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A note on the problem of scattering from a single atomic plane and a stack of planes. Differences between the Ewald and other diffraction theories

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The scattering of a scalar plane wave (neutrons) from a single atomic plane consisting of any two-dimensional lattice with a basis is studied using the Ewald dynamical theory of diffraction. Formulae for the reflection and transmission coefficients obtained by evaluating the optical plane lattice sums are valid for general geometries, including nonsymmetrical and noncoplanar diffractions. The approach adopted is different from and more general than that by Yashiro & Takahashi [*Acta Cryst.* (2000), A**56**, 1663–167]. The structure factor yielded by this procedure differs from that used in the kinematical or Laue dynamical diffraction theories.

1. Introduction

Today's sophisticated experimental equipment enables the study of the atomic structures of crystal surfaces. Thus, the problem of radiation scattering on a single atomic plane has become important. In particular, the study of the intensity of scattered radiation far from Bragg peaks (crystal truncation rod scattering) (Robinson, 1986) has awoken the interest of some authors (Caticha, 1994; Nakatani & Takahashi, 1994; Takahashi & Nakatani, 1995; Yashiro & Takahashi, 2000) in Darwin's papers (Darwin, 1914), which were the first work in the field of the dynamical diffraction theory.

The crucial point of the Darwin theory is to find the reflection and transmission coefficients of a single atomic plane. To evaluate them, it is necessary to sum the waves emitted by the atomic oscillators forced by the incoming external wave, the interactions among the oscillators not being considered. In the Darwin theory, the sum at a distant point is calculated by using the phase differences of the waves emitted by different scatterers in the atomic plane.

The original Darwin theory concerned symmetrical Bragg reflection. Later, his method was generalized to nonsymmetrical reflection (Warren, 1990) and, in the recent paper by Yashiro & Takahashi (2000), nearly 90 years after Darwin, to noncoplanar reflection or transmission. Another procedure, used for the coplanar case, in which the plane is divided into Fresnel zones can be found in James (1950) and Borie (1967).

In the present paper, we study the interaction of the radiation with a single atomic plane in the framework of the exact dynamical diffraction theory based on the discrete model of the crystal developed in our former papers (Litzman, 1980, 1986). This approach leads to the evaluation of the optical plane lattice sums defined in Appendix *A*.

The paper is structured as follows. In §2, we apply this method to the reflection and transmission of neutrons by a single plane, Ewald's dipole model being addressed briefly. Results obtained are valid for general scattering geometry. §3 is devoted to comparison of our results with those of the kinematical theory by Yashiro & Takahashi (2000) and of the dynamical theory by Laue (see *e.g.* Rauch & Petraschek, 1978). In particular, the new form of the structure factor yielded by our theory is analyzed. In §4, the basic ideas of how to handle the problem of scattering by a stack of planes are outlined.

2. Reflection and transmission by a plane lattice

We shall study the reflection and transmission of a plane wave

$$f(r) = A\exp(i\mathbf{kr}), \quad \mathbf{k} = \mathbf{k}^{\parallel} + \mathbf{e}_3 k_z, \quad k_z > 0, \tag{1}$$

by a system of scatterers forming an ideal plane crystal lattice with a basis formed by s atoms, fixed at points

$$\mathbf{R}^{\mu}_{\mathbf{m}} = m_1\mathbf{a}_1 + m_2\mathbf{a}_2 + \mathbf{r}_{\mu}, \tag{2}$$

where $m_1, m_2 = 0, \pm1, \pm2, \ldots, \pm\infty$, $\mu = 1, 2, 3, \ldots, s$, with $\mathbf{r}_{\mu}$ lying in the $(\mathbf{a}_1\mathbf{a}_2)$ plane.

Owing to the translation symmetry of the problem, the components of the wave vectors of the reflected and transmitted waves parallel to the plane lattice are of the form

$$\mathbf{k}^{\parallel}_{pq} = \mathbf{k}^{\parallel} + p\mathbf{b}_1 + q\mathbf{b}_2.$$

Here p, q are arbitrary integers and $\mathbf{b}_1$, $\mathbf{b}_2$ are vectors of the two-dimensional reciprocal lattice, *i.e.* $\mathbf{b}_i\mathbf{a}_j = 2\pi\delta_{ij}$, $i, j = 1, 2$. Further, $\mathbf{c}^{\parallel}$ and $\mathbf{c}^{\perp}$ denote the components of the vector

$\mathbf{c} = \mathbf{c}^{\parallel} + \mathbf{c}^{\perp}$ parallel and perpendicular to the plane lattice, respectively.

The wave vectors $\mathbf{K}^{-}_{pq}(\mathbf{k})$ and $\mathbf{K}^{+}_{pq}(\mathbf{k})$ of the reflected and transmitted waves, respectively, are

$$\mathbf{K}^{\pm}_{pq} = \mathbf{k}^{\parallel}_{pq} \pm \mathbf{e}_3 K_{pqz}. \tag{3}$$

Considering merely elastic scattering processes, $|\mathbf{K}^{\mp}_{pq}(\mathbf{k})| = k$ must hold, so that

$$K_{pqz}(\mathbf{k}) = +[k^2 - (\mathbf{k}^{\parallel}_{pq})^2]^{1/2}. \tag{4}$$

Let us consider the diffraction of particles (neutrons) in a system of point scatterers. The Ewald dynamical (self-consistent) theory of diffraction leads to the following system of algebraic equations (Sears, 1989; Dederichs, 1972):

$$\Psi(\mathbf{r}) = A\exp(i\mathbf{kr}) - \sum_{\mathbf{n},\nu} Q_\nu \frac{\exp(ik|\mathbf{r} - \mathbf{R}^\nu_{\mathbf{n}}|)}{|\mathbf{r} - \mathbf{R}^\nu_{\mathbf{n}}|}\varphi^{\mathbf{n}}_\nu(\mathbf{R}^\nu_{\mathbf{n}}), \tag{5}$$

$$\varphi^{\mathbf{m}}_\mu(\mathbf{R}^\mu_{\mathbf{m}}) = A\exp(i\mathbf{kR}^\mu_{\mathbf{m}}) - {\sum_{(\mathbf{n},\nu)\neq(\mathbf{m},\mu)}}' Q_\nu \frac{\exp(ik|\mathbf{R}^\mu_{\mathbf{m}} - \mathbf{R}^\nu_{\mathbf{n}}|)}{|\mathbf{R}^\mu_{\mathbf{m}} - \mathbf{R}^\nu_{\mathbf{n}}|}\varphi^{\mathbf{n}}_\nu(\mathbf{R}^\nu_{\mathbf{n}}). \tag{6}$$

The total field $\Psi(\mathbf{r})$ is the superposition of the incident wave $A\exp(i\mathbf{kr})$ and of the spherical waves generated by all scatterers in the atomic plane. The scattering amplitude of the $(\mathbf{n}\nu)$th atom is $Q_\nu\varphi^{\mathbf{n}}_\nu(\mathbf{R}^\nu_{\mathbf{n}})$, where $\varphi^{\mathbf{n}}_\nu(\mathbf{R}^\nu_{\mathbf{n}})$ is the effective field incident on the point-like scatterer located at $\mathbf{R}^\nu_{\mathbf{n}}$ and Q_ν is the scattering length of the νth atom, $Q_\nu = Q^0_\nu/(1 + ikQ^0_\nu)$. Note that $\operatorname{Im} Q^0_\nu \to 0^-$ when the absorption is missing.

The solution of the Ewald equations proceeds as follows: First we evaluate $\varphi^{\mathbf{n}}_\nu(\mathbf{R}^\nu_{\mathbf{m}})$ from (6) and then perform the summation in (5).

Owing to the translational symmetry, we may put

$$\varphi^{\mathbf{n}}(\mathbf{R}^\nu_{\mathbf{n}}) = A\exp[i\mathbf{k}^{\parallel}(n_1\mathbf{a}_1 + n_2\mathbf{a}_2)]\exp(i\mathbf{k}^{\parallel}\mathbf{r}_\nu)w_\nu. \tag{7}$$

After inserting (7) into (6), we obtain for the amplitudes w_μ a nonhomogeneous system of algebraic equations:

$$\begin{aligned} w_\mu = 1 &- {\sum_{\substack{n_1,n_2\\-\infty}}^{+\infty}}{\sum_{\substack{\nu=1\\\nu\neq\mu}}^{s}}' Q_\nu \frac{\exp(ik|n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + \mathbf{r}_\nu - \mathbf{r}_\mu|)}{|n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + \mathbf{r}_\nu - \mathbf{r}_\mu|} \\ &\times \exp[i\mathbf{k}^{\parallel}(n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + \mathbf{r}_\nu - \mathbf{r}_\mu)]w_\nu \\ &- {\sum_{\substack{n_1,n_2\\(n_1,n_2)\neq(0,0)\\-\infty}}^{+\infty}} Q_\mu \frac{\exp(ik|n_1\mathbf{a}_1 + n_2\mathbf{a}_2|)}{|n_1\mathbf{a}_1 + n_2\mathbf{a}_2|} \\ &\times \exp[i\mathbf{k}^{\parallel}(n_1\mathbf{a}_1 + n_2\mathbf{a}_2)]w_\mu. \end{aligned} \tag{8}$$

Using the notation for the above lattice sums introduced in (18) and (19) of Appendix A, (8) reads

$$\begin{aligned} w_\mu = 1 &- \sum_{\nu\neq\mu} Q_\nu S(\mathbf{k}, \mathbf{0}, \mathbf{r}_\nu - \mathbf{r}_\mu)\exp[i\mathbf{k}^{\parallel}(\mathbf{r}_\nu - \mathbf{r}_\mu)]w_\nu \\ &- Q_\mu S'(\mathbf{k})w_\mu, \qquad \mu, \nu = 1, 2, \ldots, s. \end{aligned} \tag{9}$$

The solution of (9) for a single case with $s = 2$ is given in Appendix B.

Further, we insert (7) into (5). Then,

$$\begin{aligned} \Psi(\mathbf{r}) &= A\exp(i\mathbf{kr}) \\ &\quad - A{\sum_{\substack{n_1,n_2\\-\infty}}^{+\infty}}\sum_{\nu=1}^{s} Q_\nu \frac{\exp(ik|n_1\mathbf{a}_1 + n_2\mathbf{a}_2 - \mathbf{r}^{\parallel} - \mathbf{r}^{\perp} + \mathbf{r}_\nu|)}{|n_1\mathbf{a}_1 + n_2\mathbf{a}_2 - \mathbf{r}^{\parallel} - \mathbf{r}^{\perp} + \mathbf{r}_\nu|} \\ &\quad \times \exp[i\mathbf{k}^{\parallel}(n_1\mathbf{a}_1 + n_2\mathbf{a}_2 - \mathbf{r}^{\parallel})]w_\nu\exp[i\mathbf{k}^{\parallel}(\mathbf{r}^{\parallel} + \mathbf{r}_\nu)] \\ &= A\exp(i\mathbf{kr}) \\ &\quad - A\sum_{\nu} Q_\nu w_\nu \exp[i\mathbf{k}^{\parallel}(\mathbf{r}^{\parallel} + \mathbf{r}_\nu)]S(\mathbf{k}, \mathbf{r}^{\parallel}, \mathbf{r}_\nu - \mathbf{r}^{\perp}). \end{aligned} \tag{10}$$

The crucial point of the above procedure is the evaluation of the optical plane lattice sums over (n_1, n_2) in (8) and (10). How to evaluate them is shown in Appendix A. Expressing the lattice sum $S(\mathbf{k}, \mathbf{r}^{\parallel}, \mathbf{r}_\nu - \mathbf{r}^{\perp})$ in (10) by means of (20), we get the reflected and transmitted fields in the form

$$\begin{aligned} \Psi(\mathbf{r}) = A\exp(i\mathbf{kr}) &- \frac{2\pi iA}{|\mathbf{a}_1 \times \mathbf{a}_2|}\sum_{p,q}\sum_{\nu} Q_\nu w_\nu \exp[-i\mathbf{r}_\nu(p\mathbf{b}_1 + q\mathbf{b}_2)] \\ &\times \frac{1}{K_{pqz}}\begin{cases} \exp(i\mathbf{K}^{+}_{pq}\mathbf{r}) \text{ for } z > 0 \\ \exp(i\mathbf{K}^{-}_{pq}\mathbf{r}) \text{ for } z < 0. \end{cases} \end{aligned} \tag{11}$$

Here,

$$\mathbf{r}_\nu(p\mathbf{b}_1 + q\mathbf{b}_2) = \mathbf{r}_\nu(\mathbf{K}^{\pm}_{pq} - \mathbf{k})$$

since $\mathbf{K}^{\pm}_{pq} = \mathbf{k}^{\parallel} + p\mathbf{b}_1 + q\mathbf{b}_2 \pm \mathbf{e}_3 K_{pqz}$ and $\mathbf{r}_\nu\mathbf{e}_3 = 0$.

The amplitudes w_μ are given by the nonhomogeneous system of algebraic equations (9). The wavevectors $\mathbf{K}^{+}_{pq}$ and $\mathbf{K}^{-}_{pq}$ in (11) are given by (3), their z components being determined by (4). From (4), it can be seen that there is a finite number (depending on the wavevector of the incident radiation, $\mathbf{k}$) of reflected and transmitted waves with real $K_{pqz}(\mathbf{k})$, and an infinite number of nonradiative (evanescent) waves with pure imaginary $K_{pqz}(\mathbf{k})$.

In the simple case of the lattice with a trivial basis ($s = 1$), (9) yields $w = 1/[1 + QS'(\mathbf{k}^{\parallel})]$ and then the total field (11) reads

$$\begin{aligned} \Psi(\mathbf{r}) = A\exp(i\mathbf{kr}) &- \frac{2\pi i}{|\mathbf{a}_1 \times \mathbf{a}_2|}AQ\frac{1}{1 + QS'(\mathbf{k}^{\parallel})} \\ &\times \sum_{p,q}\frac{1}{K_{pqz}}\begin{cases} \exp(i\mathbf{K}^{+}_{pq}\mathbf{r}) \text{ for } z > 0 \\ \exp(i\mathbf{K}^{-}_{pq}\mathbf{r}) \text{ for } z < 0. \end{cases} \end{aligned}$$

Let us mention at this point the relation between the dynamical and kinematical approaches. In the kinematical approximation, interactions among the scatterers are neglected. Thus, the second term on the right-hand side of dynamical equation (6) is missing and then (5) reads

$$\Psi^{\text{kin}} = A\exp(i\mathbf{k}r) - A\sum_{\mathbf{n},\mu} Q_\mu \frac{\exp(ik|\mathbf{r} - \mathbf{R}^\mu_{\mathbf{n}}|)}{|\mathbf{r} - \mathbf{R}^\mu_{\mathbf{n}}|}\exp(i\mathbf{kR}^\mu_{\mathbf{n}}). \tag{12}$$

In this expression, we recognize the sum of spherical waves generated by all atoms in the plane which is treated by using the phase-difference method in the Darwin theory (Darwin, 1914; Warren, 1990; Yashiro & Takahashi, 2000). Using for the sum in (12) again the result derived in Appendix A, we obtain

$$\Psi^{\rm kin} = A\exp(i\mathbf{kr}) - \frac{2\pi i}{|\mathbf{a}_1\times\mathbf{a}_2|}A\sum_{\substack{p,q\\ \nu}} Q_\nu \exp[-i\mathbf{r}_\nu(p\mathbf{b}_1+q\mathbf{b}_2)] \times \frac{1}{K_{pqz}}\begin{cases}\exp(i\mathbf{K}^+_{pq}\mathbf{r}) \text{ for } z>0\\ \exp(i\mathbf{K}^-_{pq}\mathbf{r}) \text{ for } z<0.\end{cases} \quad (13)$$

Formula (13) was derived exactly for point-like scatterers. If we consider the field at a distant point from the plane, it is possible to replace the scattering length Q_ν by a factor $Q_\nu f_\nu(\mathbf{K}^\pm_{pq}-\mathbf{k})$ taking into account the inner structure of non-point-like scatterers.

We have dealt with the reflection and transmission of neutrons since in this case the lattice may be considered as a system of point-like scatterers. To describe the interaction of electromagnetic radiation with an atomic plane in the frame of the Darwin theory, the plane is considered to be a system of classical dipoles. The dipoles generate the radiation, which is given in papers by Darwin (1914), James (1950), Warren (1990) and Yashiro & Takahashi (2000) by the formula $r_e f(\theta)\exp(-ikr)/r$, valid in the region far from a dipole. In the dynamical theory, it is necessary to consider the interaction of an atom with near neighbors in a plane, thus the above-mentioned formula is not adequate. To render this interaction, it is convenient to use the Ewald dipole model of a crystal where the wave generated by a dipole is expressed by the Hertz vector (Ewald, 1916*a*,*b*). The Ewald discrete dipole model of the crystal was studied in our previous papers (Litzman & Rózsa, 1977; Litzman, 1978, 1980).

3. Comparison with Darwin theory. Are the forbidden reflections allowed?

Using the 'method of phase differences', Yashiro & Takahashi (2000) obtained for the amplitude of the scattered wave from an atomic plane, in the kinematical approximation, the expression [see formulae (10), (14) and (21) in Yashiro & Takahashi (2000)]

$$E = -iqE_0\exp[2\pi ik(-ct+r)]$$

with

$$q = -CMr_e f\lambda/\sin\theta_H, \quad M = 1/|\mathbf{a}_1\times\mathbf{a}_2|. \quad (14)$$

Here f is the atomic scattering factor, C the polarization factor, r_e the classical electron radius, $k=1/\lambda$ and θ_H the angle between the crystal surface and the wavevector of the scattered wave.

The coefficient q should be compared to the corresponding term in the amplitude of the scattered wave in formula (13) derived by using the kinematical approximation, *i.e.* with the expression (for a lattice with a trivial basis)

$$-\frac{2\pi}{|\mathbf{a}_1\times\mathbf{a}_2|}\frac{Q}{K_{pqz}}. \quad (15)$$

Using our notation, where $K=2\pi/\lambda$ and $K_{pqz}=K\sin\theta_H$, and neglecting the polarization factor C, which is missing in our model, we can see the coincidence of the two results in the frame of the kinematical theory.

For a lattice with basis, the scattering length Q should be replaced in the kinematical theory by the structure factor [see (13)]

$$\sum_\nu Q_\nu\exp[-i\mathbf{r}_\nu(p\mathbf{b}_1+q\mathbf{b}_2)]. \quad (16)$$

On the other hand, in the dynamical theory, the structure factor (16) is replaced by a more complicated expression [see (11)]:

$$\sum_\nu Q_\nu w_\nu\exp[-i\mathbf{r}_\nu(p\mathbf{b}_1+q\mathbf{b}_2)]. \quad (17)$$

Here, w_ν are the solutions of the algebraic equations (9) and thus they depend on Q_μ and $\mathbf{r}_\mu$ for all $\mu=1,2,\ldots,s$ (see also Appendix *B*). It follows that in our dynamical theory some diffractions forbidden according to (16) may be allowed. Nevertheless, as Q_ν are of order 10^{-15} m and the lattice sums of order $1/a$ (a being the lattice parameter of order 10^{-10} m), we can see from (9) that $w_\nu = 1+O(Q/a)$. Thus, the dynamical corrections yielded by (17) to the kinematical value (16) are very small.

Finally, let us note that in the dynamical theory of diffraction by von Laue the crystal is characterized by the Fourier transform of the potential, *i.e.* by $(1/\Omega)\int V(\mathbf{r})\exp(-i\mathbf{Gr})\,\mathrm{d}\mathbf{r}$ (Rauch & Petraschek, 1978), which for neutron diffraction leads to the kinematical structure factor of the form (16).

4. The scattering from a stack of planes

After evaluating the transmission and reflection of a single plane, the problem of reflection and transmission of a stack of planes in Darwin's procedure (Darwin, 1914) is similar to that in thin-film optics. It leads to a nonhomogeneous system of algebraic equations. In the two-beam approximation, the matrix of this system is a tridiagonal matrix and the properties of these matrices and the determinants of these matrices (continuants) can be utilized (Dub & Litzman, 1999).

But another more consistent approach may be followed, which is based on the solution of Ewald's equations (5) and (6) for a slab. However, in this case, it is necessary to solve the dispersion relation yielding the perpendicular components of the wave vectors inside the crystal.

In our paper (Litzman, 1986), we found the structure of the solution of Ewald equations (5) and (6) for a slab formed by a lattice with basis, where

$$\mathbf{R}^\mu_{\mathbf{n}} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 + \mathbf{r}_\mu,$$

with $n_1, n_2 = 0, \pm1, \ldots, \pm\infty, n_3 = 0, 1, 2, \ldots, N$. The general formulae derived for both the coplanar or noncoplanar multiwave transmission or reflection near or far from the Bragg or Laue diffraction positions have a transparent algebraic form suitable for analytical or numerical approximations. Note that the expressions

$$\alpha^\pm(j) = \sum_\nu Q_\nu\exp[-i\mathbf{r}_\nu(p\mathbf{b}_1+q\mathbf{b}_2\pm\mathbf{e}_3K_{pqz})]u_\nu(\psi_j)$$

(depending on the solutions ψ_j of the dispersion equation), which appeared in the above paper by Litzman (1986), could

be considered as the generalized structure factors analogous to (17).

5. Summary

We have shown that the formulae for scattering of a plane wave from an atomic plane can be effectively obtained for both coplanar and noncoplanar cases as a simple application of the optical plane lattice sums. Our theory taking into account the interaction of the scatterers yields a structure factor different from that used in the kinematical or in Laue's dynamical diffraction theories and thus it may allow some forbidden reflections.

APPENDIX *A*
The evaluation of two-dimensional lattice sums

To describe the interaction of radiation with layered structures in the frame of the discrete model of a crystal, we have to evaluate two-dimensional lattice sums of two kinds:

$$S(\mathbf{k}, \mathbf{R}^{\parallel}, \mathbf{u}) = \sum_{\substack{n_1,n_2\\-\infty}}^{+\infty} \frac{\exp(ik|n_1\mathbf{a}_1 + n_2\mathbf{a}_2 - \mathbf{R}^{\parallel} + \mathbf{u}|)}{|n_1\mathbf{a}_1 + n_2\mathbf{a}_2 - \mathbf{R}^{\parallel} + \mathbf{u}|} \times \exp[i\mathbf{k}^{\parallel}(n_1\mathbf{a}_1 + n_2\mathbf{a}_2 - \mathbf{R}^{\parallel})], \quad (18)$$

$$S'(\mathbf{k}) = {\sum_{\substack{n_1,n_2\\(n_1,n_2)\neq(0,0)\\-\infty}}^{+\infty}}' \frac{\exp(ik|n_1\mathbf{a}_1 + n_2\mathbf{a}_2|)}{|n_1\mathbf{a}_1 + n_2\mathbf{a}_2|} \times \exp[i\mathbf{k}^{\parallel}(n_1\mathbf{a}_1 + n_2\mathbf{a}_2)]. \quad (19)$$

The main difference between (18) and (19) is that in (19) the term with $(n_1, n_2) = (0, 0)$, describing the interaction of the atom with its own secondary field, is excluded from the summation. Both sums converge slowly. But because (18) is a periodic function of $\mathbf{R}^{\parallel}$, it can be transformed into a sum over the reciprocal lattice, which, as we shall see, converges rapidly. Standard Fourier procedure yields

$$S(\mathbf{k}, \mathbf{R}^{\parallel}, \mathbf{u}) = \sum_{p,q} f(p, q) \exp[i(p\mathbf{b}_1 + q\mathbf{b}_2)\mathbf{R}^{\parallel}],$$

where

$$f(p, q) = \frac{1}{|\mathbf{a}_1 \times \mathbf{a}_2|} \iint_{-\infty}^{+\infty} \frac{\exp(ik|\mathbf{R}^{\parallel} - \mathbf{u}|)}{|\mathbf{R}^{\parallel} - \mathbf{u}|} \exp(-i\mathbf{k}_{pq}^{\parallel}\mathbf{R}^{\parallel})\, \mathrm{d}\mathbf{R}^{\parallel}.$$

This integral may be evaluated easily by using the Weyl representation of the diverging spherical wave (Mandel & Wolf, 1995)

$$\exp(ik\rho)/\rho = \frac{i}{2\pi} \iint_{-\infty}^{+\infty} \nu^{-1} \exp[i(u\xi + v\eta + \nu|\mu|)]\, \mathrm{d}u\, \mathrm{d}v,$$

where $\overline{\rho} = (\xi, \eta, \mu)$ and $\nu = +(k^2 - u^2 - v^2)^{1/2}$. Then, we get

$$f(p, q) = \frac{2\pi i}{|\mathbf{a}_1 \times \mathbf{a}_2|} \exp(-i\mathbf{u}^{\parallel}\mathbf{k}_{pq}^{\parallel}) \frac{\exp(i|u_z|K_{pqz})}{K_{pqz}}$$

and finally

$$S(\mathbf{k}, \mathbf{R}^{\parallel}, \mathbf{u}) = \frac{2\pi i}{|\mathbf{a}_1 \times \mathbf{a}_2|} \sum_{p,q} \exp(-i\mathbf{u}^{\parallel}\mathbf{k}_{pq}^{\parallel}) \times \frac{\exp(i|u_z|K_{pqz})}{K_{pqz}} \exp[i(p\mathbf{b}_1 + q\mathbf{b}_2)\mathbf{R}^{\parallel}]. \quad (20)$$

The evaluation of the sum (19) is much more difficult. Using the Ewald procedure (Ewald, 1932), we transformed (19) into the sum of two rapidly convergent sums, one over the direct lattice and the other over the reciprocal one (Dub & Litzman, 1983; Litzman, 1986). Note that

$$\mathrm{Im}\, S'(\mathbf{k}) = \frac{2\pi}{|\mathbf{a}_1 \times \mathbf{a}_2|} \sum_{\substack{p,q\\K_{pqz}^2>0}} \frac{1}{K_{pqz}} - k. \quad (21)$$

Looking for an approximate value of the sum (19), we can write (Dub *et al.*, 1996)

$$S'(\mathbf{k}) = \frac{1}{a^2} \int_a^{\infty} \int_0^{2\pi} \exp(ikr) \exp(ik^{\parallel} r \cos\varphi)\, \mathrm{d}\varphi\, \mathrm{d}r = \frac{2\pi}{a^2} \int_a^{\infty} \exp(ikr) J_0(k^{\parallel} r)\, \mathrm{d}r.$$

As $\int_0^{\infty} \cos(kr) J_0(k^{\parallel} r)\, \mathrm{d}r = 0$ for $k^{\parallel} < k$, in the region where $ak \approx 1$, we can put $|\mathrm{Re}\, S(\mathbf{k}')| \approx 2\pi \sin(ak)/ka^2$.

APPENDIX *B*
Evaluation of amplitudes w_μ for μ = 1, 2

The system of equations (9) for $s = 2$ reads

$$\begin{aligned} w_1 &= 1 - a_{12}w_2 - a_{11}w_1 \\ w_2 &= 1 - a_{21}w_1 - a_{22}w_2, \end{aligned} \quad (22)$$

where

$$a_{\mu\mu} = Q_\mu S'(\mathbf{k})$$
$$a_{\mu\nu} = Q_\nu \alpha_{\mu\nu}(\mathbf{k})$$

and

$$\alpha_{\mu\nu} = S(\mathbf{k}, \mathbf{O}, \mathbf{r}_\nu - \mathbf{r}_\mu) \exp[i\mathbf{k}^{\parallel}(\mathbf{r}_\nu - \mathbf{r}_\mu)],$$

whereby $\alpha_{\mu\nu} \neq \alpha_{\nu\mu}$.

From (22), it follows that

$$w_1 = \frac{Q_2(S' - \alpha_{12}) + 1}{\Delta},$$
$$w_2 = \frac{Q_1(S' - \alpha_{21}) + 1}{\Delta}$$

with

$$\Delta = 1 + (Q_1 + Q_2)S' + Q_1Q_2(S'^2 - \alpha_{12}\alpha_{21}).$$

Thus, generally $w_1 \neq w_2$. Moreover, since the lattice sums are of order $1/a$ (a being the lattice parameter of order 10^{-10} m) and scattering lengths Q_μ are of order 10^{-15} m, the amplitudes w_μ differ from 1 by terms of order 10^{-5}.

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