Calculation of Reflected Intensities for Medium and High Energy Electron Diffraction *

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Dedicated to Professor K. MOLIÈRE *on the occasion of his sixtieth birthday*

The Bethe theory of electron diffraction is used to calculate reflection electron diffraction intensities for medium and high energy electrons. A generalized Hill's determinant method is used for the numerical calculations instead of the more common but slower matrix-eigenvalue technique. Results of a "systematics" calculation of the specular intensity as a function of incident angle are compared with some experimental values for the Si (111) surface. The application of the Bethe theory to crystals where the surface structure differs from the bulk is also considered.

1. Introduction

The Bethe theory[1] of electron diffraction, so useful in Transmission microscopy (TM) studies[2], has also been used for calculating reflection electron diffraction intensities[3-5]. The infinite number of dynamical equations obtained from the theory is first reduced to a finite number N in a manner similar to that used in TM calculations. These N coupled equations of second order in the wave vector component normal to the crystal surface may be transformed into a $2N \times 2N$ matrix eigenvalue equation[5]. (The small λ, linearisation approximations of TM are no longer valid for reflection calculations.) Bloch wave components corresponding to each of the $2N$ eigenvalues are then calculated and the amplitudes of the various Bloch waves are found from the boundary condition (BC) equations. Here a difficulty arises. In the transmission case there are exactly enough BC equations to provide solutions for all unknown quantities. In the reflection case this is no longer so. This problem arises because some of the eigenvalues are physically equivalent to each other and thus produce identical Bloch wave components. If the amplitudes of the Bloch waves associated with these equivalent eigenvalues are then treated as separate and distinct unknown quantities, then it is not surprising that there are insufficient BC equations. Thus to calculate the reflected intensities using matrix eigenvalue techniques one eigenvalue from each set should be chosen and only these eigenvalues should be used to calculate the Bloch wave components and amplitudes.

Unfortunately, because of the equivalence of many of the eigenvalues, matrix eigenvalue techniques are inefficient in use of computer time. Eigenvalue algorithms generally calculate *all* eigenvalues even though only one from each set of equivalent eigenvalues is required in the intensity calculation. A more efficient procedure in such cases is the generalized Hill's determinant method proposed by LAMLA[6, 7].

This article describes the development of the Hill's determinant (HD) approach, showing how the problem of equivalent eigenvalues arises, is resolved and efficiently solved. As far as possible Lamla's notation has been retained. The application of the Bethe theory to crystals where the surface structure differs from the bulk is also discussed.

2. Bethe Theory

An electron incident on a crystal finds itself in a region of potential $V(\boldsymbol{r})$. For an electron of energy E (eV) the Schroedinger equation is

$$\nabla^2 \Psi + (2\,m\,e/\hbar^2)\,(E+V)\;\Psi = 0 \qquad (1)$$

which has solution in vacuum

$$\Psi = \exp\{-2\,\pi\,i\,\boldsymbol{k}^{\mathrm{a}} \cdot \boldsymbol{r}\}\,,$$

where $|\boldsymbol{k}^{\mathrm{a}}| = 1/\lambda \cong \sqrt{E/150}$ Å^{-1}. The primitive translations of the crystal lattice $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, $\boldsymbol{a}_3$ are so

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chosen that $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ lie on the boundary plane of the crystal surface. The corresponding vectors of the reciprocal net are defined by $\mathbf{b}_i = \boldsymbol{a}_j \times \boldsymbol{a}_k / \Omega$, where $\Omega = \boldsymbol{a}_i \cdot \boldsymbol{a}_j \times \boldsymbol{a}_k$. A right hand cartesian coordinate system is chosen such that the boundaries of the crystal are defined by $z=0$ and $z=D$ (which may be finite or infinite). The potential V possesses the lattice periodicity and may be expanded in a Fourier series

$$(2\,m\,e\,V/\hbar^2) = \sum_{g} v_g \exp\{-2\,\pi\,i\,\mathbf{b}_g \cdot \boldsymbol{r}\} \qquad (2)$$

where $\boldsymbol{g}$ represents the number triple such that $\mathbf{b}_g = g_1\,\mathbf{b}_1 + g_2\,\mathbf{b}_2 + g_3\,\mathbf{b}_3$. The wave function may be expanded as a linear combination of Bloch wave expressions of the form

$$\psi = \sum_{g} \psi_g \exp\{-2\,\pi\,i\,\boldsymbol{k}_g \cdot \boldsymbol{r}\} \qquad (3)$$

where $\boldsymbol{k}_g = \boldsymbol{k}_0 + \mathbf{b}_g$. Substitution of the expressions for Ψ and V into (1) yields (after rearrangement)

$$\sum_{h} \{(\boldsymbol{k}_g{}^2\,\lambda^2 - 1)\,\delta_{gh} - \lambda^2/4\,\pi^2\,v_{g-h}\}\,\psi_h = 0\,, \qquad (4)$$

where δ_{gh} is the Kronecker δ-function. The condition for solution of the (infinite) equation system is the vanishing of the determinant of the coefficients

$$\det\left|(\boldsymbol{k}_g{}^2\,\lambda^2 - 1)\,\delta_{gh} - \lambda^2/4\,\pi^2\,v_{g-h}\right| = 0\,. \qquad (5)$$

The X- and Y-components of k_0 (crystal) are written as α_0/λ, β_0/λ (λ is the vacuum wavelength) and the Z-component as x_0/λ. Defining

$$\varrho_g = \lambda\,b_g{}^x = \lambda(g_1\,b_1{}^x + g_2\,b_2{}^x), \qquad (6\,\text{a})$$
$$\sigma_g = \lambda\,b_g{}^y = \lambda(g_1\,b_1{}^y + g_2\,b_2{}^y) \quad \text{and} \qquad (6\,\text{b})$$
$$\tau_g = \lambda\,b_g{}^z = \lambda(g_1\,b_1{}^z + g_2\,b_2{}^z + g_3\,b_3{}^z) \qquad (6\,\text{c})$$

then

$$\boldsymbol{k}_g = (\alpha_g/\lambda,\ \beta_g/\lambda,\ x_g/\lambda)$$

where

$$\alpha_g = \alpha_0 + \varrho_g\,, \quad \beta_g = \beta_0 + \sigma_g \quad \text{and} \quad x_g = x_0 + \tau_g\,.$$

Now $k_g{}^2\,\lambda^2 - 1$ may be rewritten as

$$x_g{}^2 - \gamma_g{}^2 = (x_0 + \tau_g)^2 - \gamma_g{}^2$$

where

$$\gamma_g = +\sqrt{1 - \alpha_g{}^2 - \beta_g{}^2} \qquad (7)$$

and writing $v_0\,\lambda^2/4\,\pi^2 = q = \overline{V}/E$ and $v_g = a_g\,v_0$ the dynamical equations may be rewritten as

$$\sum_{h} [((x_0 + \tau_g)^2 - \gamma_g{}^2)\,\delta_{gh} - a_{g-h}]\,\psi_h = 0 \qquad (8)$$

which have a solution provided

$$\det\left|[((x_0 + \tau_g)^2 - \gamma_g{}^2)\,\delta_{gh} - a_{g-h}\,q]\right| = 0. \qquad (9)$$

Distinguishing the various solutions x_0 of this equation by the index i the wave function in the interior may be written as

$$\Psi = \sum_{g,i} \psi_g^i \exp\{-2\,\pi\,i/\lambda\,(\alpha_g\,X + \beta_g\,Y + x_g{}^i\,Z)\}\,. \qquad (10)$$

Now a plane wave (direction cosines α, β, γ and amplitude 1) has wave function

$$\Psi^a = \exp\{-2\,\pi\,i/\lambda\,(\alpha\,X + \beta\,Y + \gamma\,Z)\}. \qquad (11)$$

Continuity conditions at the surface require that

$$\alpha_0 = \alpha \quad \text{and} \quad \beta_0 = \beta$$

and thus $\alpha_g = \alpha + \varrho_g$ and $\beta_g = \beta + \sigma_g$.

Now because of the existence of the waves $\boldsymbol{k}_g$ in the crystal diffracted waves appear in the vacuum with wave vectors α_g/λ, β_g/λ, $\pm\gamma_g/\lambda$ where γ_g is determined by Equation (7). The negative sign corresponds to a reflected wave and the positive sign to the transmitted wave. The wave function (in vacuum) for the reflected wave ($Z \leqq 0$) is

$$\Psi^R = \sum_{g} \varphi_g \exp\{-2\,\pi\,i/\lambda\,(\alpha_g\,X + \beta_g\,Y - \gamma_g\,Z)\} \qquad (12)$$

and for the transmitted wave ($Z \geqq D$)

$$\Psi^T = \sum_{g} \Phi_g \exp\{-2\,\pi\,i/\lambda\,(\alpha_g\,X + \beta_g\,Y + \gamma_g\,Z)\}\,. \qquad (13)$$

The requirements of continuity of the wave function and its normal derivative on the upper surface $Z=0$ yields the equations [6]

$$1 + \varphi_0 = \sum_{g_3,\,i} \psi_{00g_3}^i\,, \qquad \gamma(1 - \varphi_0) = \sum x_{0g_3}^i\,\psi_{00g_3}^i\,,$$
$$g_1\,,\,g_2 = 0 \qquad (14)$$

and

$$\varphi_g = \sum_{g_3,\,i} \psi_g{}^i \qquad (15)$$
$$-\gamma_g\,\varphi_g = \sum_{g_3,\,i} x_g{}^i\,\psi_g{}^i \quad \text{for all other cases.}$$

On the lower surface $Z=D$ the corresponding equations are found

$$\Phi_g \exp\{-2\,\pi\,i/\lambda\,\gamma_g\,D\} = \sum_{g_3,\,i} \psi_g{}^i \exp\{-2\,\pi\,i/\lambda\,x_g{}^i\,D\}\,, \qquad (16)$$

$$\gamma_g \Phi_g \exp\{-2\,\pi\,i/\lambda\,\gamma_g\,D\} = \sum_{g_3,\,i} x_g{}^i\,\psi_g{}^i \exp\{-2\,\pi\,i/\lambda\,x_g{}^i\,D\}\,. \qquad (17)$$

Eliminating the quantities Φ_g and φ_g from these equations the boundary condition equations are obtained.

$$\sum_{g_3,\, i} (\gamma_g + x_g{}^i)\, \psi_g{}^i = 2\,\gamma \text{ for } \quad g_1\,, g_2 = 0$$

$$= 0 \quad \text{for all other cases} \qquad (18)$$

$$\sum_{g_3,\, i} (\gamma_g - x_g{}^i)\, \psi_g{}^i \exp\{-2\,\pi\, i/\lambda\, x_g{}^i\, D\} = 0\,. \qquad (19)$$

From the direction cosines α, β, γ of the incident wave the (infinitely) many corresponding directions α_g, β_g, γ_g of the diffracted wave vector in vacuum are calculated. The various $x_0{}^i$ are calculated from Eq. (9) and back-substitution into the dynamical equations (8) provides the ratios $\psi_g{}^i/\psi_0{}^i$. The $\psi_0{}^i$ are calculated from the BC equations (18) and (19), and finally the amplitudes of the reflected and transmitted waves are calculated from the Equations (14) – (16). If absorption processes are included in the description of the potential, and provided D is sufficiently large, all Φ_g will be zero and thus only those $x_0{}^i$ corresponding to waves propagating down into the crystal need be considered.

If the calculation is limited to N different $\boldsymbol{g}$ values (including $\boldsymbol{g} = 0$) then the determinant (9) is of order N and yields then an equation of order $2\,N$ for x_0. The solution of an equation

$$\det(Q - B\,x + x^2) = 0\,,$$

such as Eq. (9), is provided by the eigenvalue solutions of the equation

$$\det \left| \begin{pmatrix} B - x\,I & -Q \\ I & 0 - x\,I \end{pmatrix} \right| = 0 \qquad (20)$$

where the matrices B, Q, I, 0 are of order N, and I and 0 are the identity and null matrices respectively[5]. To each of the $2\,N$ values $x_0{}^i$ correspond N values $x_g{}^i$ and thus there are, in toto, $2\,N^2$ values $x_g{}^i$ and correspondingly $2\,N^2$ values $\psi_g{}^i$ ($2\,N$ wave fields each with N waves). From (8) the $\psi_g{}^i$ may be expressed as ratios of the $\psi_0{}^i$ leaving $2\,N$ $\psi_0{}^i$ to be found from the BC Eqs. (18) and (19). The totality of these equations is twice the number of different pairs $(g_1\,, g_2)$ and is equal to $2\,N$ only if, of the N number triples originally chosen, no two triples are such that they differ *only* in their g_3 values. If such number triples do occur then the number of BC equations is insufficient to solve for all unknowns. This problem arises because the eigenvalues with number triples differing only in their g_3 values are physically equivalent to each other, and including them in the calculation means counting the same Bloch wave more than once. If matrix eigenvalue techniques are used to calculate the eigenvalues only *one* eigenvalue from each set of equivalent eigenvalues should be used.

It is assumed of course that N was chosen large enough to ensure that the eigenvalues had converged in value. For reflection calculations the generalized Hill's determinant[6, 7] method is a more efficient technique in cases where many number triples must be included which differ only in their g_3 values.

3. The Hill's Determinant Method

The dynamical equations (8) may be rewritten as

$$\psi_{\boldsymbol{g}} - \sum_{\boldsymbol{h}} \frac{\varrho\, a_{g-h}}{(x + t_g + g_3)^2 - c_g{}^2}\, \psi_{\boldsymbol{h}} = 0 \qquad (21)$$

where

$$\varrho = q/c^2, \quad x = x_0/c, \quad t_g = \lambda\,(g_1\, b_1{}^z + g_2\, b_2{}^z)\,, \quad c = \lambda\, b_3{}^z \qquad (22)$$

and

$$c_g{}^2 = (\gamma_g{}^2 + q)/c^2\,. \qquad (23)$$

The quantities $a_g = v_g/v_0$ are such that the sum $\sum_{\boldsymbol{h}} \varrho\, a_g$ is absolutely convergent. The equation system (21) has solutions provided the determinant $\Delta_1(x)$ of the coefficient vanishes. If only three pairs $(g_1\,, g_2)$ need be considered (0, **G** and ***H***), then this determinant $\Delta_1(x)$ may be written as[7]

$$\Delta_1(x) = \begin{bmatrix} 1 & \dfrac{-a_{-1}\,\varrho}{(x-1)^2 - c_0{}^2} & \cdots & \dfrac{-a_{-G-1}\,\varrho}{(x-1)^2 - c_0{}^2} & \\ \dfrac{-a_1\,\varrho}{(x-0)^2 - c_0{}^2} & 1 \cdots\cdots & & \dfrac{-a_{-G}\,\varrho}{(x-0)^2 - c_0{}^2} & \\ \vdots & & & \vdots & \\ \dfrac{-a_{G+1}\,\varrho}{(x+t_G)^2 - c_G{}^2} & \cdots\cdots & & 1 \cdots\cdots & \vdots \\ \vdots & & & \vdots & \\ \dfrac{-a_{H+1}\,\varrho}{(x+t_H)^2 - c_H{}^2} & \cdots\cdots\cdots & \cdots\cdots\cdots & \cdots\cdots & 1 \end{bmatrix}. \qquad (24)$$

Apart from simple poles at the positions

$$x = \pm\, c_0 + n, \quad \pm\, c_g - t_g + n \quad \text{and} \quad \pm\, c_h - t_h + n$$
$$(n \text{ any integer})$$

this infinite determinant is unconditionally convergent, since the products of the main diagonal elements $(=1)$ and the sum of all elements not on the main diagonal are absolutely convergent (because of the convergence of the sums $\sum_g \varrho\, a_g$ and $\sum 1/n^2$) [8]. In addition $\Delta_1(x)$ is a simple periodic function of x with period 1. Thus if x is a solution of the equation $\Delta_1(x)=0$ then so is $x+n$, where n is any integer. These solutions $x(+n)$ are physically equivalent. The simplest periodic function of x with period 1 and simple poles at the points $x=\pm c_0+n$ is the function $\cot\pi(x\mp c_0)$. If constants $A_0, B_0, A_G, B_G, A_H, B_H$, etc., are determined such that the function

$$f(x)=\Delta_1(x)-\sum_g \{A_g \cot\pi(x+t_g-c_g) + B_g \cot\pi(x+t_g+c_g)\} \qquad (25)$$

has no poles at the positions $\pm c_0$, $-t_g \pm c_g$, etc., then $f(x)$ has no poles at all, and is a simple periodic function of x which remains finite at infinity. As a result, according to Liouville's theorem [8] $f(x)$ is a constant, whose value may be found (by considering the limit $x \rightarrow \pm i\infty$) as equal to 1. The coefficients A_g, B_g, etc., are then found to satisfy the condition $\sum_g (A_g+B_g)=0$. The solutions of the equation $\Delta_1(x)=0$ are then found as solutions of the polynomial equation

$$1+\sum_g \{A_g \cot\pi(x+t_g-c_g) + B_g \cot\pi(x+t_g+c_g)\} = 0\,. \qquad (26)$$

The coefficients A_g, B_g may simply be found by expanding (26) in the vicinity of $x=c_g-t_g$, etc., and thus

$$A_g=\pi \operatorname*{Lt}_{x\rightarrow c_g-t_g} [(x+t_g-c_g)\,\Delta_1(x)]$$

and
$$B_g=\pi \operatorname*{Lt}_{x\rightarrow -c_g-t_g} [(x+t_g+c_g)\,\Delta_1(x)]\,. \qquad (27)$$

It is assumed that $\pm c_0$ and $\pm c_g - t_g$ differ by more than an integer. The determinants may be evaluated conveniently using the Gaussian elimination procedure [9]. The order of the determinant is increased until convergence of the coefficients (to working accuracy) is achieved. The approximation suggested by LAMLA [7] for the evaluation of the coefficients [expansion of (27) in powers of ϱ^2] is insufficiently accurate, at least for the low order expansion.

For a centro-symmetric crystal where the a_3 axis is normal to the crystal surface, all $t_g=0$ and $A_g=-B_g$. Defining

$$y=\tan\pi x, \quad y_0=\tan\pi c_0, \quad y_g=\tan\pi c_g, \text{ etc.,}$$

the Eq. (26) reduces to a bi-cubic equation in y,

$$\sum_{i=0}^{3} K_i (y^2)^i = 0\,.$$

If only two pairs 0, **G** need be considered (26) reduces to a bi-quadratic equation in y, and if a "systematics" calculation only is required [i. e., only reciprocal lattice points $(0, 0, g_3)$ need be considered] then the equation system reduces to a bi-linear equation in y.

$$(1+2A_0 y_0)\, y^2 + (2A_0 y_0 - y_0^2) = 0\,. \qquad (28)$$

In the general case where many pairs (g_1, g_2) must be considered a polynomial in y must be solved. Nickel's algorithm [10] readily provides the roots of such a general polynomial.

4. An Application

The simplest application of this theory is to the "systematics" case. If it is possible to choose azimuth angles experimentally so that the interference from non-systematic diffracted beams is greatly minimized, then in the theoretical calculation only those reciprocal lattice (RL) points lying on the 00-rod (the RL rod through the RL point 000 and normal to the surface) need be considered. To calculate the Fourier coefficients of the potential, Doyle-Turner parameters [11] were used for the electron scattering factors. The approximations inherent in the calculations leading to these parameters should remain valid for both MEED (1 – 10 keV) and RHEED (10 – 50 keV) energy regions. (The likely advantages of MEED over both RHEED and LEED have been pointed out elsewhere [12].) The effect of absorption on the intensity may be included by means of an imaginary part aded to the potential coeffi-

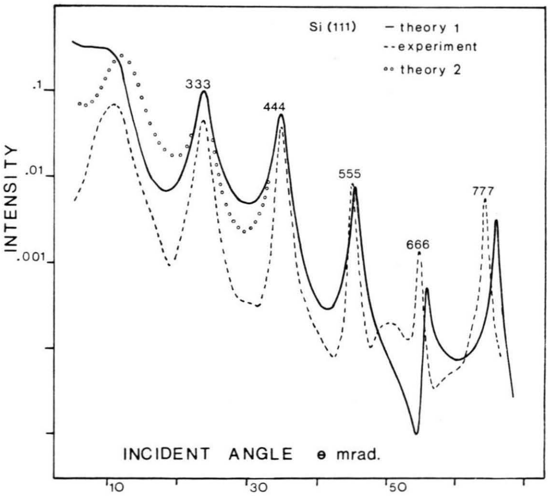

Fig. 1. A "systematics" calculation of the specular intensity as a function of incident angle compared with the experimental values of MENADUE [13] for the Si (111) surface. The incident energy is 40 keV and the inner potential is 12 V for curve 1 and 8 V for curve 2. The origin has been displaced in curve 2 so that the peak position still coincide.

cients. In the absence of good theoretical values the absorptive part of the potential may be treated as a parameter in the calculations.

Figure 1 is a comparison of the experimental results of MENADUE[13] for the Si (111) surface with a "systematics" calculation. The incident energy was 40 keV. To provide best agreement with the 555 peak V_0, the inner potential, was chosen as 12 volt and $V^{\text{imaginary}}$ was chosen as $V^{\text{real}}/8.0$ to account for absorption. A Debye parameter of 0.5 Å^2 was assumed. Using the HD method each intensity point required one second computation time (using a CDC 6400 computer). Matrix eigenvalue methods (e. g., the QR algorithm[14]) are at least an order of magnitude slower. The discrepancy between theory (curve 1) and experiment, especially noticeable at very low angles of incidence, may be attributed to two main factors:

1. Neglect of non-systematic interactions. This would cause the minima to be greater than observed experimentally. The peak intensities should not be significantly changed because the azimuth angles were chosen experimentally to minimize non-systematic interactions at the Bragg positions.
2. "Surface flatness." At very low angles of incidence there will be a significant variation in penetration and refraction effects if the surface departs at all from the ideal flat state. In addition, especially at very low angles, the abrupt potential cut-off required by the Bethe theory (planar surface at $Z=0$) causes the reflected intensity to be much larger than would be expected for a potential which actually decreases gradually.

Curve 2 (Fig. 1) shows the effect of decreasing the inner potential on the reflected intensity at low angles. (The origin has been shifted in this curve so that the peak positions still coincide with the experimental positions.) Similar effects occur in LEED calculations[15].

5. An Extension of the Bethe Theory to Non-Perfect Crystals

The crystal model assumed by the Bethe theory is an infinitely (3-D) periodic array of scattering units (Figure 2 a). The BC equations account for the finite nature of the actual crystal by providing the right linear combination of Bloch waves (infinite crystal solutions). If absorption is included in the theory this linear combination is such that the electron wave is strongly attenuated within the first few layers of atoms. That is to say, the reflected intensity is largely unaffected by the crystal structure below the first few layers of atoms. By applying the Bethe theory to a model crystal whose unit cell corresponds in structure to the uppermost layers of the actual crystal, reflection calculations can be performed for non-perfect crystals, i. e., those crystals whose surface layers differ from the bulk. This model crystal will have an elongated unit cell (Fig. 2 b) and reciprocal lattice points in the direction of the surface normal will thus be very close together. To achieve convergence, many Fourier coefficients must then be included in the calculations. While this would present a serious problem if matrix-eigenvalue techniques were used, this should not be the case for the Hill's determinant method.

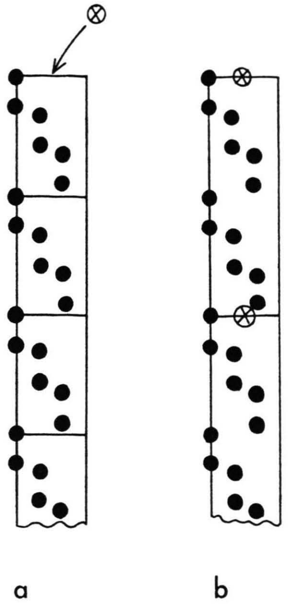

Fig. 2 a. Perfect crystal with normal unit cell dimensions *a*.

Fig. 2 b. Model crystal used for calculations. The unit cell now has dimensions 2 *a*. It is assumed that absorption is so strong that the electron beam does not penetrate deeper than 2 *a*. The top unit cell of this model crystal corresponds in structure to the actual crystal (perfect crystal + adsorbed atoms on the surface).

This approach is formally equivalent to the multi-layer scattering matrix approach suggested for LEED[16] and RHEED[5] calculations. It corresponds however to the case where absorption is so strong and the first layer so thick that the back-scattering from the second and subsequent layers may be neglected in the calculations. A comparison of these two approaches is now under way.

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Berücksichtigung der Gitterperiodizität bei der Elektron-Plasmon-Streuung. I.

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Herrn Prof. Dr. K. Molière *zu seinem 60. Geburtstag gewidmet*

Consideration of Lattice Periodicity at the Electron Plasmon Scattering. I.

The scattering of electrons by solid-state plasmons is investigated, the system of valence electrons being treated with Green's function method. The lattice periodicity is taken into account for the wave field of the incident electrons as well as for the plasma oscillations of the valence electrons. Scattering processes which contain a reciprocal-lattice vector in the momentum balance appear in addition to the usual inelastic small-angle scattering. Their influence upon the imaginary part of the complex scattering potential is discussed. In a following paper, the reason for the additional scattering processes will be given in terms of the form of the Fermi surface of the solid.

Einleitung

Bei der Elektronenbeugung an Kristallen werden neben den elastisch gestreuten Elektronen auch die unelastisch gestreuten vornehmlich in die durch die Bragg-Bedingung bestimmten Reflexionsrichtungen gestreut. Diese unelastisch gestreuten Elektronen haben vor oder nach der elastischen Streuung am Gitter Energie durch Wechselwirkung mit den Festkörperelektronen verloren. So führt die Anregung von Plasmaschwingungen der Festkörperelektronen durch schnelle Elektronen zur unelastischen Kleinwinkelstreuung. Der Wirkungsquerschnitt für den zuletzt erwähnten Prozeß wurde nach der Bohm-Pines-Theorie von Ferrell[1] berechnet. Im wesentlichen basieren alle Erklärungen der Experimente auf der Theorie des homogenen Elektronengases[2]. Dort wird zur Vereinfachung eine dielektrische Funktion eingeführt, die von Wellenzahl und Frequenz der Störung abhängig ist. Es wurde jedoch zusätzlich von Ishida u. a.[3] und Cundy[4] experimentell eine schwache Abhängigkeit der freien Weglänge für Elektronen von der Bragg-Bedingung festgestellt. Im Gegensatz dazu wurde von Meyer[5] und Hirsch[6] keine solche Abhängigkeit angegeben. Ob und in welcher Form bei der Elektron-Plasmon-Streuung eine Abhängigkeit von der Bragg-Bedingung und damit von der Gitterstruktur des Festkörpers vorliegt, soll in der vorliegenden Arbeit theoretisch geklärt werden. Ausgegangen wird von Kainumas[7] Theorie der Kikuchi-Linien und Yoshiokas[8] Theorie der anomalen Absorptionskoeffizienten. Es werden zunächst zwei Probleme behandelt:

1. Es wird untersucht, ob zusätzlich zu der oben beschriebenen elastisch-unelastischen Zweifachstreuung eine direkte unelastische Streuung in die Reflexrichtung erfolgt. Eine schematische Darstellung dieses Sachverhalts ist aus Abb. 1 zu entnehmen (s. Diskussion).

2. Es wird eine Formel für den Imaginärteil des komplexen Streupotentials angegeben, die die wegen der zusätzlichen Streuprozesse zu erwartende Änderung der Absorption beschreibt (anomale Absorption).

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