ROBERTO, J. B. & BATTERMAN, B. W. (1970). MSC Report No. 1357, Cornell Univ.
RUSSELL, G. J. (1970). *Surface Sci.* **19**, 217.
RUSSELL, G. J. & HANEMAN, D. (1967). *J. Electrochem. Soc.: Solid State Sci.* **114**, 398.
SCHLIER, R. E. & FARNSWORTH, H. E. (1959). *J. Chem. Phys.* **30**, 917.
SEWELL, P. B. (1970). Private communication.
SIEGEL, B. M. & MENADUE, J. F. (1967). *Surface Sci.* **8**, 206.
STROZIER, J. A. & JONES, R. O. (1970). MSC Report No. 1363, Cornell Univ.
TAYLOR, N. (1969). *Surface Sci.* **15**, 169.
TULL, V. F. G. (1951). *Proc. Roy. Soc.* A**206**, 219.
VAINSHTEIN, B. K. (1964). *Structure Analysis by Electron Diffraction.* Oxford: Pergamon.

Acta Cryst. (1972). A**28**, 11

n-Beam Dynamical Diffraction of High-Energy Electrons at Glancing Incidence. General Theory and Computational Methods*

BY R. COLELLA†

Department of Materials Science and Engineering, Cornell University, Ithaca, New York 14850, *U.S.A.*

(*Received* 9 *October* 1970)

The *n*-beam dynamical theory of high-energy electrons is currently used in transmission (Laue case) for accurate determination of the Fourier components of the crystal potential. The same theory is expected to provide information about the surface potential when used to interpret diffraction patterns in reflection at glancing incidence (Bragg case). Some peculiar aspects are elucidated in detail, insofar that they are different from the transmission case, particularly the boundary conditions. Inelastic scattering effects are introduced by means of a complex potential. Changes of the Fourier components of the potential near the surface are considered, and a model has been developed which incorporates these changes into the theory. A slice treatment developed in the frame of Bethe's theory is presented.

1. Introduction

Diffraction of electrons from a flat surface of a single crystal has been widely used in the last few years for surface investigations. When the energy of the primary beam is of the order of a few keV (high-energy electron diffraction, HEED) the actual penetration of the electron beam is much higher than in low-energy electron diffraction (LEED), but owing to the small grazing angle (of the order of 1 to 3°), it is to be expected that a HEED diffraction pattern will reflect the properties of the first few atomic layers. This is confirmed by the streaky character of the diffraction spots observed at different stages during heat treatment in the case, for instance, of tungsten (Siegel & Menadue, 1967).

The essential tool for understanding a HEED pattern from a quantitative point of view is of course the *n*-beam dynamical theory such as that developed for the transmission case (Laue case) (Hirsch, Howie, Nicholson, Pashley & Whelan, 1965).* In transmission experiments the *n*-beam dynamical theory has been successfully used for the accurate determination of structure factors (Cowley, 1969), in the frame of a scattering theory based upon the first Born approximation. Within the limits of such an approximation it is permissible to express the Fourier components of the crystal potential in terms of the scattering cross section for each atom within the crystal cell, a kinematic approximation being made within each cell. Such an approximation, to be sure, is not permissible in LEED.

It is expected, in principle, that the same theory applied to the Bragg case should be able to give information on the surface charge density *via* the atomic potential.

Although the basic formalism of the *n*-beam dynamical theory for the Bragg case is essentially the same as for the Laue case, there are some differences in the practical developments of the calculations, especially as far as the boundary conditions are concerned.

This paper will give a description of how the *n*-beam dynamical theory for electrons has been applied to the Bragg case of diffraction. It will be shown in detail how the original theory developed by Bethe (1928) has been used for this purpose.

A model will be described in which possible changes of the crystal inner potential can be taken into account in the frame of such a theory. Rocking curves (reflectivity *vs.* angle of incidence) have been computed in

* Work supported by the Air Force Office of Scientific Research.

† Present address: Department of Physics, Purdue University, Lafayette, Indiana 47907, U.S.A.

* Diffraction theory is an alternative but equivalent approach to band theory, as pointed out by Stern, Perry & Boudreaux (1969). *E vs. k* plots are replaced here by the dispersion hypersurface.

some particular cases, and their comparison with available experimental results will be discussed in the next paper (Colella & Menadue, 1972).

2. General theory

It is assumed that the surface of discontinuity between vacuum and crystal is plane, with infinite lateral extent, characterized by a normal unit vector **n** pointing inwards. The crystal is assumed to be semi-infinite, with the origin of coordinates on the surface.

We will consider the case in which a limited number $m \geq 1$ of diffracted beams are appreciably excited within the crystal. They will be labelled $H_1, H_2 \ldots H_m$ $(m=n-1)$* where the H_j's are the nodes which lie on or are very close to the Ewald sphere. No distinction will be made in what follows between Laue and Bragg beams.

In the frame of the quantum mechanical formulation of electron diffraction in crystals as developed originally by Bethe (1928), the electron field is described in terms of Bloch waves:

$$\psi^{\text{cryst}}(\mathbf{r}) = C_0 \exp(2\pi i\, \boldsymbol{\beta}_0 \cdot \mathbf{r}) + C_{H_1} \exp(2\pi i\, \boldsymbol{\beta}_{H_1} \cdot \mathbf{r}) + \ldots + C_{H_m} \exp(2\pi i\, \boldsymbol{\beta}_{H_m} \cdot \mathbf{r})$$

where the amplitudes C_{H_j} are the solutions of the following linear system of simultaneous homogeneous equations (see, Hirsch *et al.*, 1965)

$$\left.\begin{aligned} (K^2-\beta_0^2)C_0 + V_{0-H_1}C_{H_1} + \ldots + V_{0-H_m}C_{H_m} &= 0 \\ V_{H_1-0}C_0 + (K^2-\beta_{H_1}^2)C_{H_1} + \ldots + V_{H_1-H_m}C_{H_m} &= 0 \\ V_{H_m-0}C_0 + V_{H_m-H_1}C_{H_1} + \ldots + (K^2-\beta_{H_m}^2)C_{H_m} &= 0 \end{aligned}\right\} \quad (1)$$

where K is the magnitude of the electron wave-vector in the crystal corrected for the change of wavelength due to the mean inner potential V_0, V_{H_j} is the Fourier component of the crystal potential pertinent to the reciprocal-lattice node H_j,† β_0 is the magnitude of the wave-vector for that particular plane wave, within the crystal, which has the same tangential component as the external incident beam $\mathbf{k}_0$. In addition

$$\beta_{H_j} = |\boldsymbol{\beta}_{H_j}| = |\boldsymbol{\beta}_0 + \mathbf{B}_{H_j}|$$

where $\mathbf{B}_{H_j}$ is a reciprocal-lattice vector. The system (1) will have a non-trivial solution only if the determinant is zero. This condition involves an algebraic equation for β_0, whose roots are the allowed eigenvalues. As the tangential component of $\boldsymbol{\beta}_0$ is fixed by the boundary conditions, the normal component γ_0 can be chosen as an eigenvalue. From the definition of K it follows that: $K^2-\beta_{H_j}^2 = \Gamma_{H_j}^2 - \gamma_{H_j}^2 + 2meV_0/h^2$ where m and e are mass and charge for electron respectively, h is Planck's constant, $\Gamma_{H_j} = |\mathbf{k}_{H_j} \cdot \mathbf{n}|$,‡ $\mathbf{k}_{H_j}$ is the H_j-diffracted vacuum wave, and $\gamma_{H_j} = (\boldsymbol{\beta}_{H_j} \cdot \mathbf{n})$. In the Bragg case of diffraction, at glancing angle, Γ_{H_j} and $|\gamma_{H_j}|$ can be appreciably different, as opposed to the Laue case. It is not allowed, therefore, to use the approximation $\Gamma_{H_j} \simeq |\gamma_{H_j}|$ (Hirsch *et al.*, 1965) which would enable to transform the secular equation for γ_0 into an algebraic equation of order n. The $2n$ eigenvalues γ^i must be retained, giving rise to $2n$ independent solutions $C_{H_j}^i$ $(i=1,2,3,\ldots 2n)$. In the approximation of an infinitely thick absorbing crystal, however, only n Bloch waves will contribute significantly to the total wave field inside the crystal. These are the Bloch waves whose amplitudes decrease downwards in the crystal, as it will be shown later.

The total electron wave field inside the crystal can be written:

$$\psi^{\text{cryst}}(\mathbf{r}) = \sum_1^{2n} \psi^i \sum_0^{H_m} {}_{H_j} C_{H_j}^i \exp(2\pi i\, \boldsymbol{\beta}_{H_j}^i \cdot \mathbf{r}) \quad (2)$$

where the ψ^i's give the actual strength of the various Bloch waves and are determined by the boundary conditions.

3. Determination of the eigenvalues

The secular equation for the normal component of the electron momentum is of the form:

$$\begin{vmatrix} Q_0-\gamma_0^2 & V_{0-H_1} & \cdots & V_{0-H_m} \\ V_{H_1-0} & Q_{H_1}-\gamma_{H_1}^2 & & V_{H_1-H_m} \\ \cdots & \cdots & \cdots & \cdots \\ V_{H_m-0} & V_{H_m-H_1} & \cdots & Q_{H_m}-\gamma_{H_m}^2 \end{vmatrix} = 0 \quad (3)$$

where $Q_{H_j} = \Gamma_{H_j}^2 + 2meV_0/h^2$ and $\gamma_{H_j} = \gamma_0 + \mathbf{B}_{H_j} \cdot \mathbf{n}$.
In matrix notation the equation (3) can be written

$$\mathbf{I}\gamma_0^2 - \mathbf{B}\gamma_0 + \mathbf{Q} = 0 \quad (4)$$

where $\mathbf{B}$ is a diagonal matrix with $B_1 = 0$ and $B_j = -2(\mathbf{B}_{H_j} \cdot \mathbf{n}) = -2B_{H_j,n}$, $\mathbf{I}$ is the n-order identity matrix and

$$\mathbf{Q} = -\begin{bmatrix} Q_0 & V_{0-H_1} & \cdots & V_{0-H_m} \\ V_{H_1-0} & Q_{H_1}-B_{H_1,n}^2 & & V_{H_1-H_m} \\ V_{H_m-0} & V_{H_m-H_1} & \cdots & Q_{H_m}-B_{H_m,n}^2 \end{bmatrix}. \quad (5)$$

It can be easily shown (Faddeeva, 1959) that the $2n$ roots of the $2n$-order matrix polynomial (4) are given by the solutions of the first order matrix polynomial

---

* The symbol H_j will sometimes include the origin of the reciprocal space, which is associated with the incident beam.

† V_0 and V_{H_j} are assumed to be complex, in order to take into account inelastic scattering effects (Yoshioka, 1957).

‡ $\Gamma_{H_j} = \sqrt{k^2-(k_{H_j}^{\text{tang}})^2}$ where $k=1/\lambda$ is the magnitude of the wave-vector for the vacuum waves and $\mathbf{k}_{H_j}^{\text{tang}}$ is the tangential component of the H_j-diffracted vacuum beam. $\mathbf{k}_{H_j}^{\text{tang}} = \mathbf{k}_0^{\text{tang}} + \mathbf{B}_{H_j}^{\text{tang}}$. In some cases Γ_{H_j} is imaginary, which corresponds to the circumstance of an internal total reflection for the H_j-diffracted beam. In such a situation $\mathbf{k}_{H_j}$ does not exist except in close proximity to the surface (within a few ångströms).

$\mathbf{A}-\mathbf{I}\gamma_0=0$, where $\mathbf{A}$ is a $2n\times 2n$ matrix given by

$$\mathbf{A}=\begin{bmatrix}\mathbf{B} & -\mathbf{Q}\\ \mathbf{I} & \mathbf{0}\end{bmatrix} \tag{6}$$

and $\mathbf{0}$ is the n-order null matrix. The eigenvalues can now be determined by means of standard methods for which computer programs are available.

4. Boundary conditions

For each eigenvalue γ_0^i a solution $C_{H_j}^i$ can be determined from (1). Only the ratios between the various C_{H_j}'s are defined, however, not their absolute values.

The actual strengths of the various Bloch waves are given by the constants ψ^i [equation (2)] which are determined by the boundary conditions. In order to write down the proper boundary conditions for the Bragg case, we will consider a crystal slab of finite thickness t_0, and take the limiting form of the system of linear equations involving ψ^i as t_0 goes to infinity. The crystal slab, of infinite lateral extent, will divide the vacuum space into two regions, an 'upper' region, where the incident beam and the Bragg diffracted beams are travelling, and a 'lower' region, where only the transmitted beam (*i.e.* the incident beam after transmission through the crystal slab) and the Laue-diffracted beams can exist.* There are two parallel discountinuity surfaces which will produce mirror reflection of each plane wave. In both vacuum regions, therefore, for each active node H_j, we will consider, in general, two vacuum waves $\mathbf{k}_{H_j}$ and $\bar{\mathbf{k}}_{H_j}$ symmetric to the crystal surface. The Fourier expansion of the vacuum waves in the upper region will be of the form

$$\psi_{\text{vac}}^{\text{upper}}(\mathbf{r})=\exp(2\pi i\,\mathbf{k}_0\cdot\mathbf{r})+\sum_0^{Hm}{}_{H_j}\,X_{H_j}\times\exp\left[2\pi i\,(\mathbf{k}_{H_j}^{\text{tang}}-\mathbf{n}\,\Gamma_{H_j})\cdot\mathbf{r}\right] \tag{7}$$

where the first term represents the incident beam (of unit amplitude), X_{H_j} are the (unknown) amplitudes of the waves leaving the crystal, $\mathbf{k}_{H_j}^{\text{tang}}$ is the tangential component of $\mathbf{k}_{H_j}$ on the crystal surface.

The physical meaning of the plane waves grouped under the summation sign is as follows. The plane wave with $H_j=0$ is the specular reflected beam. When H_j denotes a Bragg beam, X_{H_j} is the amplitude of the Bragg-diffracted beam H_j. When H_j denotes a Laue beam, X_{H_j} is the amplitude of a specular beam reflected by the bottom surface.* In the lower region

$$\psi_{\text{vac}}^{\text{lower}}(\mathbf{r})=\sum_0^{Hm}{}_{H_j}\,\varphi_{H_j}\exp\left[2\pi i\,(\mathbf{k}_{H_j}^{\text{tang}}+\mathbf{n}\,\Gamma_{H_j})\cdot\mathbf{r}\right] \tag{8}$$

* The distinction between Laue and Bragg beams is not clearly defined at glancing angle when the n-beam interaction is strong. However we will retain this distinction only on an intuitive basis, for the sake of convenience, as though we were dealing with a situation of a large angle of incidence.

where the φ_{H_j}'s are the (unknown) amplitudes of the waves leaving the bottom surface. For the Bragg-diffracted beams, these waves can be viewed as those reflected within the crystal from the top surface.

The continuity requirements imposed on the electron wave function and on its normal derivative give the boundary conditions on the upper and lower surface. There is a total of $4n$ unknowns (X_{H_j}, φ_{H_j}, ψ^i, where $H_j=0,H_1,H_2\ldots H_m$; $i=1,2,\ldots 2n$) and $4n$ linear equations. By suitable linear combinations, however, it is possible to eliminate $2n$ unknowns (the X_{H_j}'s and the φ_{H_j}'s) and $2n$ equations. The following equations are obtained (Lamla, 1938):

$$\begin{aligned}&\delta_{H_j}=\sum_1^{2n}{}_i C_{H_j}^i\,(\Gamma_{H_j}+\gamma_{H_j}^i)\,\psi^i\\ &\delta_{H_j}=2\Gamma_0 \text{ for } H_j=0\\ &\delta_{H_j}=0 \text{ in all other cases}\end{aligned} \tag{9}$$

and

$$0=\sum_1^{2n}{}_i C_{H_j}^i\,(\Gamma_{H_j}-\gamma_{H_j}^i)\exp(2\pi\,i\,\gamma_{H_j}^i\,t_0)\,\psi^i\,. \tag{9'}$$

These are $2n$ equations which determine the $2n$ unknowns ψ^i. The X_{H_j}'s can be subsequently calculated from the eliminated equations (see §3 of Colella & Menadue, 1972).

Let us now assume that the eigenvalues have been ordered so that their imaginary parts are in decreasing order. Each of the last n equations (9') can be divided by $\exp(2\pi i\,B_{H_j,n})$

$$0=\sum_1^{2n}{}_i C_{H_j}^i(\Gamma_{H_j}-\gamma_{H_j}^i)\exp(2\pi\,i\,\gamma_0^i\,t_0)\,\psi^i\,. \tag{10}$$

The imaginary part of γ_0^i is related to absorption. For reasonable values of t_0 (1 or 2 mm) the real parts of the exponential factors in (10) have magnitudes differing in increasing order, by several orders of magnitude. Cramer's rule can be applied to express the ψ^i's as ratios of determinants. When these determinants are decomposed into partial products, consideration of the leading terms will show at once that it is possible to set $\psi^{n+1}=\psi^{n+2}=\ldots=\psi^{2n}=0$ and solve only the first n equations for the first n unknowns.

In the secular equation (3), the off-diagonal terms are smaller than the terms Q_{H_j}. On the other hand, the imaginary parts of all the Q_{H_j}'s are the imaginary parts of the inner potential and therefore are all the same. These two circumstances can explain why it is to be expected that each eigenvalue γ_0^i can be coupled with another one $\bar{\gamma}_0^i$ with approximately the same imaginary part, of different sign. The actual calculations have always confirmed this expectation.

The procedure described above, which leads to the elimination of the last n unknowns, is therefore equivalent to neglecting the Bloch waves whose amplitudes increase downwards into the crystal. These Bloch waves always exist in a non absorbing crystal. They can be interpreted as due to internal reflection on the

bottom surface of the crystal, and are absent when the crystal is much thicker than the absorption length of the radiation, as in our case.

Once the ψ^i's are known, the electron field in the crystal is completely determined. The boundary conditions on the upper surface of the crystal give the proper expressions for the amplitudes of the diffracted vacuum waves, as will be described in detail in the next paper (Colella & Menadue, 1972).

5. Change of the inner potential near the surface

The treatment given in the previous paragraphs assumes that the crystal is semi-infinite, and whose properties can be described as periodic functions of the primitive crystal translations defining the lattice in real space. The Fourier components involved are assumed to be the same throughout the crystal.

On the other hand, it is expected that HEED patterns at glancing incidence will sample the first few atomic layers, whose properties can be appreciably different from the bulk. Changes of the mean inner potential V_0 have been investigated both theoretically and experimentally (Pinsker, 1953). It is expected that the other Fourier components of the potential, V_{H_j}, will be similarly affected.

Changes in the lattice constants are also to be expected, which would entail a change of structure near the surface. Such changes, however, would not amount to more than a few per cent (Park & Farnsworth, 1964). They should not produce, therefore, any significant effect on the rocking curves whose widths are appreciable fractions (~0·075) of the whole diffraction angle, as shown by computations and experiments (see Colella & Menadue, 1972). The assumption of a uniform structure throughout the crystal brings on a considerable simplification in this problem.

We will not consider for the moment reconstructed surfaces. This question will be discussed in the next paper (Colella & Menadue, 1972).

The crystal is divided into an arbitrary number k of slices parallel to the surface, of different thicknesses (in general), $t_1, t_2 \ldots t_k$. In each slice the n-beam diffraction problem can be solved as in the case of the infinite crystal, with the appropriate values for the V_{H_j}'s. Each slice has therefore its own system of Bloch waves. The system of the reciprocal-lattice vectors $\mathbf{B}_{H_j}$ corresponding to the excited nodes is the same in every slice, and so is the tangential component $\boldsymbol{\beta}_{H_j}^{\text{tang}} = \boldsymbol{\beta}_0^{\text{tang}} + \mathbf{B}_{H_j}^{\text{tang}}$. In each slice there are $2n$ Bloch waves, whose amplitudes ψ^i are determined by the boundary conditions obtained by matching the wave function and its normal derivative on the lower and on the upper surface (§4). When the bulk is labelled as 0 and the k slices are numbered in increasing order from the top of the bulk upwards, the following system of linear equations is obtained:*

$$\left.\begin{aligned} 0 &= \sum_{1}^{2n}{}_i \; {}^{1}\psi^i \; {}^{1}C^i_{H_j} \exp(2\pi i \, {}^{1}\gamma^i_{H_j} z_1) - \sum_{1}^{n}{}_i \; {}^{0}\psi^i \; {}^{0}C^i_{H_j} \exp(2\pi i \, {}^{0}\gamma^i_{H_j} z_1) \\ 0 &= \sum_{1}^{2n}{}_i \; {}^{1}\gamma^i_{H_j} \; {}^{1}\psi^i \; {}^{1}C^i_{H_j} \exp(2\pi i \, {}^{1}\gamma^i_{H_j} z_1) - \sum_{1}^{2n}{}_i \; {}^{0}\gamma^i_{H_j} \; {}^{0}\psi^i \; {}^{0}C^i_{H_j} \exp(2\pi i \, {}^{0}\gamma^i_{H_j} z_1) \end{aligned}\right\} \quad (11a)$$

. . . . . .

. . . . . .

$$\left.\begin{aligned} 0 &= \sum_{1}^{2n}{}_i \; {}^{r+1}\psi^i \; {}^{r+1}C^i_{H_j} \exp(2\pi i \, {}^{r+1}\gamma^i_{H_j} z_{r+1}) - \sum_{1}^{2n}{}_i \; {}^{r}\psi^i \; {}^{r}C^i_{H_j} \exp(2\pi i \, {}^{r}\gamma^i_{H_j} z_{r+1}) \\ 0 &= \sum_{1}^{2n}{}_i \; {}^{r+1}\gamma^i_{H_j} \; {}^{r+1}\psi^i \; {}^{r+1}C^i_{H_j} \exp(2\pi i \, {}^{r+1}\gamma^i_{H_j} z_{r+1}) - \sum_{1}^{2n}{}_i \; {}^{r}\gamma^i_{H_j} \; {}^{r}\psi^i \; {}^{r}C^i_{H_j} \exp(2\pi i \, {}^{r}\gamma^i_{H_j} z_{r+1}) \end{aligned}\right\} \quad (11b)$$

. . . . . .

. . . . . .

$$\left.\begin{aligned} \delta &= \sum_{1}^{2n}{}_i \; {}^{k}\psi^i \; {}^{k}C^i_{H_j} ({}^{k}\Gamma_{H_j} + {}^{k}\gamma^i_{H_j}) \\ H_j &= 0, H_1, H_2, \ldots, H_m \end{aligned}\right\} \quad (11c)$$

where δ is $2\Gamma_0$ when $H_j = 0$ and zero otherwise.

---

* In order to determine the electron wave field in each slice, the boundary conditions must be applied simultaneously on both surfaces of the slice. This prevents one from using a 'sequential' procedure (Hirsch *et al.*, 1965, ch. 12). In other words, the amplitudes of the Bloch waves in each slice do not depend only on the preceding slices, but also on those which follow. The ψ's must therefore be self-consistent and are determined simultaneously throughout the crystal.

Equations (11*a*) are referred to the interface between the bulk and the first slice, equations (11*b*) are referred to the interface between the rth and the $(r+1)$th slice, and the last group of equations (11*c*) concern the interface between the kth slice and vacuum.

The indexes on top of the symbols indicate the particular slice to which they are referred and $z_r = t_k + t_{k-1} + \ldots + t_r$ is the total thickness between the top surface of the crystal and the interface where the boundary conditions are applied. There is a total of $2nk+n$ equations and unknowns. The $2n$ amplitudes ψ^i will be used to build up the total electron wave field in the last slice, and the vacuum diffracted amplitudes will be calculated in the same way as for the uniform crystal (Colella & Menadue, 1972).

6. Discussion

The dynamical theory of electron diffraction as developed by Bethe (1928) is based upon a triply periodic expansion of the crystal potential in reciprocal space. The validity of such expansion in a crystal plate whose thickness is of the order of a few ångströms is a matter of discussion.

Takagi (1969) put forward a dynamical theory of electron diffraction for distorted crystals, where the amplitudes of the Bloch waves (ψ^i) vary with position in the crystal, and are given by a system of first order linear differential equations, provided that these amplitudes are almost constant along the distance of the order of few lattice constants. One of the computational procedures to solve such a system consists of dividing the crystal in slices and integrating analytically within each slice, by matching the solutions at each interface between two adjacent slices. This procedure, which is equivalent to that described in §5, has been employed in a two-beam case of X-ray diffraction where dynamical theory was applied to a crystal irradiated with α particles (Burgeat & Colella, 1969).

A strict justification of the procedure described above would require an accurate knowledge on the way the Fourier components of the potential change with depth near the crystal surface. Nevertheless, it is worthwhile to perform some calculations using this model with reasonable assumptions concerning V_0 and V_{Hj}, and to observe how the computed diffraction profiles are affected. These calculations will be discussed in the next paper (Colella & Menadue, 1972).

7. Conclusions

The dynamical theory of electron diffraction originally developed by Bethe (1928) has been applied to the Bragg case of diffraction, in the general case in which $n(\geq 2)$ strong beams are excited, either towards or away from the entrance surface. The general solution of the dispersion equations, without the usual approximations valid in the transmission case, gives rise to $2n$ Bloch waves. Of these only n survive in the semi-infinite crystal, those which are exponentially damped inwards. The boundary conditions on the top surface allow the calculation of the absolute amplitudes of the various Bloch waves. A slice treatment, based on the present theory, has been attempted, in order to take into account possible changes of the inner potential near the surface. Some computational details have been elucidated, while actual calculations and comparison with experimental results are described by Colella & Menadue (1972).

The author is indebted to Professor B. W. Batterman, for pointing out the interest for this work, and also for a number of fruitful discussions. His thanks are also due to Dr I. Galligani of C. C. R. Euratom, Ispra, Italy, who gave useful suggestions for the numerical computation of the eigenvalues. This work was made possible through a grant from the Air Force Office of Scientific Research (AF-AFOSR-1652-69) and was aided by the support facilities of the Materials Science Center at Cornell University.

References

BETHE, H. A. (1928). *Ann. Phys. Lpz.* **87**, 55.
BURGEAT, J. & COLELLA, R. (1969). *J. Appl. Phys.* **40**, 3505.
COLELLA, R., & MENADUE, J. F. (1972). *Acta Cryst.* A**28**, 16.
COWLEY, J. M. (1969). *Acta Cryst.* A**25**, 129.
FADDEEVA, V. N. (1959). *Computational Methods of Linear Algebra.* New York: Dover.
HIRSCH, P. B., HOWIE, A., NICHOLSON, R. B., PASHLEY, D. W. & WHELAN, M. J. (1965). *Electron Microscopy of Thin Crystals.* London: Butterworths.
LAMLA, E. (1938). *Ann. Physik*, **32**, 178.
PARK, R. L. & FARNSWORTH, H. E. (1964). *Surface Sci.* **2**, 527.
PINSKER, Z. G. (1953). *Electron Diffraction.* London: Butterworths.
SIEGEL, B. M. & MENADUE, J. F. (1967). *Surface Sci.* **8**, 206.
STERN, R. M., PERRY, J. J. & BOUDREAUX, D. S. (1969). *Rev. Mod. Phys.* **41**, 275.
TAKAGI, S. (1969). *J. Phys. Soc. Japan*, **26**, 1239.
YOSHIOKA, H. (1957). *J. Phys. Soc. Japan*, **12**, 618.