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Linearization of the Basic Equations of the Dynamical Theory of Electron Diffraction by Crystals

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Abstract

The dynamical theory based on the plane-wave expansion of Bloch waves is applied to problems of electron diffraction by reflection at crystal surfaces. It is mainly aimed at reflection high-energy electron diffraction (RHEED), but may be applied also to medium- and low-energy electron diffraction (MEED and LEED). It is shown that the theory leads to a quadratic matrix eigenvalue problem, which can be expanded into a linear matrix eigenvalue problem by applying two alternative standard methods of matrix theory, the Günther expansion and the diagonal expansion of Falk. These methods are shown to be equivalent to the expansions of the system of second-order ordinary differential equations, obtained by the two-dimensional Fourier expansion of the Schrödinger equation, into systems of first-order differential equations. The equivalence enables a physical interpretation of the quantities introduced in the matrix methods to be given.

1. Introduction

The dynamical theory of electron diffraction by crystals has been developed in two alternative ways. One originates from the theory (Bethe, 1928; Sommerfeld & Bethe, 1930) of low-energy electron diffraction (LEED) using the plane-wave expansion of Bloch waves inside the crystal. The other uses the layer-by-layer scheme, which has its origin in Darwin's (1914) theory of X-ray diffraction, and has found powerful extensions in the multi-slice method of Cowley & Moodie (1957) [see also Cowley (1981)] for high-energy electrons in the transmission case and in the mixed scheme using both plane waves and spherical waves in the LEED theory (Pendry, 1974).

Particularly in the case of reflection at crystal surfaces (RHEED, MEED, LEED) the layer-by-layer method can be seen to be the proper one, because the non-periodic variation of the potential in the normal direction at the surface can be naturally incorporated. Nevertheless, there are cases in which the development of the theory in Bethe's original form is necessary. This is true when we have to compare the results with those of corresponding transmission cases. An example is the recent findings of Lehmpfuhl & Dowell (1986) revealing a much closer parallelism of the many-beam diffraction effects between the transmission and reflection cases than would have been expected in view of their quite different geometries.

One of the main reasons for the success of the dynamical theory in the transmission case is that the forward-scattering approximation is valid. This is true for both the Bloch-wave theory and the multi-slice theory. For the Bloch-wave theory using the plane-wave expansion one arrives at a *linear* matrix eigenvalue problem in virtue of the forward-scattering approximation. In the reflection case, on the other hand, one arrives at a *quadratic* matrix eigenvalue problem, which needs special care in treatment.

In the recent book of Zurmühl & Falk (1984) the present author has encountered a method of linearization of matrix eigenvalue problems which has been newly developed by Falk (1984) and called by him the diagonal expansion method. The method proves to be quite suitable for our problem and to be closely connected to the well known two-dimensional Fourier expansion of the Schrödinger equation. The purpose of the present paper is to introduce the method in parallel to the usual one, which is called by Falk 'the Günther expansion', and to give a physical interpretation by means of comparison with the two-dimensional Fourier expansion.

2. Quadratic matrix eigenvalue problem

The usual dynamical theory in the form of plane-wave expansion is developed here along the lines of Lehmpfuhl & Molière (1961) and Lehmpfuhl & Reissland (1968) [*cf.* Kambe & Molière (1970)].

We write the incident wave in vacuum as

$$\psi_e(\mathbf{r}) = \exp(iK_0\mathbf{S}_e \cdot \mathbf{r}), \tag{2.1}$$

where K_0 is given by

$$K_0 = (2mE)^{1/2}/\hbar, \tag{2.2}$$

and $\mathbf{S}_e$ is the unit vector in the direction of progagation. The wave function inside the crystal is written as

$$\psi(\mathbf{r}) = \sum_g \psi_g \exp(iK_0\mathbf{S}_g \cdot \mathbf{r}), \tag{2.3}$$

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where g represents the triple index g_1, g_2, g_3,

$$\mathbf{S}_g = \mathbf{S}_0 + \mathbf{B}_g, \tag{2.4}$$

and

$$\mathbf{B}_g = 2\pi\mathbf{g}/K_0, \tag{2.5}$$

$\mathbf{g}$ being the reciprocal-lattice vector. We specify the choice of $\mathbf{S}_0$ by requiring its tangential component to be equal to that of $\mathbf{S}_e$ (see Fig. 1), and put

$$\mathbf{S}_0 = \mathbf{S}_e + \tau\mathbf{N}_e, \tag{2.6}$$

where $\mathbf{N}_e$ is the unit vector representing the inward normal of the surface.

Substituting (2.3) into the Schrödinger equation,

$$(\hbar^2/2m)\nabla^2\psi(\mathbf{r}) + [E - V(\mathbf{r})]\psi(\mathbf{r}) = 0, \tag{2.7}$$

we obtain the system of 'basic equations of the dynamical theory',

$$(1 + \varphi_0 - S_g^2)\psi_g + \sum_{h \neq g} \varphi_{g-h}\psi_h = 0, \tag{2.8}$$

where the φ_g's are defined by the Fourier expansion of the periodic potential divided by E,

$$-V(\mathbf{r})/E = \sum_g \varphi_g \exp(iK_0\mathbf{B}_g \cdot \mathbf{r}), \tag{2.9}$$

φ_0 being the constant term. We put

$$\rho_g = (1 - |\mathbf{S}_e + \mathbf{B}_g|^2)/2 \tag{2.10}$$

and get the coefficient of ψ_g in (2.8) in the form

$$1 + \varphi_0 - \mathbf{S}_g^2 = \varphi_0 + 2\rho_g - 2\beta_{ge}\tau - \tau^2 \equiv D_g(\tau), \tag{2.11}$$

where

$$\beta_{ge} = (\mathbf{S}_e + \mathbf{B}_g) \cdot \mathbf{N}_e. \tag{2.12}$$

In the case of transmission problems β_{ge} is much larger than ρ_g and φ_g, so that we can neglect τ^2 in (2.11) from the beginning. This leads to a linear eigenvalue problem for τ. For reflection problems β_{ge} can become small or even vanish, so that the term τ^2 cannot be neglected. It is then convenient to put

$$\gamma_g^2 = \varphi_0 + 2\rho_g + \beta_{ge}^2 \tag{2.13}$$

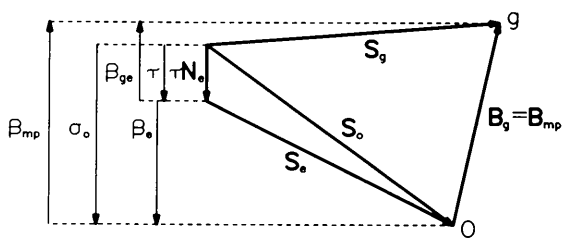

Fig. 1. Geometry of wave vectors and their normal components indicated on the left. Note that β_{ge}, τ and σ_0 are in reality complex numbers.

and write (2.11) as

$$D_g(\tau) = \gamma_g^2 - (\beta_{ge} + \tau)^2. \tag{2.14}$$

The system (2.8) is written in the matrix form

$$\begin{pmatrix} \vdots & \vdots & \vdots & \\ \cdots\ D_0(\tau) & \varphi_{-g} & \varphi_{-h} & \cdots \\ \cdots\ \varphi_g & D_g(\tau) & \varphi_{g-h} & \cdots \\ \cdots\ \varphi_h & \varphi_{h-g} & D_h(\tau) & \cdots \\ & \vdots & \vdots & \end{pmatrix} \begin{pmatrix} \vdots \\ \psi_0 \\ \psi_g \\ \psi_h \\ \vdots \end{pmatrix} = 0, \tag{2.15}$$

representing a quadratic matrix eigenvalue problem.

In the context of reflection problems (Colella, 1972; Moon, 1972) it is important to recognize the particular structure of the matrix of (2.15). For this purpose the reflection indices g are decomposed into m, indices of the reciprocal-lattice rods lying normal to the surface, and p, along one rod. We write $g = mp$. It can easily be seen from (2.10), (2.11) and (2.13) that γ_g depends only on the rod index m, that is,

$$\gamma_g = \gamma_m. \tag{2.16}$$

Geometrically (see Fig. 2) γ_m is the half of the segment of the surface normal going through $\mathbf{S}_e$ cut out by the sphere centred at the reciprocal-lattice point $g = mp$ with the radius $(1 + \varphi_0)^{1/2}$ (all measured in units of K_0), if φ_0 was real. [The sphere is the gth branch of the dispersion surface (Kambe & Molière, 1970) if all φ_g's vanish except φ_0.] Further we find from (2.12) that β_{ge} is given by

$$\beta_{ge} = \beta_{mp} + \beta_e, \tag{2.17}$$

where β_{mp} and β_e are the normal components of $\mathbf{B}_g = \mathbf{B}_{mp}$ and $\mathbf{S}_e$ (see Fig. 1). We write

$$\beta_{ge} + \tau = \beta_{mp} + \sigma_0, \tag{2.18}$$

where

$$\sigma_0 = \beta_e + \tau \tag{2.19}$$

is the normal component of $\mathbf{S}_0$ (see Fig. 1).

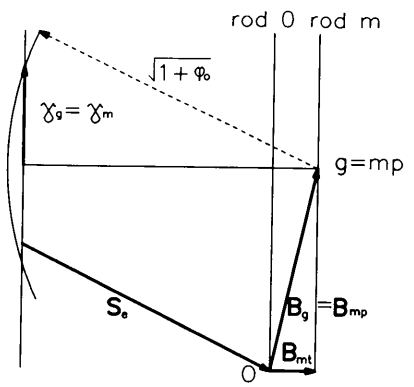

Fig. 2. Geometry of $\gamma_g = \gamma_m$ and $\mathbf{B}_{mt}$. Note that φ_0 and γ_g are in reality complex numbers.

The expression (2.14) becomes

$$D_g(\tau) = D_{mp}(\sigma_0) = \gamma_m^2 - (\beta_{mp} + \sigma_0)^2, \quad (2.20)$$

and the system (2.15) can be written

$$\begin{pmatrix} \vdots & \vdots & \\ \cdots\ D_{mp}(\sigma_0) & \varphi_{n-m,q-p} & \cdots \\ \cdots\ \varphi_{m-n,p-q} & D_{nq}(\sigma_0) & \cdots \\ & \vdots & \vdots \end{pmatrix} \begin{pmatrix} \vdots \\ \psi_{mp} \\ \psi_{np} \\ \vdots \end{pmatrix} = 0. \quad (2.21)$$

We find that a submatrix of (2.21) pertaining to one rod m is equivalent to the matrix, the determinant of which is known as Hill's determinant (Moon, 1972). The determinant of the matrix of (2.21) is called by Lamla (1938*a*, *b*) the generalized Hill's determinant and is shown to have only $2N_{\text{rod}}$ non-equivalent eigenvalues if we take into account N_{rod} rods. Naturally we are interested only in N_{rod} eigenvalues which lead to Bloch waves decaying *into* the crystal. Here we are not going further into the evaluation and selection of solutions.

3. Linearization methods

We go back to the form (2.15) mainly for brevity of the notation. The diagonal elements $D_g(\tau)$ are quadratic polynomials of τ given by (2.11) or (2.14). In order to have access to various standard treatments of linear eigenvalue problems it is convenient to transform (2.15) into an *exactly* equivalent linear form. Thus, the term linearization is used here not as a kind of approximation.

3.1. *Günther expansion*

The simplest form of linearization is to introduce new unknowns χ_g in the form

$$\chi_g = (\beta_{ge} + \tau)\psi_g. \quad (3.1)$$

Then the diagonal elements become

$$D_g(\tau)\psi_g = [\gamma_g^2 - (\beta_{ge} + \tau)^2]\psi_g = \gamma_g^2\psi_g - (\beta_{ge} + \tau)\chi_g. \quad (3.2)$$

Combining (3.1) with (2.15), into which (3.2) is substituted, we have the system

$$\begin{pmatrix} \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \\ \cdots\ -\beta_{0e}-\tau & 0 & 0 & \cdots & 1 & 0 & 0 & \cdots \\ \cdots\ 0 & -\beta_{ge}-\tau & 0 & \cdots & 0 & 1 & 0 & \cdots \\ \cdots\ 0 & 0 & -\beta_{he}-\tau & \cdots & 0 & 0 & 1 & \cdots \\ & \vdots & \vdots & & \vdots & \vdots & \vdots & \\ \cdots\ \gamma_0^2 & \varphi_{-g} & \varphi_{-h} & \cdots & -\beta_{0e}-\tau & 0 & 0 & \cdots \\ \cdots\ \varphi_g & \gamma_g^2 & \varphi_{g-h} & \cdots & 0 & -\beta_{ge}-\tau & 0 & \cdots \\ \cdots\ \varphi_h & \varphi_{h-g} & \gamma_h^2 & \cdots & 0 & 0 & -\beta_{he}-\tau & \cdots \\ & \vdots & \vdots & & \vdots & \vdots & \vdots & \end{pmatrix} \begin{pmatrix} \vdots \\ \psi_0 \\ \psi_g \\ \psi_h \\ \vdots \\ \chi_0 \\ \chi_g \\ \chi_h \\ \vdots \end{pmatrix} = 0. \quad (3.3)$$

This transformation from an $N \times N$ matrix to a $2N \times 2N$ matrix is called the Günther transformation (Zurmühl & Falk, 1984, p. 320). The physical interpretation of the χ_g's is given below.

3.2. *Diagonal expansion*

The method introduced by Falk (1984) (see Zurmühl & Falk 1984, p. 323) is adapted here to our problem without going into the details of derivation. The system (2.15) can be shown to be equivalent to

$$\begin{pmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \\ \cdots\ D_{01}(\tau) & 0 & \varphi_{-g} & \varphi_{-g} & \varphi_{-h} & \varphi_{-h} & \cdots \\ \cdots\ 0 & D_{02}(\tau) & \varphi_{-g} & \varphi_{-g} & \varphi_{-h} & \varphi_{-h} & \cdots \\ \cdots\ \varphi_g & \varphi_g & D_{g1}(\tau) & 0 & \varphi_{g-h} & \varphi_{g-h} & \cdots \\ \cdots\ \varphi_g & \varphi_g & 0 & D_{g2}(\tau) & \varphi_{g-h} & \varphi_{g-h} & \cdots \\ \cdots\ \varphi_h & \varphi_h & \varphi_{h-g} & \varphi_{h-g} & D_{h1}(\tau) & 0 & \cdots \\ \cdots\ \varphi_h & \varphi_h & \varphi_{h-g} & \varphi_{h-g} & 0 & D_{h2}(\tau) & \cdots \\ & \vdots & \vdots & \vdots & \vdots & \vdots & \end{pmatrix} \begin{pmatrix} \vdots \\ t_0 \\ r_0 \\ t_g \\ r_g \\ t_h \\ r_h \\ \vdots \end{pmatrix} = 0. \quad (3.4)$$

Each diagonal element $D_g(\tau)$ of (2.15) is replaced here by a 2×2 diagonal matrix with diagonal elements given by

$$D_{g1}(\tau) = (\tau_{g1} - \tau_{g2})(\tau_{g1} - \tau), \quad (3.5)$$

$$D_{g2}(\tau) = (\tau_{g2} - \tau_{g1})(\tau_{g2} - \tau), \quad (3.6)$$

where τ_{g1}, τ_{g2} are the roots of the quadratic equation

$$D_g(\tau) = 0. \quad (3.7)$$

The roots are assumed to be different from each other. In (3.4) each non-diagonal element φ_{g-h} of (2.15) is replaced by a 2×2 matrix having all its elements equal to φ_{g-h}. Each unknown ψ_g is replaced by two unknowns,

$$t_g = \frac{\tau_{g2} - \tau}{\tau_{g2} - \tau_{g1}}\psi_g, \quad (3.8)$$

$$r_g = \frac{\tau_{g1} - \tau}{\tau_{g1} - \tau_{g2}}\psi_g. \quad (3.9)$$

Obviously

$$\tau_g + r_g = \psi_g, \quad (3.10)$$

and

$$D_{g1}(\tau)t_g = D_g(\tau)\psi_g, \quad (3.11)$$

$$D_{g2}(\tau)r_g = D_g(\tau)\psi_g, \quad (3.12)$$

verifying that the gth *two* equations of (3.4) are both equivalent to the gth equation of (2.15). Conversely, (2.15) can be derived from (3.4), regarded as given, by constructing the difference and sum of the gth two equations,

$$D_{g1}(\tau)t_g - D_{g2}(\tau)r_g = 0, \quad (3.13)$$

$$D_{g1}(\tau)t_g + D_{g2}(\tau)r_g + 2\sum_{h \neq g}(\varphi_{g-h}t_h + \varphi_{g-h}r_h) = 0. \quad (3.14)$$

Equation (3.13) allows with (3.5) and (3.6) the introduction of ψ_g by (3.8) and (3.9), and their substitution into (3.14) leads to an equation exactly twice the gth equation of (2.15).

From our special form of $D_g(\tau)$ given by (2.14) we choose

$$\tau_{g1} = -\beta_{ge} + \gamma_g, \tag{3.15}$$

$$\tau_{g2} = -\beta_{ge} - \gamma_g. \tag{3.16}$$

Then

$$\begin{aligned} D_{g1}(\tau) &= 2\gamma_g(-\beta_{ge} + \gamma_g - \tau) \\ &= 2\gamma_m(\gamma_m - \beta_{mp} - \sigma_0), \end{aligned} \tag{3.17}$$

$$\begin{aligned} D_{g2}(\tau) &= -2\gamma_g(-\beta_{ge} - \gamma_g - \tau) \\ &= -2\gamma_m(-\gamma_m - \beta_{mp} - \sigma_0), \end{aligned} \tag{3.18}$$

where we have taken into account (2.16) and (2.18), and

$$t_g = \frac{-\beta_{ge} - \gamma_g - \tau}{2\gamma_g}\psi_g = \frac{-\gamma_m - \beta_{mp} - \sigma_0}{2\gamma_m}\psi_g, \tag{3.19}$$

$$r_g = \frac{-\beta_{ge} + \gamma_g - \tau}{-2\gamma_g}\psi_g = \frac{\gamma_m - \beta_{mp} - \sigma_0}{-2\gamma_m}\psi_g. \tag{3.20}$$

Putting again $g = mp$ we have from (3.4) the equivalent form

$$\begin{pmatrix} \vdots & \vdots & \vdots & \vdots & \\ \cdots\ 2\gamma_m(\gamma_m - \beta_{mp} - \sigma_0) & 0 & \varphi_{m-n,p-q} & \varphi_{m-n,p-q} & \cdots \\ \cdots\ 0 & -2\gamma_m(-\gamma_m - \beta_{mp} - \sigma_0) & \varphi_{m-n,p-q} & \varphi_{m-n,p-q} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix} \begin{pmatrix} \vdots \\ t_{mp} \\ r_{mp} \\ \vdots \end{pmatrix} = 0. \tag{3.21}$$

For the applicability of the method it is essential that the two roots of the quadratic equation (3.7) given by (3.15) and (3.16) be different from each other. This means

$$\gamma_g \neq 0 \tag{3.22}$$

for all g's. According to (2.13) this means

$$\varphi_0 + 2\rho_g + \beta_{ge}^2 \neq 0. \tag{3.23}$$

After (2.10) and (2.12) ρ_g and β_{ge} are always real. They may be, under the conditions of reflection, negative or vanish. The potential φ_0 is, however, a complex constant. The magnitude of the imaginary part of φ_0, representing the 'absorption' (Kambe & Molière, 1970), may be comparable to ρ_g or β_{ge}^2 and, therefore, should not be neglected even in the first approximation. This guarantees that the condition (3.23) is always satisfied.

It is to be noted that we have to deal with the diagonalization of a complex non-Hermitian matrix of (3.4) or (3.21). We obtain complex eigenvalues τ or σ_0, from which we are interested, as already mentioned, only in N_{rod} eigenvalues.

4. Two-dimensional Fourier expansion

It is known that the system of quadratic equations (2.8) is equivalent to the system of second-order ordinary differential equations, which are derived by Fourier expansion of the Schrödinger equation in the two dimensions parallel to the surface (e.g. Lamla, 1938*a*, *b*; Tournarie, 1962; Kambe, 1967; Lynch & Moodie, 1972; Maksym & Beeby, 1981; Ichimiya, 1983). The linearizations carried out above are shown here to be equivalent to the expansion of the system into a system of first-order differential equations.

The potential is expanded in the form

$$-V(\mathbf{r})/E = \sum_m \varphi_m(z) \exp(iK_0 \mathbf{B}_{mt} \cdot \mathbf{r}_t), \tag{4.1}$$

where z and $\mathbf{r}_t$ are the normal and tangential components of $\mathbf{r}$, m is again the rod index, $\mathbf{B}_{mt}$ is the vector in the reciprocal space (in units of K_0) directed from the origin perpendicular to the rod m (Fig. 2). The wave function is written as

$$\psi(\mathbf{r}) = \sum_m \psi_m(z) \exp[iK_0(\mathbf{S}_{0t} + \mathbf{B}_{mt}) \cdot \mathbf{r}_t], \tag{4.2}$$

where $\mathbf{S}_{0t}$ is the tangential component of $\mathbf{S}_0$ or $\mathbf{S}_e$ [*cf.* (2.6)]. Substituting (4.1) and (4.2) into (2.7) we obtain the system of second-order differential equations

$$\frac{1}{K_0^2}\frac{d^2}{dz^2}\psi_m(z) + \gamma_m^2\psi_m(z) + \sum_n{}' \varphi_{m-n}(z)\psi_n(z) = 0, \tag{4.3}$$

where

$$\gamma_m^2 = 1 + \varphi_0 - |\mathbf{S}_{0t} + \mathbf{B}_{mt}|^2. \tag{4.4}$$

The prime in the summation of (4.3) indicates that the term $\varphi_0\psi_m(z)$ is excluded. It can easily be seen that γ_m given by (4.4) is identical to γ_g given by (2.13). Various alternative ways may be conceived for expanding the system (4.3) into a system of first-order differential equations (Tournarie, 1962; Lynch & Moodie, 1972; Maksym & Beeby, 1981; Ichimiya, 1983). We present here two typical ones which are equivalent to the matrix expansions described above.

It is to be noted that the method using (4.3) can be regarded as one of the multi-slice methods. The finite small increments of z used in a numerical solution of (4.3) may be regarded as the slice thicknesses. The potential need not be periodic in the z direction. If, however, the potential is periodic, then the plane-wave expansion can be introduced and shown to lead to the same equations as (3.3) or (3.21).

4.1. *Equivalent method to the Günther expansion*

The most usual method, used by Tournarie (1962) and Lynch & Moodie (1972), is to introduce new functions

$$\chi_m(z) = (iK_0)^{-1}\, d\psi_m(z)/dz. \tag{4.5}$$

From (4.3) we have

$$-(iK_0)^{-1}\,\mathrm{d}\chi_m(z)/\mathrm{d}z+\gamma_m^2\psi_m(z)+\sum_n{}'\varphi_{m-n}(z)\psi_n(z)=0. \tag{4.6}$$

The system of first-order differential equations (4.5) and (4.6) replaces (4.3). We are interested here in the case of a periodic potential given by

$$\varphi_m(z)=\sum_p \varphi_{mp}\exp(iK_0\beta_{mp}z), \tag{4.7}$$

where β_{mp} is again the normal component of $\mathbf{B}_{mp}$ (*cf.* § 2). The functions $\psi_m(z)$, $\chi_m(z)$ are expanded in the form

$$\psi_m(z)=\sum_p \psi_{mp}\exp[iK_0(\beta_{mp}+\sigma_0)z], \tag{4.8}$$

$$\chi_m(z)=\sum_p \chi_{mp}\exp[iK_0(\beta_{mp}+\sigma_0)z], \tag{4.9}$$

where σ_0 is again the normal component of $\mathbf{S}_0$ (*cf.* § 2).

From (4.5) and (4.6) we have

$$\chi_{mp}=(\beta_{mp}+\sigma_0)\psi_{mp}, \tag{4.10}$$

$$-(\beta_{mp}+\sigma_0)\chi_{mp}+\gamma_m^2\psi_{mp}+\sum_{nq}{}'\varphi_{m-n,p-q}\psi_{nq}=0. \tag{4.11}$$

We find that (4.10) and (4.11) are identical to (3.3), taking into account (2.16) and (2.18).

4.2. *Equivalent method to the diagonal expansion*

A similar method used by Maksym & Beeby (1981) and Ichimiya (1983) is to introduce two functions, assuming that γ_m given by (4.4) does not vanish,

$$t_m(z)=\frac{1}{i2\gamma_m}\left[\frac{\mathrm{d}}{\mathrm{d}z}\psi_m(z)+i\gamma_m\psi_m(z)\right], \tag{4.12}$$

$$r_m(z)=-\frac{1}{i2\gamma_m}\left[\frac{\mathrm{d}}{\mathrm{d}z}\psi_m(z)-i\gamma_m\psi_m(z)\right], \tag{4.13}$$

and derive from (4.3)

$$2\gamma_m[\mathrm{d}t_m(z)/\mathrm{d}z-i\gamma_m t_m(z)]-i\sum_n \varphi_{m-n}(z)[t_m(z)+r_m(z)]=0, \tag{4.14}$$

$$-2\gamma_m[\mathrm{d}r_m(z)/\mathrm{d}z+i\gamma_m r_m(z)]-i\sum_n \varphi_{m-n}(z)[t_m(z)+r_m(z)]=0. \tag{4.15}$$

This is the system of first-order differential equations. In the case of the periodic potential (4.7) we put

$$t_m(z)=\sum_p t_{mp}\exp[iK_0(\beta_{mp}+\sigma_0)z], \tag{4.16}$$

$$r_m(z)=\sum_p r_{mp}\exp[iK_0(\beta_{mp}+\sigma_0)z], \tag{4.17}$$

and obtain from (4.14) and (4.15)

$$2\gamma_m(\gamma_m-\beta_{mp}-\sigma_0)t_{mp}+\sum_{nq}\varphi_{m-n,p-q}(t_{nq}+r_{nq})=0, \tag{4.18}$$

$$-2\gamma_m(-\gamma_m-\beta_{mp}-\sigma_0)r_{mp}+\sum_{nq}\varphi_{m-n,p-q}(t_{nq}+r_{nq})=0. \tag{4.19}$$

We find that these equations are identical to (3.21). We note again that the applicability of this method depends on the non-vanishing value of γ_m, just as discussed in § 3.2.

5. Discussion

The equivalence demonstrated above enables us to give a physical interpretation of the new variables introduced in the linearization of the matrix eigenvalue problem.

Thus, the equivalence between (3.3), (4.10) and (4.11) indicates that the quantities χ_g in § 3.1 are nothing but the expansion coefficients of the derivative of the wave function in the z direction.

The quantities t_{mp} and r_{mp} in § 3.2 can be interpreted as follows. From (4.3) we find immediately that if all φ_m's except φ_0 vanish the solution is given by

$$\psi_m(z)=t_m^{(0)}\exp(i\gamma_m z)+r_m^{(0)}\exp(-i\gamma_m z), \tag{5.1}$$

and the transformation of $\psi_m(z)$ to $t_m(z)$, $r_m(z)$ given by (4.12) and (4.13) leads to

$$t_m(z)=t_m^{(0)}, \tag{5.2}$$

$$r_m(z)=r_m^{(0)}. \tag{5.3}$$

We see that these are the amplitudes of the forward and backward propagating waves which constitute the wave function in the constant potential φ_0. This property is approximately maintained by $t_m(z)$ and $r_m(z)$ in the periodic potential if the potential modulation is not too large. The forward and backward waves are also periodically modulated, and t_{mp}, r_{mp} are their Fourier coefficients. In the layer-by-layer schemes in LEED or RHEED (Pendry, 1974; Pendry & Gard, 1975) these forward and backward waves are also explicitly used in the constant (muffin-tin zero) potential regions between the atomic layers. Obviously an equivalent form to the usual forward-scattering formulation of the transmission case can be obtained by neglecting the backward waves r_{mp} or $r_m(z)$.

In conclusion, the diagonal expansion of the quadratic matrix appears to be the proper way of applying the Bloch-wave theory in the plane-wave expansion form to the reflection case. It enables us rather naturally to find the relation to the transmission case as well as to other methods (multi-slice *etc.*) of treating the reflection case.

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References

BETHE, H. (1928). *Ann. Phys. (Leipzig)*, **87**, 55-129.
COLELLA, R. (1972). *Acta Cryst.* A**28**, 11-15.
COWLEY, J. M. (1981). *Diffraction Physics.* Amsterdam: North-Holland.
COWLEY, J. M. & MOODIE, A. F. (1957). *Acta Cryst.* **10**, 609-619.
DARWIN, C. G. (1914). *Philos. Mag.* **27**, 315-333, 675-690.
FALK, S. (1984). *Z. Angew. Math. Mech.* **64**, 445-456.
ICHIMIYA, A. (1983). *Jpn. J. Appl. Phys.* **22**, 176-180.
KAMBE, K. (1967). *Z. Naturforsch. Teil A*, **22**, 422-431.
KAMBE, K. & MOLIÈRE, K. (1970). In *Advances in Structure Research by Diffraction Methods*, Vol. 3, edited by R. BRILL & R. MASON, p. 53. Oxford: Pergamon Press.
LAMLA, E. (1938*a*). *Ann. Phys. (Leipzig)*, (5. *Folge*), **32**, 178-189, 225-241.
LAMLA, E. (1938*b*). *J. Rein. Angew. Math.* **179**, 134-142.
LEHMPFUHL, G. & DOWELL, W. C. T. (1986). *Acta Cryst.* A**42**, 569-577.
LEHMPFUHL, G. & MOLIÈRE, K. (1961). *Z. Phys.* **164**, 389-408.
LEHMPFUHL, G. & REISSLAND, A. (1968). *Z. Naturforsch. Teil A*, **23**, 544-549.
LYNCH, D. F. & MOODIE, A. F. (1972). *Surf. Sci.* **32**, 422-438.
MAKSYM, P. A. & BEEBY, J. L. (1981). *Surf. Sci.* **110**, 423-438.
MOON, A. R. (1972). *Z. Naturforsch. Teil A*, **27**, 390-395.
PENDRY, J. B. (1974). *Low Energy Electron Diffraction.* London: Academic Press.
PENDRY, J. B. & GARD, P. (1975). *J. Phys. C*, **8**, 2048-2058.
SOMMERFELD, A. & BETHE, H. (1930). *Handbuch der Physik*, Vol. 24, No. 2. Berlin: Springer. (Available as a paperback, *Heidelberger Taschenbücher*, Vol. 19, 1967).
TOURNARIE, M. (1962). *J. Phys. Soc. Jpn*, **17** Suppl. B-II, 98-100.
ZURMÜHL, R. & FALK, S. (1984). *Matrizen und Ihre Anwendungen*, Vol. 1. Berlin: Springer.

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Interpretation of the Shape of Electron Diffraction Spots from Small Polyhedral Crystals by Means of the Crystal Shape Amplitude

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Abstract

The influence of the crystal shape on the fine structure of transmission electron diffraction (TED) patterns described by the crystal shape amplitude is discussed. A general algebraic expression for the crystal shape amplitude of any crystal polyhedron is used for computing the intensity distribution of TED reflections. The computer simulation method is applied to the analysis of the fine structure of TED patterns of small gold and palladium crystals having octahedral and tetrahedral habits.

1. Introduction

In electron diffraction of small crystals spots are frequently observed which have distinct fine structure consisting of streaks, satellites or elongations. The shape of any diffraction spot is mainly determined by the shape of the crystal as well as by the presence of crystal defects. The contribution of the crystal shape to the fine structure of the reflections can be described within the framework of the kinematical diffraction theory. The intensity distribution around each reciprocal-lattice point **g** is then given by

$$I_{hkl}(\mathbf{p}) = |F_{hkl}|^2 |S(\mathbf{p})|^2 \qquad (1)$$

where, for the lattice point **g**, F_{hkl} is the structure amplitude and S is the shape amplitude, which is the same around every reflection. In electron diffraction the kinematical approximation usually fails and the exact calculation of the scattered intensities requires a dynamical treatment. A dynamical theory of the

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