveal the fundamental features characteristic of this phenomenon. An is shown in sections 3 and 4, in a general case of realization of ES neither electric nor magnetic vectors of the wave field in the crystal turn to zero at the points of equilibrium positions of the nuclei. For the reaction to be suppressed, it is necessary that the total amplitude of the excited nucleus formation be zero. In this case, a rather peculiar picture of the electromagnetic field within the crystal sets in which depends on the character of the hyperfine splitting and on the multiplicity of the transition.

In this work, conditions have been found of the coexistence of ES for both polarizations, and with these conditions being fulfilled, the strongly resonantly absorbing crystal becomes transparent for the whole of radiation. Special attention has been paid to the proof that lattice vibrations do not restore the nuclear absorption of gamma-quanta. It is interesting that all this takes place during resonant interaction with a separate nucleus when the cross-section of the inelastic process may be large as compared with the elastic scattering cross-section. Although all these features (and a number of others discussed in detail in the text) essentially distinguish ES from the Borrmann effect for X-rays, there is a circumstance which makes them related. In both cases it is necessary to produce a coherent superposition of waves within the crystal owing to the Bragg diffraction of the incident quanta, and in the both cases the crystal becomes more transparent for the radiation that comes through.

## I. Introduction

The effect of "anomalous transmission" of X-rays, discovered by G. Borrmann three decades ago<sup>1, 2</sup>, has clearly demonstrated for the first time the possibility of a radical change of the electromagnetic field interaction with the particles of a medium which gives rise, in particular, to the strong diminishing of the photoelectric absorption. M. v. Laue's theory<sup>3, 4</sup> has led to the very transparent physical interpretation of the phenomenon. In a sufficiently thick crystal, under the Bragg diffraction condition, the total electric field from both waves for one polarization turns out to be strictly zero at all sites of the crystal lattice.

This phenomenon has essentially regenerated the interest in the principal problems of X-rays physics and initiated a great number of experimental, theoretical, and applied works.

In fact, the abrupt spatial readjustment of the electromagnetic field of the incident radiation in the crystal is not a privilege of X-rays, but takes place each time when the coherence is conserved during the scattering process on an individual centrum. In papers<sup>5, 6</sup> (see also<sup>7</sup>), the present authors have predicted that it is possible to stop completely the nuclear reaction when gamma quanta or neutrons interact resonantly with nuclei in crystals. In spite

of the fact that the process goes through the formation of the excited longliving nucleus which decays mainly by the inelastic channel (conversion electrons in the case of gamma quanta and  $n\gamma$  reaction in the case of neutrons), the coherency turns out to be fully conserved and this makes possible the strong readjustment of the radiation field. This phenomenon, being called the effect of suppression of inelastic channels (ES), has been discovered experimentally both for Mössbauer gamma quanta<sup>8-12</sup> and neutrons<sup>13</sup>.

The ES reveals itself in the experiment as an increase of the transparency of a strongly absorbing crystal for the gamma quanta incident under the Bragg angle. In this sense the ES comes forward as an analogy to the Borrmann effect. Nevertheless, these effects differ from each other essentially in the physical nature.

Perhaps, the most principal difference consists in the fact that the suppression of nuclear reactions takes place, in a general case, under conditions when neither electric nor magnetic fields become zero at the sites occupied by the nuclei.

Instead of this, the requirement arises for the total amplitude of excited nucleus formation to be zero, which in turn leads to a number of new phenomena. First of all, this concerns the temperature dependence of



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the effects. In the case where the width of the resonant level is small compared to the characteristic phonon energy (as it always takes place for the Mössbauer transitions), it turns out that lattice vibrations, and therefore temperature, do not influence the ES at all (see <sup>5-7</sup>). In the case of the Borrmann effect, the atom vibrations from its equilibrium positions, naturally, lead to a restoration of the photoelectric absorption.

Another interesting circumstance is the possibility to realize the ES simultaneously for both directions of polarization (see below) and, therefore, to make the crystal completely unabsorbing for the whole radiation.

Finally note that the accomplishment of the Borrmann effect assumes the equality of the phases or the corresponding partial structural factors for all atoms in the unit cell. This requirement is absent for the ES. There exists a number of cases where the partial structural factors are different and nevertheless the ES takes place in a full degree.

The nontrivial picture of the electromagnetic field distribution in the crystal and the consequences mentioned above reveal itself most vividly under conditions where the nuclei are influenced by the internal electric and magnetic fields and where hyperfine splitting of the nuclear levels occurs.

As is known (cf. e.g. <sup>14</sup>), owing to the unique narrowness of Mössbauer lines, the interaction of the gamma quanta with an individual nucleus is very sensitive to the hyperfine structure, and it is possible to alter sharply the character of this interaction in one and the same crystal by slightly changing the gamma quanta energy, as it usually can be done with the help of the Doppler shift.

In the present paper a detailed analysis is given of the ES in the presence of hyperfine splitting, the main attention being paid to the conditions of the full ES realisation and to the structure of the electromagnetic field arising in these cases.

## II. Derivation of the Set of the Dynamical Equations

Suppose that an electromagnetic radiation enters a perfect crystal and the wave length of the radiation is of the order of the interatomic distance, so that strong diffractive Bragg scattering can arise under a proper direction of the incident wave. If the crystal is sufficiently thick and its perfection is high

enough, the scattering wave amplitude can come up to the amplitude of the incident wave. As a result, a radical change of the electromagnetic field distribution over the crystal takes place. The diffractive scattering is a purely elastic coherent process, and the quantum mechanical state of the crystal on the whole remains unchanged during this process. This circumstance permits us to use the classical Maxwell equations for the description of the electromagnetic field inside the crystal in spite of the fact that the problem requires to take into account both the incoherent processes (lattice vibrations, spin and isotopic incoherency in the case of gamma quanta) and the especially quantum ones (photoeffect, Compton scattering, inelastic nuclear reaction). All these processes can be taken into account by calculating the current induced in the crystal by the electromagnetic radiation.

The Maxwell equation for the Fourier component of the electric field  $\mathbf{E}(\mathbf{k}, \omega)$  has the form

$$[k^2 - (\omega^2/c^2)] \mathbf{E}(\mathbf{k}, \omega) = \mathbf{k}(\mathbf{k} \cdot \mathbf{E}(\mathbf{k}, \omega)) = 4\pi c^{-2} i \omega \mathbf{j}(\mathbf{k}, \omega). \quad (1)$$

Here  $\mathbf{j}(\mathbf{k}, \omega)$  is the Fourier component of the current density which, in accordance with its physical meaning, is a quantum mechanical average of the Fourier component of the current density operator  $\hat{\mathbf{j}}(\mathbf{k}, \omega)$  over the state of the crystal in the presence of the electromagnetic field  $\mathbf{E}(\mathbf{k}, \omega)$  (cf. e.g. <sup>5, 15</sup>

$$\begin{aligned} j^i(\mathbf{k}, \omega) &= \langle \hat{j}^i(\mathbf{k}, \omega) \rangle \\ &= \int [d\mathbf{k}' / (2\pi)^3] \sigma_{\omega}^{il}(\mathbf{k}, \mathbf{k}') E^l(\mathbf{k}', \omega). \end{aligned} \quad (2)$$

Owing to the translation symmetry, the conductivity tensor  $\sigma_{\omega}^{il}(\mathbf{k}, \mathbf{k}')$  is unequal zero only in the cases when the wave vectors  $\mathbf{k}$  and  $\mathbf{k}'$  differ from each other by a reciprocal lattice vector  $\mathbf{K}_h$ :

$$\begin{aligned} \sigma_{\omega}^{il}(\mathbf{k}, \mathbf{k}') &= (2\pi)^3 \sum_h \delta(\mathbf{k}', \mathbf{k} + \mathbf{K}_h) \\ &\quad \cdot \tilde{\sigma}_{\omega}^{il}(\mathbf{k}', \mathbf{k} + \mathbf{K}_h). \end{aligned} \quad (3)$$

Substituting now Eq. (2) and (3) into Eq. (1), we get the set of the dynamical equations

$$\begin{aligned} (k_h^2 - \kappa^2) E^i(\mathbf{k}_h) - \mathbf{k}_h^i (\mathbf{k}_h \cdot \mathbf{E}(\mathbf{k}_h)) \\ = \kappa^2 \sum_{h'} g_{hh'}^{il} E^l(\mathbf{k}_{h'}), \end{aligned} \quad (4)$$

$$\begin{aligned} g_{hh'}^{il} &= \frac{4\pi i}{\omega} \tilde{\sigma}_{\omega}^{il}(\mathbf{k}_h, \mathbf{k}_{h'}), \\ \mathbf{k}_h &= \mathbf{k}_0 + \mathbf{K}_h, \quad \kappa = \omega/c. \end{aligned} \quad (5)$$

which connect the incident wave amplitude  $\mathbf{E}(\mathbf{k}_0)$  with the amplitudes of the waves scattered on a reciprocal lattice vector  $\mathbf{K}_h$ .

In the case of gamma quanta with the energy close to that of a nuclear transition, both atomic electrons and nuclei will contribute to the current. In a general case

$$\mathbf{j}(\mathbf{k}, \omega) = \mathbf{j}^{(\text{el})}(\mathbf{k}, \omega) + \mathbf{j}^{(\text{nucl})}(\mathbf{k}, \omega).$$

Consistent calculations of the nuclear part of the current, and therefore of the coefficients  $g_{hh'}^{il}$ , have been carried out in <sup>5, 16</sup>. Along with the extremely strong absorption caused by a resonant character of the interaction, the lattice vibrations and the incoherent spin and isotopical incoherency have been taken into account in <sup>5</sup>; besides, the complete analysis has been made of the process of the inelastic scattering of gamma quanta by phonons in <sup>16</sup>.

A detailed derivation was given in <sup>15, 16</sup> of the dynamical equations coefficients for the case of an interaction of the electromagnetic field (in particular of X-rays) with atomic electrons. Here we shall not repeat these calculations but give only the final results which are convenient for us to be presented in the form

$$g_{hh'}^{il} = g_{hh'}^{il}(\text{nucl}) + g_{hh'}^{il}(\text{el}), \quad (6)$$

$$g_{hh'}^{il}(\text{nucl}) = - \frac{4\pi\eta}{\omega^2 \Omega_0} \frac{1}{2I_0 + 1} \sum_p \sum_{\zeta_0, \zeta} A_h^i(p, \zeta_0, \zeta) A_{h'}^{I*}(p, \zeta_0, \zeta) \frac{1}{\hbar \omega - E_p(\zeta_0, \zeta) + i\Gamma/2} \quad (7)$$

where

$$A_h(p, \zeta_0, \zeta) = \exp(i\mathbf{k}_h \mathbf{q}_p) \times \exp\left(\frac{1}{2} Z_p(\mathbf{k}_h)\right) \times (\mathbf{j}_p(\mathbf{k}_h))_{\zeta_0 \zeta}. \quad (8)$$

Here the index  $p$  labels positions  $\mathbf{q}_p$  in the unit cell that can be occupied by a resonant nucleus,  $\eta$  is the abundance of the resonant isotope;  $\Omega_0$  is the volume of the unit cell. The indices  $\zeta_0, \zeta$  denote the quantum numbers for the ground and excited states of the  $p$ -th nucleus, respectively;  $E_p(\zeta_0, \zeta)$  is the energy of the corresponding nuclear transition,  $\Gamma$  is the total width of the nuclear level,  $I_0$  is the nuclear spin of the ground state;  $\hat{\mathbf{j}}_p(\mathbf{k}_h)$  is the current operator corresponding to the  $p$ -th nucleus;  $\exp\{-\frac{1}{2} Z_p(\mathbf{K}_h)\}$  are the usual Mössbauer factors.

For the electron part of the coefficients  $g_{hh'}^{il}$  we have

$$g_{hh'}^{il}(\text{el}) = -\delta^{il} \frac{4\pi r_0}{\kappa^2 \Omega_0} \left\{ \sum_j \exp\{i(\mathbf{k}_{h'} - \mathbf{k}_h) - \frac{1}{2} Z_j(\mathbf{k}_{h'} - \mathbf{k}_h)\} f_j(\mathbf{k}_{h'} - \mathbf{k}_h) \right\} + F_T^{il}(\mathbf{k}_{h'}, \mathbf{k}_h). \quad (9)$$

Here  $r_0$  is the classical radius of an electron,  $\mathbf{q}_j$

determines the position of the  $j$ -th atom in the unit cell;  $f_j(\mathbf{k}_{h'} - \mathbf{k}_h)$  is the temperature independent atomic form factor in which, along with the Thompson scattering, the photoelectric absorption and the Compton scattering have been taken into account. The term  $F_T^{il}(\mathbf{k}_h, \mathbf{k}_{h'})$  describes the contribution from the process of the inelastic scattering by phonons.

In the case of the nuclear interaction one has to know the explicit form of the matrix elements of the current operator  $\hat{\mathbf{j}}_p(\mathbf{k})$ . We shall restrict ourselves the cases of the  $E1$ - and  $M1$ -type transition. Then

$$\begin{aligned} \hat{\mathbf{j}}(\mathbf{k}) &= i\omega \hat{\mathbf{d}}, \quad (E1); \\ \hat{\mathbf{j}}(\mathbf{k}) &= ic[\mathbf{k} \times \hat{\boldsymbol{\mu}}], \quad (M1). \end{aligned} \quad (10)$$

Here  $\hat{\mathbf{d}}$  and  $\hat{\boldsymbol{\mu}}$  are the nuclear electric and magnetic dipole momentum operators, respectively. Denote by  $M_0$  and  $M$  the quantum numbers of the nuclear spin projection on the quantization axis  $\mathbf{n}_0$  for the ground and excited state of the nucleus, respectively. Then

$$(\hat{\mathbf{d}})_{M_0 M} = -i \left( \frac{3(2I+1) \Gamma_1}{4\kappa^3} \right)^{1/2} (-1)^q \begin{pmatrix} I_0 & 1 & I \\ M_0 & q & M \end{pmatrix} \mathbf{n}_q. \quad (11)$$

Just the same formula holds for the operator  $\hat{\boldsymbol{\mu}}$  in the case of  $M1$ -transitions. Here  $I$  is the nuclear spin of the excited state;  $\Gamma_1$  is the elastic part of the total width which corresponds to the gamma quanta emission;  $\begin{pmatrix} I_0 & 1 & I \\ M_0 & q & M \end{pmatrix}$  are the 3  $j$ -symbols (cf. e.g. <sup>17</sup>),  $q = M_0 - M$ ;  $\mathbf{n}_{\pm 1} = \mp (\mathbf{n}_x \pm i\mathbf{n}_y)$  are two arbitrary mutually orthogonal unit vectors, which in turn are orthogonal to the vector  $\mathbf{n}_0$ .

If the hyperfine splitting is absent, that is if  $E(\zeta_0, \zeta)$  does not depend on  $\zeta_0, \zeta$ , one can carry out the summation over  $\zeta_0, \zeta$  in formula (7). As a result, one has

$$g_{hh'}^{il} = \delta^{il} g_{hh'}, \quad (E1), \quad (12')$$

$$g_{hh'}^{il} = \{ [k_h^i k_h^l - \delta^{il} (k_h k_h)] / \kappa^2 \} g_{hh'}(M1), \quad (12'')$$

where

$$g_{hh'} = -\eta \frac{4\pi}{\kappa^3 \Omega_0} \frac{2I+1}{2(2I_0+1)} \cdot \frac{\Gamma_1/2}{\hbar \omega - E_0 + i\Gamma/2} \cdot \sum_p \exp\left\{ -\frac{1}{2} (Z_p(\mathbf{k}_h) + Z_p(\mathbf{k}_{h'})) + i(\mathbf{k}_{h'} - \mathbf{k}_h) \mathbf{q}_p \right\}.$$

For  $E2$ -transitions,  $g_{hh'}^{il}$  is determined by (12'') where the sign before the symbol  $\sigma^{il}$  should be changed.

The coefficients (7) of the general set of the dynamical Eq. (4) are in fact the coherent elastic scattering amplitudes of gamma quanta in the crystal.

It is essential that the pure elastic scattering amplitude is always finite although the incoherent inelastic processes can be very large. Apparently, every channel of the coherency lack decreases the elastic amplitude which can be seen directly from formulae (7) and (12).

The presence of the inelastic channel (in our case it is the process of the internal conversion) displays itself in (7), (12) by means of the total width  $\Gamma = \Gamma_1 + \Gamma_2$  which is the sum of the elastic part  $\Gamma_1$  and the inelastic one  $\Gamma_2$ . As a rule,  $\Gamma_2 \gg \Gamma_1$  and therefore, at the exact resonance ( $\hbar \omega = E_0$ ), the coherent amplitude decreases by the factor  $\Gamma_1/\Gamma_2$ .

The factors  $\exp\{-\frac{1}{2} Z_p(\mathbf{k}_n)\}$  are just the relative probability amplitudes of the absorption and the emission of the gamma quantum by the nucleus without any excitement of the phonon system. It is interesting that, owing to the large value of the life time of the excited nucleus  $\tau_0 (\tau_0 \gg 1/\omega_{ph}, \omega_{ph}$  is the characteristic phonon frequency), the excitement of the phonon system on the steps of the absorption and of the emission of the gamma quanta are statistically independent. Therefore the coherency conservation requires the phononless transition at each step separately. Note, that the phononless nuclear scattering amplitude differs radically from the Debye-Waller factor which stands in the electron part of the coefficients  $g_{hh'}^{il}$  (9).

In particular, the nuclear coherent scattering amplitude can be strongly diminished due to the temperature factors even at small reciprocal lattice vectors  $\mathbf{K}$ . Forestalling note that, in spite of this fact, the lattice vibrations do not prevent completely the SE.

Finally, the presence of the ground state nuclear spin gives rise to incoherent scattering of gamma quanta which is accompanied by a change of the spin projection. This circumstance causes an additional diminishing of the coherent scattering amplitude.

The set of the dynamical Eq. (4) with the coefficients (6) – (9) can be utilized both for resonant gamma quanta and X-rays. In the latter case, one has to put  $g_{hh'}^{il}(\text{nucl}) = 0$ .

### III. The Conditions for the Realization of the Suppression Effect

Suppose that the Bragg requirement is satisfied only for one reciprocal lattice vector  $\mathbf{K}_1$ , one can

neglect all the amplitudes except  $\mathbf{E}(\mathbf{k}_0)$  and  $\mathbf{E}(\mathbf{k}_1)$  in Equation (4). Owing to the smallness of the gamma quanta interactions with nuclei and electrons, the electromagnetic field inside the crystal remains practically transverse, i. e.  $\mathbf{E}(\mathbf{k}_h) \cdot \mathbf{k}_h = 0$ . Therefore, under the approximation considered, the set (4) is a set of four equations. If one chooses arbitrarily two mutually orthogonal transverse polarization vectors  $\mathbf{e}_0^{(1,2)}$  in the incident wave and  $\mathbf{e}_1^{(1,2)}$  in the diffracted one, one can represent the fields  $\mathbf{E}(\mathbf{k}_0)$  and  $\mathbf{E}(\mathbf{k}_1)$  as follows:

$$\mathbf{E}(\mathbf{k}_h) = \mathbf{e}_h^{(1)} E_h^{(1)} + \mathbf{e}_h^{(2)} E_h^{(2)}.$$

Then the set (4) reduces to

$$\begin{aligned} 2\varepsilon_0 E_0^{(1)} &= g_{00}^{11} E_0^{(1)} + g_{00}^{12} E_0^{(2)} + g_{01}^{11} E_1^{(1)} + g_{01}^{12} E_1^{(2)}, \\ 2\varepsilon_0 E_0^{(2)} &= g_{00}^{21} E_0^{(1)} + g_{00}^{22} E_0^{(2)} + g_{01}^{21} E_1^{(1)} + g_{01}^{22} E_1^{(2)}, \\ (2\varepsilon_0/\beta + \alpha) E_1^{(1)} &= g_{10}^{11} E_0^{(1)} + g_{10}^{12} E_0^{(2)} + g_{11}^{11} E_1^{(1)} + g_{11}^{12} E_1^{(2)}, \\ (2\varepsilon_0/\beta + \alpha) E_1^{(2)} &= g_{10}^{21} E_0^{(1)} + g_{10}^{22} E_0^{(2)} + g_{11}^{21} E_1^{(1)} + g_{11}^{22} E_1^{(2)}, \end{aligned} \quad (13)$$

where

$$g_{hh'}^{ss'} = \sum_{il} (\mathbf{e}_h^{(s)})_i^* g_{hh'}^{il} (\mathbf{e}_{h'}^{(s')})_l. \quad (14)$$

Here, we have introduced the standard notations

$$\begin{aligned} 2\varepsilon_0 &= (k_0^2/\varkappa^2) - 1, \quad \alpha = \mathbf{K}(\mathbf{K} + 2\boldsymbol{\varkappa})/\varkappa^2, \quad \beta = \gamma_0/\gamma_1, \\ \gamma_{0,1} &= \cos(\widehat{\mathbf{k}_{0,1}, \mathbf{n}}), \end{aligned}$$

where  $\boldsymbol{\varkappa}$  is the gamma quantum wave vector in vacuum;  $\mathbf{n}$  is the interior normal to the crystal surface.

For the case of X-rays, when the coefficients  $g_{hh'}^{il}$  are determined only by the interaction of X-rays with the atomic electron (9), the set of Eq. (4) splits up into two pairs of independent equations separately for the  $\sigma$ -polarized quanta with the polarization vector

$$\mathbf{e}_0^{(\sigma)} = \mathbf{e}_1^{(\sigma)} = [\mathbf{k}_0 \times \mathbf{k}_1]/|\mathbf{k}_0 \times \mathbf{k}_1| \quad (15)$$

and for  $\pi$ -polarized quanta with

$$\mathbf{e}_h^{(\pi)} = [\mathbf{k}_h \times \mathbf{e}_h^{(\sigma)}]/k_h. \quad (16)$$

One can easily perceive this splitting directly from the formulae (14), (9). In this case, the analysis of the dynamical equations is of no special difficulty.

In the gamma quanta case, when the nuclear term (7) is important then the set (13) splits up into two independent subsets only in special situations. The case, where the hyperfine interaction is absent<sup>5</sup>, is such a situation (this fact can be easily seen from (12)). In the general case, when the



hyperfine interaction takes place, the set (13) is an indivisible system of mutually connected equations.

The condition of the existence of the nontrivial solution of the (13) gives us the following equation:

$$\begin{bmatrix} g_{00}^{11} - 2\varepsilon_0, & g_{00}^{12}, & g_{01}^{11} & & g_{01}^{12} \\ g_{00}^{21}, & g_{00}^{22} - 2\varepsilon_0, & g_{01}^{21} & & g_{01}^{22} \\ g_{10}^{11}, & g_{10}^{12}, & g_{11}^{11} - 2\varepsilon_0/\beta - \alpha, & & g_{11}^{12} \\ g_{10}^{21}, & g_{10}^{22}, & g_{11}^{21} & & g_{11}^{22} - 2\varepsilon_0/\beta - \alpha \end{bmatrix} = 0. \quad (17)$$

The wave field inside the crystal will be determined by the expression

$$\mathbf{E}(\mathbf{r}) = \exp\{i\mathbf{r} \cdot \boldsymbol{\kappa}\} \sum_{m=1}^4 \exp\{i\kappa \varepsilon_0^{(m)} t/\gamma_0\} \times \left\{ \sum_{s=1,2} [\mathbf{e}_0^{(s)} E_0^{(s)}(m) + \exp\{i\mathbf{K} \cdot \mathbf{r}\} \mathbf{e}_1^{(s)} E_1^{(s)}(m)] \right\} \quad (18)$$

Here,  $\varepsilon_0^{(m)}$  are the roots of Eq. (17), and  $E_h^{(s)}(m)$  are the solutions corresponding to these roots. Because our initial set (13) is a uniform one, we have to utilize the boundary conditions for the determination of  $E_h^{(s)}(m)$ . In this paper we will be interested only in the Laue case diffraction. Then the boundary conditions have the form

$$\sum_{m=1}^4 E_0^{(s)}(m) = E_0^{(s)}, \quad \sum_{m=1}^4 E_1^{(s)}(m) = 0. \quad (19)$$

Here  $E_0^{(s)}$  is the incident "s" polarized wave amplitude on the crystal surface.

As was shown in<sup>5</sup>, under the condition of pure nuclear scattering, one of the roots  $\varepsilon^{(m)}$  can become strictly equal to zero. Therefore, according to (18), the related part of the radiation will travel through the crystal without any absorption.

We shall call the situations, where at least for one of roots

$$\text{Im } \varepsilon_0^{(m)} = 0, \quad (20)$$

the cases of the full ES realization, and these situations will be of the main interest in the following investigations.

Let us neglect at first the gamma quanta interaction with electrons. Consider the simplest case when the gamma quanta energy falls on the part of the spectrum where only one line of hyperfine structure is placed, the hyperfine splitting being assumed so large that the influence of the remaining spectral lines can be neglected. To put it in another way we mean the cases when it is possible to conserve only one term  $(p', \zeta_0', \zeta')$  in the sum over  $p', \zeta_0', \zeta'$  in (16). Choose as the polarization vectors  $\mathbf{e}_h^{(1)}$  the vectors perpendicular to the vectors  $\mathbf{A}_h(p', \zeta_0', \zeta')$ ,

i. e.,

$$\mathbf{e}_h^{(1)} \mathbf{A}_h' = 0. \quad (21)$$

It is easy to see that the gamma quanta polarized like in (21) do not interact at all with the nuclei under the considered approximation. The gamma quanta with the polarization vectors  $\mathbf{e}_h^{(2)} = [\mathbf{k}_h \times \mathbf{e}_h^{(1)}]/k_h$  interact strongly with the nuclei, their moving over the crystal being governed by the set of two dynamical equations

$$\begin{aligned} 2\varepsilon_0 E_0^{(2)} &= g_{00}^{(2)} E_0^{(2)} + g_{01}^{(2)} E_1^{(2)} \\ (2\varepsilon_0/\beta + \alpha) E_1^{(2)} &= g_{10}^{(2)} E_0^{(2)} + g_{11}^{(2)} E_1^{(2)} \end{aligned} \quad (22)$$

where

$$g_{hh'}^{(2)} = - \frac{4\pi\eta}{(2I_0 + 1)\omega^2\Omega_0} \frac{A_h^{(2)} A_{h'}^{(2)*}}{\hbar\omega - E_{p'}(\zeta_0', \zeta') + i\Gamma/2} \quad (23)$$

with  $A_h^{(2)} = (\mathbf{e}_h^{(2)} \cdot \mathbf{A}_h(p', \zeta_0', \zeta'))$ .

A straightforward analysis gives us

$$\begin{aligned} \varepsilon_0^{(1,2)} &= \frac{1}{2} (g_{00}^{(2)} + \beta g_{11}^{(2)} - \beta\alpha) \\ &\pm \frac{1}{2} \{ (g_{00}^{(2)} + \beta g_{11}^{(2)} - \beta\alpha)^2 + 4\beta g_{00}^{(2)}\alpha \}^{1/2}. \end{aligned} \quad (24)$$

It is seen from (24) that  $\varepsilon_0^{(1)} = 0$  at  $\alpha = 0$ , and therefore the full ES takes place in the case under consideration.

Of interest is the fact that  $\varepsilon_0$  turns out to be strictly zero independently from the value of the temperature factors  $\exp\{-\frac{1}{2}Z(\mathbf{k}_h)\}$  which enter the coefficients  $g_{hh'}^{(2)}$ , by means of the factors  $\mathbf{A}_h(8)$ . Therefore, if the Bragg condition is strictly satisfied, the lattice vibrations do not influence the gamma quanta interaction with the nuclei. For the case of X-rays, the lattice vibrations destroy the Borrmann effect and cause the considerable restoration of the photoelectric absorption.

Suppose now that the gamma quanta energy falls on the part of the spectrum where two lines are placed, where, in other words, one can preserve only two terms in the sum over  $p' \zeta_0' \zeta'$  in (7). In this case one has to handle the general dispersion Eq. (17) which under the above assumption takes the following form:

$$\begin{aligned} (2\varepsilon_0)^2 (2\varepsilon_0/\beta + \alpha)^2 - (g_{11}^{(11)} + g_{11}^{(22)}) (2\varepsilon_0)^2 (2\varepsilon_0/\beta + \alpha) \\ - (g_{00}^{(11)} + g_{00}^{(22)}) 2\varepsilon_0 (2\varepsilon_0/\beta + \alpha)^2 + \Delta_{11}^{12} (2\varepsilon_0)^2 + (\Delta_{01}^{11} \\ + \Delta_{01}^{11} + \Delta_{01}^{21} + \Delta_{01}^{22}) 2\varepsilon_0 (2\varepsilon_0/\beta + \alpha) \\ + \Delta_{00}^{12} (2\varepsilon_0/\beta + \alpha)^2 = 0 \end{aligned} \quad (25)$$

where  $\Delta_{hh'}^{ss'}$  are the second order determinants

$$\Delta_{hh'}^{ss'} = \begin{vmatrix} g_{hh}^{ss} & g_{hh'}^{ss'} \\ g_{h'h}^{s's} & g_{h'h'}^{s's'} \end{vmatrix}. \quad (26)$$

It follows right from (25) that, at  $\alpha=0$ , the dispersion equation has two roots which are equal to zero. The latter means that in this case the full ES takes place at the same time for both directions of polarization.

If three lines are placed at the given part of the spectrum, then we again have the full ES for one polarization. To see this, one should put  $\alpha=0$  and  $\varepsilon_0=0$  and satisfy oneself directly that the remainder determinant (17) composed only from the coefficients  $g_{hh'}^{ss'}$  is strictly equal to zero if the  $g_{hh'}^{ss'}$  are determined by formula (7) where only three terms are conserved in the sum over  $p$   $\zeta_0 \zeta$ .

We shall return to these results in the next section.

#### IV. Structure of the Electromagnetic Field in the Case of ES Realization

Let us come back to the case of one line. Making use of (22) – (24), one can easily find the following expression for the wave field which corresponds to the root  $\varepsilon_0=0$  ( $\alpha=0$ ):

$$\mathbf{E}(\mathbf{r}) = \text{const} \exp\{i \boldsymbol{\kappa} \cdot \mathbf{r}\} [A_1 \mathbf{e}_0^{(2)} - \exp\{i \mathbf{K} \cdot \mathbf{r}\} A_0 \mathbf{e}_1^{(2)}] \quad (27)$$

Let us consider the case of the  $E1$ -transition and assume that the nuclei are influenced by the internal

magnetic field perpendicular to the scattering plane. Assume also that the unit cell has only one resonant nucleus and let the gamma quantum energy be close to that of the nuclear transition with  $q = M - M_0 = 1$ . According to (10), (11), and (8),

$$A_h(M, M_0 = M - 1) = \text{const} \exp\left\{\left[-\frac{1}{2} Z(\mathbf{k}_h)\right] (\mathbf{n}_x + i \mathbf{n}_y)\right\}. \quad (28)$$

The direction of axes  $X$  and  $Y$  is shown in Figure 1. In the case under consideration, the  $\sigma$ -polarized quanta do not interact with the nuclei but the  $\pi$ -polarized ones do.

It is obvious that the electric field can not become equal to zero anywhere, and hence not at the sites occupied by the nuclei, too, because the vectors  $\mathbf{e}_0^{(\pi)}$  and  $\mathbf{e}_1^{(\pi)}$  are noncolinear. Moreover, if the scattering angle equals  $\pi/2$ , then the modulus of the electric field is constant over the crystal. Nevertheless, the polarization of the field changes from point to point. Indeed, making use of (27), (28), one has

$$\begin{aligned} A_0 &= \text{const} \exp\{i \Theta\}; \quad A_1 = \text{const} \exp\{-i \Theta\}; \\ \mathbf{E}(\mathbf{r}) &= \text{const} \exp\{i \varphi/2\} [\sin \Theta \cos(\Theta + \varphi/2) \mathbf{n}_x \\ &\quad + i \cos \Theta \sin(\Theta + \varphi/2) \mathbf{n}_y], \quad \varphi = \mathbf{K} \cdot \mathbf{r}. \end{aligned} \quad (29)$$

As follows from this expression, the electric field is circular polarized at the lattice sites. Figure 1 b shows the change of the electric field polarization at the point between the nuclei.

Consider another example. Let the gamma quanta energy be near that of the transition with  $q = M - M_0 = 0$ . In this case

$$A_h(M, M_0 = M) = \text{const} \exp\left\{-\frac{1}{2} Z(\mathbf{k}_h)\right\} \mathbf{n}_0. \quad (30)$$

Assume that the internal magnetic field lies in the  $(\mathbf{k}_0, \mathbf{k}_1)$  plane. Here again, the electric field does not equal zero anywhere, but the polarization properties change essentially (cf. Figure 1 c). The picture is analogous to the preceding case, but now we have the linearly polarized field at the lattice sites.

These examples show that the ES does not depend on the fact whether the electric or magnetic field amplitude is equal to zero or not.

In fact, a new characteristic — the amplitude of the excited nucleus formation — comes forward in the case under consideration.

The gamma quantum with the energy close to that of the nuclear transition,  $E(\zeta_0 \zeta)$ , can be absorbed by a nucleus which turns an excited state.

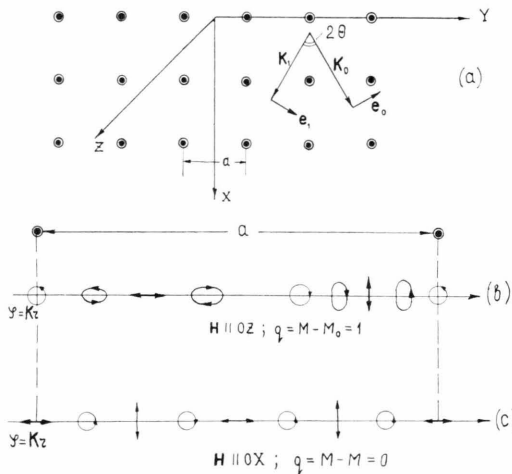


Fig. 1. Change of the electromagnetic field polarization within one unit cell under conditions of realization of the complete effect of suppression: (a) density of scattering; (b) a case, when the hyperfine magnetic field  $\mathbf{H}$  at the nuclei is perpendicular to the scattering plane and the gamma-quantum energy corresponds to the transition with  $q = M - M_0 = 1$ ; (c) a case, when  $\mathbf{H}$  lies in the scattering plane and  $q = M - M_0 = 0$ .

The amplitude of this process is proportional to

$$A_p(\mathbf{k}, s) = [\exp\{i \mathbf{k} \cdot \mathbf{e}_p\} E^{(s)}(\mathbf{k})] \times [\mathbf{e}^{(e)} \cdot \mathbf{j}(\mathbf{k})_{\mathbf{e}_p}] \times \exp\{-\frac{1}{2} Z(\mathbf{k}_h)\}. \quad (31)$$

Here the first factor shows the dependence of the amplitude on the value and the phase of the electromagnetic field at the sites occupied by the nuclei, the second one is the matrix element of the corresponding nuclear transition, and the third factor determines the relative probability of the nucleus excitation in the vibrating crystal.

If the coherent superposition of waves moves through the crystal, the amplitude of excited nucleus formation in this superposition is obviously the sum of the amplitudes of type (31), i. e.,

$$A^{\text{tot}}(p, \zeta_0, \zeta) = [A_h(p, \zeta_0, \zeta) \mathbf{e}_h^{(e)}] E_h^{(s)} \quad (32)$$

where  $A_h(p, \zeta_0, \zeta)$  is determined by (9).

The full ES corresponds to the superposition of waves in which

$$A^{\text{tot}}(p, \zeta_0, \zeta) = 0 \quad (33)$$

for all the transitions, which are essential at the given region of the spectrum. It is easy to conceive, that in all the examples considered above, the full ES corresponds exactly to the conditions (33).

The physical conditions of the full ES realization obtained above are very useful for the interpretation of the results of Section II. If the gamma quantum energy lies in the spectrum region where three lines are essential, the realization of the full ES demands the satisfaction of Eqs. (33) for the transitions simultaneously. But there are four quantities  $E_h^{(s)}$  in our disposal and therefore it is always possible to satisfy three equations of type (33). Besides, the same quantities  $E_h^{(s)}$  will be the solution of the diffraction Eq. (13) with  $\alpha = 0$  and  $\varepsilon_0 = 0$ . Indeed, if the conditions (33) are satisfied, the right part of Eq. (13) equals strictly zero.

If only two lines are in the given part of the spectrum, then it is sufficient to satisfy two Eq. (33) for the full ES realization. In this case, as it is easy to see, there are two independent solutions of Equation (33). This is completely in accordance with the results of Section II.

Consider now the case of two lines in more detail. Let us analyse the following example. Assume that the nuclei are influenced by the internal electric field of the axial symmetry. In this case, as is well known (cf. e. g. <sup>14</sup>), the energies of the transitions  $M_0 \rightarrow M$  and  $-M_0 \rightarrow -M$  exactly coincide. For  $E$  1-transi-

tions and  $|M - M_0| = 1$ , one has according to (8) – (11) the following formulae

$$A_h(M, M_0 = M - 1) = \text{const} \exp\{-\frac{1}{2} Z(\mathbf{k}_h) (\mathbf{n}_x + i \mathbf{n}_y)\}, \\ A_h(-M, -M_0) = A_h^*(M, M_0). \quad (34)$$

Here  $\mathbf{n}_x, \mathbf{n}_y$  are two arbitrary mutually orthogonal unit vectors which are in turn perpendicular to the electric field gradient axis  $\mathbf{n}_0$ . In (34) all the inessential factors are omitted.

As follows directly from (32), (34), the value of the total electric field projection on the axis  $n$  is not important for the gamma quanta interaction with the nuclei in the neighbourhood of the transition under consideration. Naturally, this circumstance enlarges the number of the possible cases of the absorption diminution in comparison with the X-ray case.

Let now the axis  $\mathbf{n}_0$  lie in the scattering plane symmetrically to the vectors  $\mathbf{k}_0$  and  $\mathbf{k}_1$ , and for simplicity assume that  $Z(\mathbf{k}_0) = Z(\mathbf{k})$ . In this case one can write down the following two combinations, one for the  $\sigma$ -polarized waves

$$\mathbf{E}^{(\sigma)}(\mathbf{r}) = \exp\{i \boldsymbol{\kappa} \cdot \mathbf{r}\} \mathbf{e}^{(\sigma)} (1 - \exp\{i \mathbf{K} \cdot \mathbf{r}\}) \quad (35)$$

and another for the  $\pi$ -polarized quanta

$$\mathbf{E}^{(\pi)}(\mathbf{r}) = \exp\{i \boldsymbol{\kappa} \cdot \mathbf{r}\} (\mathbf{e}_0^{(\pi)} - \mathbf{e}_1^{(\pi)} \exp\{i \mathbf{K} \cdot \mathbf{r}\}), \quad (36)$$

which satisfy the Eqs. (33) identically; thus for these fields the full ES is realized. While the electric field in the case (35) at the lattice sites,  $\mathbf{K} \cdot \mathbf{r} = 2\pi n$ , appears to be zero, but for the  $\pi$ -combination (36) this is not the case, because the component along  $n$  axis is still finite. But the accomplishment of the full ES requires in our case only turning into zero of the projection of the field on the plane perpendicular to  $\mathbf{n}_0$ . As it is easy to see this condition is strictly satisfied at the lattice sites.

It is of interest to know the coefficients  $g_{hh'}^{il}$  taking into account Eq. (34), Eqs. (7) and (8) lead to

$$g_{hh'}^{il} = g_{hh'}(M, M_0) (\delta^{il} - n_0^i n_0^l), \quad (37)$$

$$g_{hh'}(M, M_0) = - \frac{2\pi\eta}{(2I_0 + 1)\kappa^3\Omega_0} \cdot \frac{\Gamma_1/2}{\hbar\omega - E(M, M_0) + i\Gamma/2} \begin{pmatrix} I & 1 & I_0 \\ -M & 1 & M_0 \end{pmatrix} + \exp\{-\frac{1}{2}[Z(\mathbf{k}_h) + Z(\mathbf{k}_{h'})]\}. \quad (38)$$

If  $\mathbf{n}_0$  lies in  $(\mathbf{k}_0, \mathbf{k}_1)$  plane, the system of the dynamical equations splits into the two subsystems of the form (22) for the  $\sigma$  and the  $\pi$ -polarized

quanta separately. In this case the analysis can be easily performed not only for the case when the Bragg condition is exactly satisfied but for any arbitrary value of  $\alpha$ .

Suppose that there are two resonant nuclei in the unit cell which are influenced by the different hyperfine fields. Let us assume now that there are nuclear transitions whose energies are close to each other or which even coincide. To realize the full ES one should satisfy Eq. (33) for the corresponding transitions both for the first nucleus and for the second respectively. According to the results received earlier these conditions can always be satisfied. Herein the true sites of the nuclei in the unit cell or, in other words, the phase factors  $\exp\{i\mathbf{K}\cdot\boldsymbol{\varrho}_p\}$  are proved to be inessential. This circumstance divides distinctly the ES and the Borrmann effect. Let us consider, for example, a collinear antiferromagnet with two magnetic atoms of Mössbauer type in the unit cell. Hyperfine magnetic fields at the locations of the nuclei in the unit cell will be equaled in magnitude and will have opposite signs. As a result, the  $M_0 \rightarrow M$  transition energy for the first nucleus will coincide with the  $-M_0 \rightarrow -M$  transition energy for the second one, i. e. each line of the hyperfine spectrum will be doubly degenerated. The vectors for the first nucleus transitions are determined by the Eq. (34) and for the second one by the same equation whose right side should be multiplied by the structure factor  $\exp\{i\mathbf{k}\cdot\boldsymbol{\varrho}_2\}$ . Here the radius vector  $\boldsymbol{\varrho}_2$  gives the second nucleus site; we have supposed  $\boldsymbol{\varrho}_1$  to be equal to zero by taking the origin at the first nucleus site. If the structure factor  $\exp\{i(\mathbf{k}_1 - \mathbf{k}_0)\cdot\boldsymbol{\varrho}_2\} = 1$ , then we have the situation analogous to the case of the quadrupole splitting considered just now. So the one hundred per cent SE is realized for both polarizations and the dynamical theory coefficients are determined by the Equation (37). Let  $\exp\{i\mathbf{k}\cdot\boldsymbol{\varrho}_2\} = -1$ . Such situation in the case of X-ray diffraction would lead to the total vanishing of the corresponding reflection. In the nuclear case there is no such a compensation. Simple calculations result in the following expressions for the tensor  $g_{hh}^{il}$ :

$$\begin{aligned} g_{hh}^{il} &= g_0(\delta^{il} - n_0^i - n_0^l) \exp\{-Z(\mathbf{k}_h)\}, \\ g_{01}^{il} &= -g_{10}^{il} = i g_0 \epsilon^{ilk} n_0^k \exp\{-\frac{1}{2}[Z(\mathbf{k}_0) + Z(\mathbf{k}_1)]\}. \end{aligned} \quad (39)$$

Here  $\mathbf{n}_0$  is the unit vector in the direction of the internal magnetic field for the first nucleus,  $\epsilon^{ilk}$  is the completely antisymmetric unit tensor;  $g_0$  is determined by Equation (38).

Equation (39) results in changing of the  $\gamma$ -quantum polarization during the process of the diffraction, which is determined by then tensors  $g_{01}^{il}$  and  $g_{10}^{il}$ . Really, according to Eq. (39) the  $\gamma$ -quantum scattering amplitude with polarization changing from  $\mathbf{e}_0^{(s)}$  to  $\mathbf{e}_1^{(s')}$  is proportional to the magnitude  $(\mathbf{n}_0 \cdot [\mathbf{e}_0^{(s)} \times \mathbf{e}_1^{(s')}])$ . So if  $\mathbf{n}_0$  lies in the  $(\mathbf{k}_0, \mathbf{k}_1)$  - plane then the  $\sigma$ -polarized  $\gamma$ -quantum can be scattered only in the  $\pi$ -polarized one and conversely. In spite of such strong changing of the polarization the process is strictly coherent, i. e. the crystal state during the scattering, or to be more definite the nuclei spins projections, stay invariable.

Let us direct the vector  $\mathbf{n}_0$  in the scattering plane  $(\mathbf{k}_0, \mathbf{k}_1)$ . In this case the general system of the dynamical equations splits into two subsystems of the form (22). The first subsystem connects the amplitude of the incident  $\sigma$ -polarized wave with the amplitude of the diffracted  $\pi$ -polarized one; the second subsystem in the contrary connects the incident  $\pi$ -polarized wave with the diffracted  $\sigma$ -polarized wave.

The dynamical system coefficients (22) should be replaced by the following ones

$$\begin{aligned} g_{00}^{(2)} &\rightarrow g_{00}^{(\sigma\sigma)} = g_0 \exp\{-Z(\mathbf{k}_0)\}; \\ g_{11}^{(2)} &\rightarrow g_{11}^{(\pi\pi)} = g_0 \exp\{-Z(\mathbf{k}_1)\} \cos^2 \Theta_1, \\ g_{01}^{(2)} &\rightarrow g_{01}^{(\sigma\pi)} = i g_0 \exp\{-\frac{1}{2}[Z(\mathbf{k}_0) + Z(\mathbf{k}_1)]\} \cos \Theta_1; \\ g_{10}^{(2)} &\rightarrow g_{10}^{(\pi\sigma)} = -g_{01}^{(\sigma\pi)}. \end{aligned} \quad (40)$$

Using Eq. (40) and (24) one easily can obtain that one of the roots  $\varepsilon_0$  is equal to zero for  $\alpha=0$ , i. e. in the given case the total SE is realized in spite of the fact that we have chosen  $\exp\{i\mathbf{k}\cdot\boldsymbol{\varrho}_2\} = -1$ . The similar situation takes place for the second subsystem too. Recently, an experimental investigation of the ES was performed with an antiferromagnetic crystal<sup>12</sup>.

As it can be seen from the represented results the analysis on the base of Eq. (33) is simpler and physically obvious with respect to the analysis of the initial system of the equation. The results obtained in Sec. III for the condition of the full ES realization are valid for an arbitrary multipolarity of the nuclear transition. For the  $E1$ - and  $M1$ -type transitions the number of cases when the SE takes place is much wider.

Let us consider  $E1$ -type transition. The current operator  $\hat{\mathbf{j}}(\mathbf{k})$  [see (10)] for these transitions is independent from the vector  $\mathbf{k}$ . Now suppose that we have chosen a reflection so, that



$$S_p = \exp\{i \mathbf{K} \cdot \boldsymbol{\varrho}_p\} = 1 \quad \text{and} \quad Z(\mathbf{k}_0) = Z(\mathbf{k}_1). \quad (41)$$

Herein the vectors  $\mathbf{A}_h$  are independent of the index  $h$ . It can easily be seen that the system (33) regardless of the number of its equations always has the solution

$$E_1^{(\sigma)} = -E_0^{(\sigma)}. \quad (42)$$

Thus by the suggestions (41) the full ES is always realized in the case of  $E1$ -transition for the arbitrary hyperfine structure of the spectrum (including the case of the unresolved spectrum). If there is only one resonant nucleus in the unit cell or if the Mössbauer factors of all the nuclei are equal, then the full ES takes place even if  $Z(\mathbf{k}_0) \neq Z(\mathbf{k}_1)$ . In this case the solution of the system (33) is

$$\exp\{-\tfrac{1}{2}Z(\mathbf{k}_1)\} E_1^{(\sigma)} = -\exp\{-\tfrac{1}{2}Z(\mathbf{k}_0)\} E_0^{(\sigma)}. \quad (43)$$

A quite analogous situation takes place also for the  $M1$ -type transition.

## V. Role of the Interaction with Electrons

Up to now we neglected the gamma quanta interaction with the electrons. This assumption can be justified in a number of cases. In the first place the nuclear interaction due to its resonant character is stronger in some cases than the electronic one, and in the second place the electronic scattering in complex lattices can be suppressed by the proper choice of the reflecting plane (cf. e. g. <sup>12</sup>).

However, in the general case the question arises in which situations the full ES is maintained in the presence of the electronic scattering and in what manner the nuclear absorption is restored in the other cases.

It is clear from the considerations represented above that the electronic scattering changes by no means the conditions of the full ES. Therefore in order to answer the question one has only to check that the superposition of  $E_n^{(s)}$  satisfying conditions (33) will be the solution of the dynamical problem for some  $\alpha$  in the presence of electronic scattering. Above we have obtained the solution (42) for the  $E1$ -transition or in more general form (43). Let's substitute this solution into the Eq. (22). As a result we come to the following equations:

$$\begin{aligned} 2\varepsilon_0 \exp\{-\tfrac{1}{2}Z(\mathbf{k}_1)\} &= g_{00}^{(\sigma)}(\text{el}) \exp\{-\tfrac{1}{2}Z(\mathbf{k}_1)\} \\ &- g_{01}^{(\sigma)}(\text{el}) \exp\{-\tfrac{1}{2}Z(\mathbf{k}_0)\}, \\ &-(2\varepsilon_0/\beta + \alpha) \exp\{-\tfrac{1}{2}Z(\mathbf{k}_0)\} = g_{10}^{(\sigma)}(\text{el}) \\ &\exp\{-\tfrac{1}{2}Z(\mathbf{k}_1)\} - g_{11}^{(\sigma)}(\text{el}) \exp\{-\tfrac{1}{2}Z(\mathbf{k}_0)\}. \end{aligned} \quad (44)$$

Since the quantity  $\alpha$  must be real in the given case we arrive at the following conditions of the full ES realization with the electronic scattering taken into account:

$$\text{Im } g_{10}^{(\sigma)}(\text{el}) = \text{Im } g_{11}^{(\sigma)}(\text{el}) = 0. \quad (45)$$

We are interested in the suppression of the strong nuclear absorption; therefore we neglect a small electronic absorption. So we can neglect small imaginary parts of the atomic structure factors  $f_j(\mathbf{k}_h, \mathbf{k}_h)$ , for their contribution to the total absorption is of the order of the electronic one. Then the condition (45) reduces to

$$\text{Im} \left\{ \sum_j \exp\{i \mathbf{K} \cdot \boldsymbol{\varrho}_j - Z_j(\mathbf{K})\} \text{Re } f(\mathbf{K}) \right\} = 0. \quad (46)$$

This condition, for example, is always fulfilled in crystals with a center of symmetry.

Thus the conditions (33) not only demonstrate the physical sense of the ES but also open the direct way for the analysis of the general problem.

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## Effect of Compton Scattering on the Borrmann Effect of X-Rays in Silicon Crystals

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*Dedicated to Prof. G. Borrmann on his 65-th birthday*

The absolute integrated intensities diffracted in anomalous transmission through thick, nearly perfect crystals of silicon were measured for  $\text{AgK}\alpha$  and  $\text{MoK}\alpha$  wavelengths and for the  $\{220\}$  reflection, at room and liquid nitrogen temperatures. There is good agreement between experimental values and those calculated by using the formulas of the dynamical theory of diffraction, provided the contribution of Compton scattering  $\mu_C^*$  is included in the effective absorption coefficient  $\mu^*$ .  $\mu_C^*$  is a considerable fraction of  $\mu^*$  (from 23 to 55 per cent) for the two wavelengths and temperatures used in the present work. The experimental values of  $\mu_C^*$  agree well with those calculated by using the theory of the Compton contribution to the dynamical absorption coefficient of X-rays. A simple formula which is a good approximation of the rigorous expression of  $\mu_C^*$  is also given. The Debye temperature  $\Theta$  of Si was derived from the experimental dependence of the intensities on crystal thickness for the  $\{220\}$  reflection at room and liquid nitrogen temperatures by using  $\text{CuK}\alpha$  radiation. It was found that  $\Theta = 521 \pm 5$  and  $543 \pm 5$  °K at 295 and 77 °K, respectively, in agreement with the results of other authors.

### I. Introduction

In a previous study measurements of X-ray intensities diffracted in anomalous transmission (Borrmann effect) through nearly perfect crystals of Cu were found to be in good agreement with the intensity values calculated by means of the dynamical theory of diffraction<sup>1</sup>. The diffracted intensities in anomalous transmission depend greatly on the effective absorption coefficient  $\mu^*$ , that is, on the difference between the average and the dynamical absorption coefficients. Therefore, as Prof. Borrmann suggested many years ago<sup>2</sup>, it is important to evaluate the contributions of the various X-ray scattering processes to  $\mu^*$ . In the case of Cu crystals only the photoelectric effect contributes significantly to absorption at the X-ray wavelengths used in diffraction. However, this fact is not generally valid: the relative importance of the Compton scattering contribution to the absorption of X-rays increases with a decrease in the atomic number or the wavelength

of X-rays. Experiments on the anomalous transmission of  $\text{MoK}\alpha$  radiation ( $\lambda = 0.711$  Å) through nearly perfect crystals of silicon have shown that there is a discrepancy between experimental and calculated values of the diffracted intensities when only photoelectric absorption is included in the formulas of the dynamical diffraction theory. The measured intensities, diffracted at room temperature by the  $\{220\}$  planes of a thick Si crystal ( $\mu_0 t \approx 50$ ), were about half the calculated ones<sup>3</sup>. Although the photoelectric effect accounted for more than 96% of the total average absorption coefficient, it was suggested that the origin of the discrepancy be in the neglect of the Compton scattering contribution to  $\mu^*$ . In fact, the contribution of photoelectric absorption to the static part of the dynamical absorption coefficient is nearly independent from the scattering angle, the K-shell electrons being responsible for most of the absorption. The Compton contribution instead, should rapidly decrease with the scattering angle because the outside electrons of the atom are responsible for a great part of the Compton scattering.