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Dynamical Theory of X-ray Diffraction – A Review

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ABSTRACT

A brief review is given of the development of the dynamical theory of x-ray diffraction from crystals. It begins with the geometrical theory and kinematical theory and then goes on to the dynamical theories, where the plane-wave and spherical-wave approximations for perfect crystals and distorted crystals are discussed. The statistical dynamical theory and the calculation schemes for multiple diffraction and grazing incidence geometry are also reviewed.

Key Words: dynamical theory, interaction of x-rays with crystal lattices, x-ray diffraction

I. Introduction

X-rays, discovered by Wilheim Conrad Rontgen more than one hundred years ago, have had a tremendous impact on the evolution and development of modern sciences and technologies, where x-ray diffraction from crystals has played an important role in basic research and industrial applications. For example, x-ray diffraction from single crystals makes possible crystal-structure determination and lattice defect mapping; x-ray diffraction from polycrystalline materials (powders) provides various means of phase identification, structure recognition, and materials characterization; and x-ray diffraction from surface/interface reveals quasi two-dimensional structures and related phenomena in magnetic, metallic, semiconducting, superconducting, and even biological systems. Moreover, with the advent of synchrotron radiation, x-ray diffraction from perfect crystals has become important in designing x-ray optical components for beamlines.

1996 marked the centennial of the discovery of x-rays, but it is not too late to celebrate this great achievement in science. Thus, it seems appropriate to give the following review of the development of x-ray diffraction theories, especially the dynamical theories, based upon which various diffraction mechanisms have been understood and useful experimental techniques designed.

II. Geometrical/Kinematical Theories of X-ray Diffraction

Theoretical investigation into the propagation of electromagnetic waves in a three-dimensional periodic array of dipoles, a few angstroms (A) apart, was initiated by P. P. Ewald in 1911 (Ewald, 1962a), even before the discovery of x-ray diffraction by Laue, Friedrich, and Knipping (Ewald, 1962a). This theory of the dispersion of light in crystals later formed the basis for the then called 'dynamical theory of x-ray diffraction' (Ewald, 1916a, 1916b, 1917, 1937).

In 1912, soon after Friedrich's and Knipping's x-ray diffraction experiments on a copper sulfate crystal, Laue derived a simple theory based on the diffraction and interference of waves in three-dimensional gratings. This is Laue's well-known geometrical theory, which specifies diffractions via three vector equations:

$$\vec{a}\cdot(\vec{s}-\vec{s_0})=h\lambda,\quad \vec{b}\cdot(\vec{s}-\vec{s_0})=k\lambda,$$

$$\vec{c}\cdot(\vec{s}-\vec{s_0})=l\lambda, \tag{1}$$

where $\vec{a}$, $\vec{b}$, and $\vec{c}$ are the basis vectors of a crystal lattice, $\vec{s}$ and $\vec{s_0}$ stand for the scattered and the incident unit wavevectors, and λ is the x-ray wavelength. Here, h, k, and l are integers for constructive interference.

This theoretical treatment is also called Laue's kinematical theory because Laue considered x-ray diffraction by a simple space lattice as the scattering of a set of plane waves by the lattice points, where these lattice points become the centers of spherical scattered wavelets. The following assumptions were made by Laue to simplify this scattering problem: (1) The

interaction between the incident waves and the scattered waves is neglected; (2) each scattered wave travels through the crystal without being rescattered by other lattice points; and (3) no absorption is considered for both the incident and the scattered waves within the crystal. As a result, the scattered amplitude is governed only by the phase factor determined by Eq. (1). The corresponding scattered intensity then takes the familiar form of $\sin^2 n\chi/\sin^2\chi$, which is usually encountered in optics for interference (James, 1962).

III. Darwin's Kinematical Theory and Extinction

Laue's kinematical theory is not rigorous in the sense that multiple scattering of x-rays by the various lattice points, or more precisely, the atoms in a crystal, is not considered and the law of the conservation of energy is violated becasue the energy of the incident wave passing through the crystal is treated as being constant. From 1913 to 1914, C. G. Darwin developed a rather complete theory (Darwin, 1914a, 1914b), which took into account multiple scattering in the diffraction process. In his theory, x-ray reflection from a crystal is regarded as successive reflections of x-rays by the many parallel atomic planes which form the crystal. For simplicity, multiple scattering within each plane is neglected. Suppose that T_j and R_j are the amplitudes of the incident and reflected waves, respectively, at the j-th plane. By considering the interchange of energy between the incident and the reflected beams, for example, the contribution of R_j through the reflection of T_j by the j-th plane and the transmission of R_{j+1} through the j-th plane, the following recurrence relations can be established:

$$R_j=-iqT_j+(1-iq_0)e^{-i\phi}R_{j+1} \tag{2}$$

$$T_{j+1}=(1-iq_0)e^{-i\phi}T_j-i\overline{q}\ e^{-2i\phi}R_{j+1}, \tag{3}$$

where $-iq$ is the reflection coefficient, $(1-iq_0)$ a transmission coefficient, and q and q_0 are defined as (James, 1962)

$$q=-(Nd\lambda/\sin\theta)f\cdot r_e \tag{4a}$$

$$q_0=-(Nd\lambda/\sin\theta)f_0 r_e. \tag{4b}$$

N, d, and f are the number of atoms per unit volume, the inter-planar distance, and the atomic scattering factor, respectively. 2θ is the scattering angle for the given reflection, and $f_0=f(\frac{\sin\theta}{\lambda}=0)$. The phase factor ϕ is equal to $\frac{2\pi}{\lambda}d\sin\theta$. $\overline{q}$ is the reflection coefficient from the lower side of the j-th plane, and r_e is the classic radius of the electron. Equations (2) and (3) lead to the amplitude ratio given below:

$$R(\theta)=\frac{R_0}{T_0}=\frac{-q}{q_0+v\pm\sqrt{(q_0+v)^2-q\overline{q}}}, \tag{5}$$

where v is defined as $(2\pi/\lambda)d\sin\theta=m\pi+v$; $v=0$ as $\theta=\theta_0$ (Bragg angle). Accordingly, the integrated intensity from a perfect crystal plate of both σ- and π-polarization is

$$I=\int R(\theta)\,d\theta=\frac{8}{3\pi}\frac{N\lambda^2}{\sin 2\theta_0}r_e\left|f(2\theta)\right|\cdot\frac{1+\left|\cos 2\theta_0\right|}{2}, \tag{6}$$

which is Darwin's well-known formula. This is in contrast to the expression for imperfect crystals:

$$I=\frac{N^2\lambda^3}{\sin 2\theta_0}\left|f(2\theta)\right|^2 r_e^2\left(\frac{1+\cos^2 2\theta_0}{2}\right). \tag{7}$$

That is, Darwin's treatment is a dynamical rather than kinematical approach. As can be seen, Eq. (6) differs from Eq. (7) in the power of $|f(2\theta)|$. This fact has been the source of the discrepancy between the measured and the theoretical integrated intensities in many x-ray diffraction experiments. To explain this discrepancy, Darwin proposed a mosaic structure for crystals; i.e., an imperfect crystal consists of many slightly misoriented perfect crystal blocks. Darwin then predicted the so-called primary extinction (i.e., the decrease in the diffracted intensity) due to the total reflection of x-rays from perfect crystals and the secondary extinction due to gradual reflection of x-rays from separate crystal blocks satisfying Bragg's law. This consideration leads to Eq. (6) for primary extinction and Eq. (7) for secondary extinction. It should be noted that the idea of mosaic crystals is only an ideal picture for real crystals which accounts for the discrepancy in actual intensity measurements. In reality, it is difficult for real crystals to form such a mesoscopic structure.

IV. Ewald's Dynamical Theory

Ewald's dynamical theory deals also with the intensity of x-ray reflection by crystals by considering the dynamical interaction of the scattered waves and the crystal lattice. Independent of the work of Darwin, Ewald expressed the laws of crystal optics in terms of the discrete lattice, instead of in terms of the continuum. According to Ewald (1916a, 1916b, 1917, 1937), when x-rays propagate in a crystal, each lattice-point of the crystal acts as an oscillating dipole, which in turn radiates an electromagnetic wave (EM wave).

Therefore, the dipole wave and the EM wave form a dynamically self-contained system, where the wavevector $\vec{K}$ of the dipole wave and the wavevector $\vec{k}$ of the EM wave are related by $K=k(1+\epsilon)$, where ϵ is the deviation of the refractive index from unity. In this self-contained system, a dipole wave in the lattice is accompanied by an EM wave travelling at a speed very close to the speed of light, whose amplitude is inversely proportional to the difference between K and k, i.e., $k\epsilon$.

The relation between the moment $\vec{p}$ of a dipole and the excited EM field E is governed by

$$\vec{E}=\frac{2\pi}{V}\sum_m \vec{p}_{\perp m}\frac{1}{\epsilon_m}e^{2\pi i\vec{K}_m\cdot\vec{r}}, \tag{8}$$

where $\vec{p}_{\perp m}$ is the component perpendicular to the wavevector $\vec{K}_m$. Since $\vec{E}=-\frac{m}{e^2}(\omega^2-\omega_0^2)\vec{p}$ is the steady-state solution of the equation of motion of the dipole with ω_0 as its natural frequency, the maximum dipole moment b satisfies the following relation:

$$\vec{b}=-\delta\sum_m \vec{b}_{\perp m}\frac{1}{\epsilon_m}, \tag{9}$$

where $\delta=1/[\frac{m}{2\pi e^2}(\omega^2-\omega_0^2)V]=1-n$, the correction in the refractive index n.

For a simple Bragg reflection, the so-called 2-beam (O, G) case, the dispersion equation, derived from the coefficients of Eq. (9), takes the form

$$\frac{1}{\epsilon_0}+\frac{1}{\epsilon_m}=-\frac{1}{\delta}. \tag{10}$$

The starting points of the wavevectors $\vec{K}$, the so-called wave-points according to Ewald, therefore lie on a certain hyperboloid. The excitation of dipole waves to generate EM waves, namely, the excitation of the dispersion surface, depends on the crystal boundary. As is usual in optics, the tangential components of the wavevectors inside and outside the crystal at the boundary must be continuous for phase matching. This leads to the rule of selecting the proper wave-points on the dispersion surface. By applying appropriate boundary conditions for the generated EM waves, the intensities of the direct reflection O and the diffraction G can be calculated.

It should be noted that the development of the dynamical theory of Ewald was a formidable task in the early 1900s because Fourier transform was not available that time.

V. Laue's Dynamical Theory

Soon after the discovery of electron diffraction in 1927, H. A. Bethe developed a dynamical theory of electron scattering (Bethe, 1928), analogous to Ewald's x-ray dynamical theory. In Bethe's theory, the electrons are taken as the scatters with a continuous three-dimensional periodic distribution of the internal crystal potential. This work inspired Laue and a different version of dynamical theory was then developed. In his treatment, in place of the arrays of dipole resonators, Laue considered a crystal as a continuous three-dimensional periodic complex dielectric medium which represents continuous electron density with positive charges located at the centers of atoms (Laue, 1931). The polarization of the crystal by the electric field of the incident wave depends on the strength of the local electric field.

Based on the macroscopic point of view, Laue applied Maxwell's equation to describe x-ray diffraction from a crystal. The solutions to Maxwell's equation are the Bloch functions, expressed as

$$D(\vec{r},t)=\sum_G \vec{D}_G\exp(i\omega t-2\pi i\vec{K}_G\cdot\vec{r}) \tag{11}$$

for electric displacements, where $\vec{K}_G$ is the wavevector of the G-reflection satisfying Bragg's law, i.e.

$$\vec{K}_G=\vec{K}_O+\vec{g}_G \tag{12}$$

for every G-reflection involved.

Let the electric susceptibility, $\chi/4\pi$, be expressed as a Fourier series:

$$\chi=\sum_G \chi_G\exp[-2\pi i(\vec{g}_G\cdot\vec{r})], \tag{13}$$

where

$$\chi_G=-\frac{r_e\lambda^2}{\pi V}F_G. \tag{14}$$

Here, F_G is the structure-factor of the G-reflection, r_e is the classic radius of the electron (i.e. $r_e=\frac{e^2}{mc^2}$), λ is the x-ray wavelength and V the volume of a crystal unit cell.

After substituting the Bloch functions and the electric susceptibility into Maxwell's equations, the Fourier components satisfy the so-called fundamental equation of wavefield given below:

$$\frac{K_G^2-k^2}{K_G^2}\vec{D}_G=\sum_L \chi_{G-L}\vec{D}_{L(\perp\vec{K}_G)}, \tag{15}$$

where $\vec{D}_{L(\perp\vec{K}_G)}$ represents the vector component of D_L perpendicular to the wavevector $\vec{K}_G$ and $k=1/\lambda$.

Employing the approximation $\vec{D}\cong\vec{E}$ at x-ray frequencies (Laue, 1931) and considering the polarization

of x-rays, the fundamental equation can be written in the following matrix form:

$$\Phi[\vec{E}]=0,$$

where $\vec{E}$ is a column vector, expressed horizontally as $\vec{E}=[E_{\sigma O}E_{\pi O}E_{\sigma G_1}E_{\pi G_2}...E_{\sigma G_{N-1}}E_{\pi G_{N-1}}]$, and Φ is a $(2N\times 2N)$ complex matrix, with the diagonal terms equal to $\Phi(i,i)=\chi_O-2\alpha_i$ and the off-diagonal terms $\Phi(i,j)=\chi_{i-j}p_{i-j}$ with $2\alpha_i=(\vec{K}_{G_i}^2-k^2)/k$. N is the number of Bragg reflections involved, and σ and π are the polarization unit vectors perpendicular to and lying in the plane of incidence, respectively. The polarization factor p_{i-j} is the product of the corresponding polarization unit vectors. The 2α's are the eigenvalues, which can be determined from the dispersion equation $\det[\Phi]=0$ for non-trivial solutions for $\vec{E}$, where det stands for a determinant. The real parts of the 2α's describe the dispersion relation between the wavevectors and the crystal angular settings while the imaginary parts yield the absorption. The fundamental equation also gives the eigenvectors, i.e., the ratios of the wavefield amplitudes among the diffracted beams. Their absolute amplitudes can be determined from the boundary conditions usually adopted in electromagnetism. Hence, the diffracted intensities can be calculated accordingly.

Several review articles and books have been written based on this rather simple version of dynamical theory (Zachariasen, 1945; Borrmann, 1959; Laue, 1960; James, 1962, 1963; Ewald, 1962b; Kato, 1963a, 1974; Batterman and Cole, 1964; Authier, 1970; Pinsker, 1978; Chang, 1984; Authier *et al.*, 1996).

VI. Spherical-wave Dynamical Theory

The dynamical theories discussed above are mainly for x-ray diffraction from perfect crystals using plane-wave approximation. In 1959, Kato and Lang investigated interference effects in dynamical diffraction on a wedge-shaped crystal and found that the observed interference patterns could only be accounted for if the incident wave was a spherical wave (Kato and Lang, 1959). Kato then developed the spherical-wave version of dynamical theory (Kato, 1961a, 1961b, 1968a, 1968b).

The essential point of the spherical-wave theory is that the x-ray beam divergences of laboratory sources are usually one-order of magnitude or more larger than the FWHM of a dynamical diffraction. In other words, the actively excited region is not a small portion but the entire dispersion surface as far as the dynamical excitation of the crystal is concerned. Therefore, all the wavepoints on the dispersion surface are excited, and the interactions among the various x-ray waves must be considered in the dynamical diffraction process. Two-dimensional integration over those wavepoints in the reciprocal space is then needed for all the wavefield amplitudes. With the aid of Kelvin's stationary-phase approximation (Kato, 1974), the expressions for diffracted intensities involve zero-th and first-order Bessel functions of the first kind. The derivation of this theory is very lengthy, and interested readers are advised to refer to Pinsker's book (Pinsker, 1978).

VII. Dynamical Theories for Distorted Crystals

The development of a theory for dynamical diffraction from distorted crystals was initiated by Penning and Holder (1964, 1968a, 1968b) and then by Kato (1963b, 1964a, 1964b). Ray approximation in the optics of the visible spectra was adopted to handle the scattering from areas with deformation gradients. This approach is useful although in interpreting the experimental results, it is not very general as far as the application is concerned. A generalized theory, which could cover x-ray diffraction from both perfect and distorted crystals, was then needed. In 1962 Takagi proposed the fundamental equations for distorted crystals based on Darwin's recurrence relations. These were called Takagi equations or, later, Takagi-Taupin equations (Takagi, 1962, 1969; Taupin, 1964). Solutions to these equations for transmission (Laue) cases and reflection (Bragg) cases were then published by Authier and Simon (1968), Afanasiev and Kohn (1971) and Uragami (1969), respectively.

For slightly distorted crystals, the amplitudes of the electric displacement are a function of the position inside the crystal. Taking this assumption into account in Maxwell's equations, Takagi derived the following fundamental equations of wavefields for slightly distorted crystals (Takagi, 1962):

$$-i\frac{\lambda}{\pi}\frac{\partial D_O}{\partial s_O}=\chi_O D_O+p\chi_{-G}D_G \qquad (16)$$

$$-i\frac{\lambda}{\pi}\frac{\partial D_G}{\partial s_G}=(\chi_O-\alpha_G)D_G+p\chi_G D_O, \qquad (17)$$

where $\vec{s_O}$ and $\vec{s_G}$ are the unit vectors along the refracted and reflected beams, respectively. p is the polarization factor, which equals unity for σ-polarization and $\cos 2\theta_0$ for π-polarization. The geometrical factor α_G is defined as

$$\alpha_G=(K_G^2-K^2)/k^2, \qquad (18)$$

which is the unknown variable to be determined.

For a crystal with large lattice distortion, the Takagi-Taupin equations are still valid, except that now the interbranch scattering due to the jumping of excited wavepoints on the dispersion surface should be considered. This is different from the Eikonal theory (ray optics) in that the lattice distortion is so large that it is no longer possible to define a ray. Therefore, the Eikonal theory of optics is invalid. In this case, the wavefield amplitudes through the largely distorted crystal may be evaluated step by step by means of the Takagi-Taupin equations using a grid, as proposed by Authier *et al.* (1968), to divide the diffraction Borrmann fan of a given reflection (Borrmann, 1959) into a large number of small cells. Within each cell, the lattice distortion is considered to be small, so that the Takagi theory is still valid.

VIII. Statistical Dynamical Theory

Statistical dynamical theory is an extension of Kato's extinction theory (Kato, 1976a, 1976b, 1979, 1980a, 1980b, 1980c). The aim was to provide a unified theory which could deal with primary and secondary extinction simultaneously, namely, a theory valid for perfect and imperfect crystals. The theory first derives the energy-transfer equation (or reflection-power transfer) from Maxwell's (wave) equation for a small portion of the crystal. This equation is of a kinematical nature. The theory then considers the coupling between these kinematical equations of different portions and leads to the dynamical theory. In this approach, x-ray diffraction from a crystal is considered as an ensemble of various routes needed for x-ray diffraction to occur in the Borrmann-fan triangle. Within the triangle, there are millions of routes for successive x-ray reflections with a minimum step equal to an interdistance of atomic planes. Therefore, the diffracted intensities are the ensemble average of all the individual diffracted intensities associated with the routes mentioned. With this scheme, Kato was able to obtain an analytical expression for the intensities of x-ray diffraction for perfect and imperfect crystals; or more precisely, for primary, secondary, and even mixed extinction (Kato, 1980b, 1980c).

IX. Dynamical Theories for Many-beam Cases

Many-beam diffraction, or so-called multiple diffraction, is a combination of several two-beam diffractions. Hence, one can regard multiple diffraction as generalized two-beam diffraction. Diffraction theories for multi-beam cases have, therefore, been derived from the two-beam diffraction theories. In 1928, Mayer (Chang, 1984) attempted to account for his four-beam experiments using Ewald's dynamical theory. Later Renninger (Renninger, 1937) presented a semi-quantitative theoretical treatment for Renninger reflection. Also, Ewald (1937) formulated the dispersion equation and the excitation of wavefields in crystals for 3-beam dynamical diffraction. In 1958, Kato (Kato, 1958) derived a matrix formulation for multi-beam diffraction and Laue then applied his dynamical theory to 3-beam cases (Laue, 1960). Other contributors to this particular theory were Saccocio and Zajac (1965a, 1965b), Hildebrandt (1966), Joko and Fukuhara (1967), Ewald and Heno (1968), Heno and Ewald (1968), and many others. It should be noted that Ewald and Heno gave a detailed analytical expression for the dispersion relation of wavevectors in reciprocal space and discussed the relationship between the dispersion surface and reflection phases. A relevant theory was also given by Penning and Polder (1968a, 1968b). Recently, a dynamical approach, interpreting the diffracted intensity in Bragg type multiple diffraction, has been pursued by Colella (1974), and Chang (1982a, 1984).

Kinematical theories for multi-beam diffraction, involving equations of power-transfer, were reported by Moon and Shull (1964), Zachariasen (1965), Caticha-Ellis (1969), and Chang (1982b).

The formalism of the dynamical theory for multiple diffraction is exactly the same as that for 2-beam cases (see Sec. III). However, unlike the case in 2-beam cases, analytical expressions for dispersion relation and diffracted intensities are difficult to derive in multi-beam cases because of complications introduced by the presence of the third reflection and by the polarization factors for three-beam diffraction geometry. Therefore, numerical calculation becomes a must in interpreting experimental results. Usually, in dynamical calculations, the σ-, π-polarization vectors, and the wavevector $\overline{K}$ of a given reflection are defined as being mutually orthogonal to one another, and the polarization unit vectors serve as the reference directions in analyzing the components of the electric displacements of the x-ray wavefields. Details about the theory and computing scheme can be found in the references (Colella, 1974; Chang, 1984).

X. Dynamical Theories for Grazing Incidence

Grazing incidence x-ray diffraction (GIXD) from crystal surfaces and interfaces has been widely used in surface structure determination. This kind of diffraction takes place when the incident angle θ_i is set close to the critical angle of the total external reflection.

The beam diffracted by a set of atomic planes perpendicular to the crystal surface is specularly reflected by the crystal surface in a direction tilted slightly off the surface. A dynamical formulation was first derived by Afanasiev and Melkonyan (1983) for dynamical GIXDs. The main difference between it and the conventional theory (wide-angle) is that the specularly reflected beams are considered in the diffraction process. That is, the specularly reflected and diffracted wavefield amplitudes are included in the boundary conditions. Further theoretical development along this line includes the geometrical analysis of GIXD (Durbin and Gog, 1989), and extension of the GIXD theory to multi-beam GIXDs (Hung and Chang, 1989; Tseng and Chang, 1990; Stepanov and Ulyanenkov, 1994).

The reciprocal lattice of a truncated crystal surface is a combination of the 2-dimensional reciprocal rods of the surface and the 3-dimensional discrete reciprocal lattice points of the crystal bulk. To analyze the quasi 2-dimensional structures of surfaces/interfaces from GIXD data, very often, the surface normal scan (the so-called crystal truncation rod scan) in the reciprocal space is employed. Interpretation of the diffracted intensity distributions of rod scans has been a difficult task in terms of the dynamical theory of GIXD. Attempts have been made (Colella, 1991; Caticha, 1993) in recent years, but only specular rods involving no surface in-plane momentum transfers can be accounted for using Darwin's dynamical theory (Nakatani and Takahashi, 1994; Caticha, 1994). The other type of rod scan, the non-specular rod, which involves surface in-plane momentum transfers, still poses a problem in developing a suitable dynamical theory for GIXD in general. The difficulty, according to Gau and Chang (1995), is the non-linear equations of high-order polynomials involved in the dispersion surface and the angle-dependent off-diagonal elements of the scattering matrix Φ. Numerical solutions to the non-linear dispersion equations can only be found asymptotically (Gau and Chang, 1995) by means of numerical calculations. Although the numerical analysis scheme proposed is useful in describing the intensity distributions of rods, it is very time-consuming to perform this type of calculation. A directly solvable scheme for this particular problem is desired. Very recently, Stetsko and Chang (1997) proposed a generalized dynamical calculation algorithm which can handle all of the wide-angle and grazing-angle x-ray diffraction from bulk crystals and surfaces/interfaces. The above stated difficulties can be eliminated by adapting a Cartesian coordinate system with one of the axes, say the z-axis, along the crystal surface normal to define the polarization unit vectors. The angle-dependent off-diagonal elements are automatically absorbed into the eigenvectors of the fundamental equations of wavefields. The eigenvalue equation then becomes a polarization-free linear equation which can be easily solved.

This generalized algorithm has recently been applied to calculate surface nonspecular rods involving three reciprocal lattice points and wide-angle three-beam diffractions. Satisfactory and correct results have been obtained. Details of these calculations will be reported elsewhere (Chien *et al.*[1]).

XI. Discussion and Concluding Remarks

We have briefly reviewed the geometrical/kinematical theories and dynamical theories for various situations, such as perfect crystals, distorted lattices, multi-beam cases, and grazing incidence. The geometrical and kinematical theories are, in general, valid for x-ray diffraction in imperfect crystals while the dynamical theories is applicable to cases involving perfect or nearly perfect crystals. The criterion for applying these theories is determined by the parameter A defined as

$$A=r_e\lambda T|F_G|/(V\sqrt{|\gamma_O\gamma_G|}),$$

where r_e and T are the classical radius of electron and the crystal thickness, respectively. V is the volume of the unit cell, γ_O and γ_G are the direction cosines of the incident beam O and the diffracted beam G with respect to the inward normal to the crystal surface. When the crystal is small, or the reflection involved is weak, or the radiation used is more penetrating, the corresponding A is small, i.e., $A\leq 1$. Under this circumstance, the kinematical theory is suitable for describing the diffraction mechanism. Otherwise ($A>1$), the dynamical theories should be used. Since the dynamical theories are much more fundamental than the kinematical ones, the kinematical theories are special cases of the dynamical theories. By making appropriate assumptions and simplifications, the dynamical theories can certainly lead to the same kinematical formalism. Moreover, the quantum theories of x-ray diffraction are an extension of the dynamical theories. Due to space limitations, we will not discuss them here. In any case, the formation of x-ray wavefields, the excitation of modes of wave-propagation, the dispersion relation, and the dynamical equilibrium of the wavefields in the

[1] Chien, H. C., T. S. Gau, S. L. Chang, and Y. Stetsko, "Dynamical calculation of crystal truncation rods using a Cartesian coordinate system." In preparation.

crystal lattice are the essence of x-ray diffraction and have contributed importantly to our understanding of x-ray crystal optics, to the design of advanced x-ray diffraction apparatus, and to solving long-standing difficult problems, such as extinction and x-ray phase problems.

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X光動力繞射理論之回顧

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摘　要

本文就X光對晶體之動力繞射理論之發展，從幾何繞射理論、靜力繞射理論、到動力繞射理論，作了簡單的回顧。動力理論中的平面波與球面波近似法、以及處理完美單晶和晶格扭曲晶體之繞射，都作了探討。此外，統計動力繞射理論和用於多光繞射及掠角繞射之動力理論計算方式，亦加以解釋說明。