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A New Approach for *n*-Beam Dynamical Calculations

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Abstract

With the use of modulated plane waves, a new method for *n*-beam dynamical calculations has been established on the basis of a paper by Watanabe, Kikuchi, Hiratsuka & Yamaguchi [*Phys. Status Solidi A* (1988), **109**, 119-126]. The computing time is reduced to about one-sixth of what it originally was and a large reduction of memory is achieved. *n*-beam dynamical calculations of aluminium, copper and gold at several accelerating voltages and orientations were carried out in a completely parallel manner by the present method, the multi-slice method and Bethe's eigenvalue method [Fujiwara (1959). *J. Phys. Soc. Jpn* **14**, 1513-1524]. The present method turned out to be competitive with respect to accuracy and speed in comparison with the latter two methods. The new method makes *n*-beam dynamical calculations of complex systems and defects possible.

1. Introduction

After direct-lattice images from a large unit cell (Allpress, Sanders & Wadsley, 1969; Uyeda, Kobayashi, Suito, Harada & Watanabe, 1972; Hashimoto, Endo, Tanji, Ono & Watanabe, 1977) were observed by high-resolution electron microscopy, the development of electron microscopy made

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it possible to observe the direct-lattice images of diamond (Izui, Furuno, Nishida, Ohtsu & Kuwabara, 1987) and zinc-blende semiconductors (Yamashita, Ponce, Pirouz & Sinclair, 1982; Shiojiri, Kaito, Sekimoto & Nakamura, 1982; Watanabe, Hiratsuka, Kikuchi & Yamaguchi, 1987; Wright, Ng & Williams, 1988). For zinc-blende semiconductors, in particular, it is worthwhile to identify the atomic species. Furthermore, the determination of complex structures such as oxide superconductors (Hiraga, Hirabayashi, Kikuchi & Sindo, 1988) has also been carried out. It is one of today's powerful techniques for examining crystal structure at an atomic scale. However, the investigation of crystal structure using high-resolution electron microscopy always demands image interpretation from n-beam dynamical calculations of electron diffraction.

Since Bethe (1928) developed the dynamical theory of electron diffraction, the problem of dynamical-scattering electrons has been tackled over the last thirty years by a variety of workers (Fujimoto, 1959; Cowley & Moodie, 1957; Hirsch, Howie, Nicholson, Pashley & Whelan, 1965; Howie & Basinski, 1968; Van Dyck, 1980). Correlations between these approaches have been discussed in detail (Jap & Glasser, 1978; Gratias & Portier, 1983). The most published theories of n-beam dynamical calculation may be roughly divided into two classes, those considering the crystal as an infinite number of successive planes of infinitesimal thickness, and those considering the crystal as an infinite three-dimensional medium. The former is called the multi-slice method and was set up by Cowley & Moodie (1957). A numerical method based on finite-slice approximation was proposed by Goodman & Moodie (1974). Ishizuka & Uyeda (1977) further reduced the calculation time to evaluate the electron transmission function with a fast-Fourier-transform algorithm, so that it became possible to calculate defect images using the periodic continuation approximation (Fields & Cowley, 1978). While the multi-slice method is the most convenient and flexible theory, the selection of slice thickness for complex systems and of slice position has not been completely solved. In the second approach, which is called Bethe's eigenvalue method (Fujiwara, 1959), the Schrödinger equation for an electron is solved under the appropriate boundary conditions by assuming three-dimensional periodicity. The problem involves the solution of a large secular equation. Unless the calculation is reduced using symmetry, it is difficult to evaluate lattice images of a complex system with the present state of computer technology. Furthermore, it is conceptually inadequate for defects because of its assumptions. There are disadvantages in either case.

A rather different approach has recently been introduced by Watanabe, Kikuchi, Hiratsuka & Yamaguchi (1988) in order to obtain accurate and manageable n-beam dynamical calculations. This has been derived from the Schrödinger equation on the assumption of two-dimensional periodicity. As shown by the results of completely parallel calculations using our method, the multi-slice method and Bethe's eigenvalue method, our method is competitive with respect to accuracy for a (100) lattice image of f.c.c. metals at 100 kV. However, our method requires much computing time and enormous amounts of memory, and it is uncertain whether this method can be precisely applied to various orientations and higher accelerating voltages than 100 kV.

In this paper, we first resolve the problem of large computing time with modulated plane waves and the position-weighted method in which the calculation of scattering is neglected if the potential of the main reflection is less than a threshold energy. Furthermore, we examine (100) and (110) n-beam dynamical calculations for aluminium, copper and gold at 100 and 300 kV, and compare our results with the multi-slice and Bethe's eigenvalue methods.

2. Theory

2.1. *Basic equations*

A detailed discussion of this new approach for n-beam dynamical calculations was given in the original paper (Watanabe *et al.*, 1988), so that it is only briefly described below. A new formula has been derived from the Schrödinger equation using two-dimensional periodicity for thin films. The wave function and its coupled equations are given as

$$\psi(\mathbf{x}, z) = \sum_{\mathbf{G}_\parallel} u_{\mathbf{G}_\parallel}(z) \exp i(\mathbf{k}_\parallel + \mathbf{G}_\parallel)\mathbf{x}/s^{1/2}, \quad (1)$$

$$[(\mathrm{d}^2/\mathrm{d}z^2) + 2E - |\mathbf{k}_\parallel + \mathbf{G}_\parallel|^2 - 2V_0]u_{\mathbf{G}_\parallel}(z) = \sum_{\mathbf{G}_\parallel'} 2V_{\mathbf{G}_\parallel' - \mathbf{G}_\parallel} u_{\mathbf{G}_\parallel'}(z), \quad (2)$$

where $\mathbf{x} = (x, y)$: $\mathbf{G}_\parallel$ = the projection of reciprocal-lattice vector $\mathbf{G}$; s = the area of surface; and $V_{\mathbf{G}_\parallel' - \mathbf{G}_\parallel}$ = the Fourier component of the crystal potential at z.

The above coupling equations were derived on the basis of the same assumptions by different workers (Tournarie, 1962; Hirsch, Howie, Nicholson, Pashely & Whelan, 1967; Howie & Basinski, 1967; Lynch & Moodie, 1972; Ichimiya, 1983). The equation is easily integrated, so that the coefficient $u_{\mathbf{G}_\parallel}(z)$ at the next step is given by

$$u_{\mathbf{G}_\parallel}(\Delta z) = 2\cos(\kappa\Delta z)u_{\mathbf{G}_\parallel}(0) - u_{\mathbf{G}_\parallel}(-\Delta z) + 4[1 - \cos(\kappa\Delta z)] \sum_{\mathbf{G}_\parallel'} V_{\mathbf{G}_\parallel' - \mathbf{G}_\parallel}(0) u_{\mathbf{G}_\parallel'}(0)/\kappa^2 \quad (3)$$

$$\kappa^2 = 2E - |\mathbf{k}_\parallel + \mathbf{G}_\parallel|^2 - 2V_0, \quad (4)$$

where $u_{\mathbf{G}_\parallel}(0)$ and $u_{\mathbf{G}_\parallel}(-\Delta z)$ are the values of the coefficients at the present and previous step, respectively. While the serious problems of numerical

Table 1. *Maximum slice thickness and minimum beam number for convergence*

(100)

	Al	Cu	Au
100 kV	11×11 $a/64$	11×11 $a/256$	11×11 $a/512$
300 kV	11×11 $a/64$	11×11 $a/256$	11×11 $a/512$

(110)

	Al	Cu	Au
100 kV	13×13 $(a/2^{1/2})/64$	13×13 $(a/2^{1/2})128$	13×13 $(a/2^{1/2})/256$
300 kV	13×13 $(a/2^{1/2})/64$	13×13 $(a/2^{1/2})128$	13×13 $a/(2^{1/2})256$

calculation seem to be perfectly bypassed by this integration, it is very time consuming. For example, in order to make the calculation converge, the slice thicknesses of f.c.c. samples must be $a/1024$ at 100 kV, and $a/2048$ at 300 kV, respectively. In this way, our method still presents a formidable problem if a large number of Bragg reflections is considered.

2.2. *Modulated-plane-wave function*

The solution of (3) shows a propagating part with both oscillating and scattering components, and the solution of (4) is greater than the crystal potential $V_{\mathbf{G}_\parallel-\mathbf{G}_\parallel}(z)$ by several orders of magnitude. The time-consuming requirement for a very thin slice is mainly attributed to the first term of (3). To reduce the computing time, therefore, the $u_{\mathbf{G}_\parallel}(z)$ is represented by a modulated plane wave

$$u_{\mathbf{G}_\parallel}(z) = u_{\mathbf{G}_\parallel} \exp(ikz). \tag{5}$$

Substituting (5) into (2), we find that the coefficient $u_{\mathbf{G}}$ satisfies the set of equations

$$[(\mathrm{d}^2/\mathrm{d}z^2)+2ik(\mathrm{d}/\mathrm{d}z)-(k^2+|\mathbf{k}_\parallel-\mathbf{G}_\parallel|^2+2E)]u_{\mathbf{G}_\parallel}(z) = 2\sum_{\mathbf{G}_\parallel'} V_{\mathbf{G}_\parallel'-\mathbf{G}_\parallel}u_{\mathbf{G}_\parallel'}(z). \tag{6}$$

Provided that $k\,\mathrm{d}u_{\mathbf{G}_\parallel}/\mathrm{d}z \gg \mathrm{d}^2u_{\mathbf{G}_\parallel}/\mathrm{d}z^2$ the result is a first-order differential equation,

$$\mathrm{d}u_{\mathbf{G}_\parallel}/\mathrm{d}z-(2ik)^{-1}(k^2+|\mathbf{k}_\parallel+\mathbf{G}_\parallel|^2-2E)u_{\mathbf{G}_\parallel} = (ik)^{-1}\sum_{\mathbf{G}_\parallel'} V_{\mathbf{G}_\parallel'-\mathbf{G}_\parallel}u_{\mathbf{G}_\parallel'}. \tag{7}$$

This equation removes the oscillating part of the propagating electron. Because the right-hand side in (7) is very small for high accelerating voltages, the integration step can be chosen to be very large compared with (3), and much time reduction can be expected. Only continuity at the entrance and exit surfaces is required since the differential equation is first order. This equation is also quite similar to the standard scattering equations (Hirsch *et al.*, 1965; Howie & Basinski, 1967) except for the crystal potential. In our treatment, the unit cell is divided into many slices, and the crystal potential is constructed at each slice position. On the other hand, the standard crystal potential is built up from the structure factor of the unit cell. The viewpoint of our treatment is quite different from the standard one in spite of its similar appearance. For RHEED, similar equations were derived by Maksym & Beeby (1981), and its Fourier transform to real space may also yield a real-space description (Van Dyck, 1980).

2.3. *Position-weighted method*

From the previous paper (Watanabe *et al.*, 1988), it is clear that the amplitude of the diffracted wave changes in the vicinity of atomic planes, and remains constant between them. In other words, scattering occurs mainly around atomic planes and can be neglected between them. Therefore, in order to reduce the calculation time, we use a position-weighted method in which the scattering term in (7) is ignored when the potential for the main reflections is less than the threshold energy. In f.c.c. simulation, these energies are selected on the basis of the 200 potential for (100) dynamical calculation, and of the 111 potential for (110), respectively. As a result, we can further reduce the computing time.

3. Results

The present method has been tested on n-beam dynamical calculations of aluminium, copper and gold, taking account of accelerating voltage and orientation. The crystal potentials were constructed from superposing free atoms (Doyle & Turner, 1968). In the calculations, the choice of beam number and slice thickness affects the accuracy and computing time for the n-beam dynamical calculation. We first discuss the above numerical parameters, and compare the present results with those from the multi-slice and Bethe's eigenvalue methods.

3.1. *Effects of beam number and slice thickness*

In order to estimate the upper limit of slice thickness and the lower limit of beam number, various calculations were carried out for each material. Converged conditions are determined by the sum of deviation functions in the same manner as by Ishizuka & Uyeda (1977). This function is given by

$$R(H,K)=\frac{\sum_{h}^{H}\sum_{k}^{K}||\psi_A(h,k)|-|\psi_B(h,k)||}{\sum_{h}^{H}\sum_{k}^{K}||\psi_A(h,k)|+|\psi_B(h,k)||}. \tag{8}$$

The value of $R(H, K)$ is selected as $R(4, 4)$ for (100), and $R(6, 4)$ for (110), respectively. The resultant conditions in which $R(H, K)$ is less than 0·05 are summarized in Table 1. From this, it is clear that the (100)

n-beam dynamical calculation demands fewer beams than the (110) one, and the beam number is independent of accelerating voltage. The slice thickness decreases with increasing atomic scattering power and is almost independent of accelerating voltage.

3.2. (100) *n-beam dynamical calculation*

The results of (100) n-beam dynamical calculation using the present method were compared with the multi-slice and Bethe's eigenvalue methods. For the simulation of the multi-slice method, slice thickness was a (lattice constant), and beam number was 32×32. The slice thickness is the common condition for aluminium, copper and gold, and this beam number is large. An 11×11 beam number was adopted for Bethe. The present method used convergent-beam number and slice thickness as shown in Table 1. Figs. 1 and 2 show the thickness series of 000 and 220 beam intensities for aluminium, copper and gold calculated with the three methods. At low atomic scattering power, the present method and the other two are superimposed independent of accelerating voltage. As the atomic scattering power is increased, the present method at 100 kV shows little difference from Bethe's method, while it yields large disagreement with the multi-slice results. A poor approximation for gold has already been suggested by Lynch (1971). However, the difference at 300 kV becomes appreciable. The discrepancy with the multi-slice method is qualitatively explained in terms of a sudden perturbed approximation as discussed in the previous paper (Watanabe *et al.*, 1988). According to this, the slice thickness must be chosen to be small enough for low accelerating voltage and high atomic scattering power. Therefore, in the case of gold, this approximation becomes far from satisfactory at 100 kV.

3.3. (110) *n-beam dynamical calculation*

For the (110) n-beam dynamical calculation, 16×16 beam number was adopted for Bethe, and 32×32 beam and $a/2^{1/2}$ slice thickness were used for the

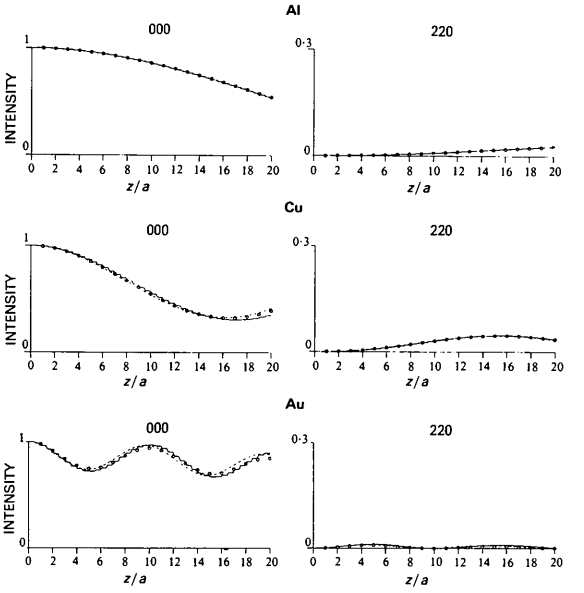

Fig. 2. Beam intensities of the 000 and 220 reflections for (100) n-beam dynamical calculations at 300 kV: multi-slice (circles), Bethe (dashed line) and new method (solid line).

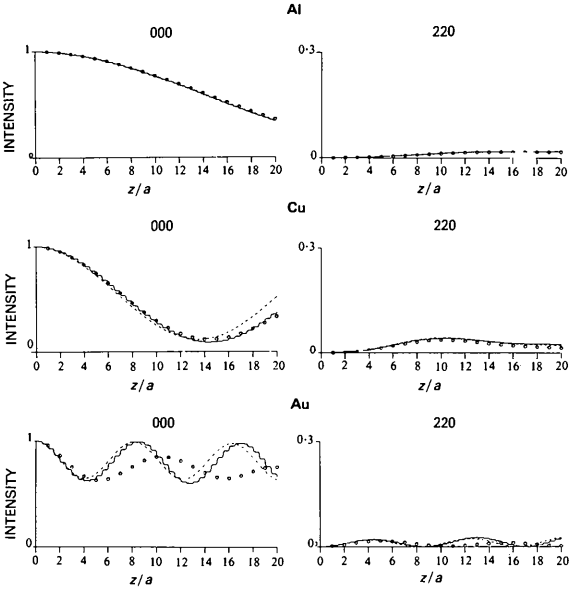

Fig. 1. Beam intensities of the 000 and 220 reflections for (100) n-beam dynamical calculations at 100 kV: multi-slice (circles), Bethe (dashed line) and new method (solid line).

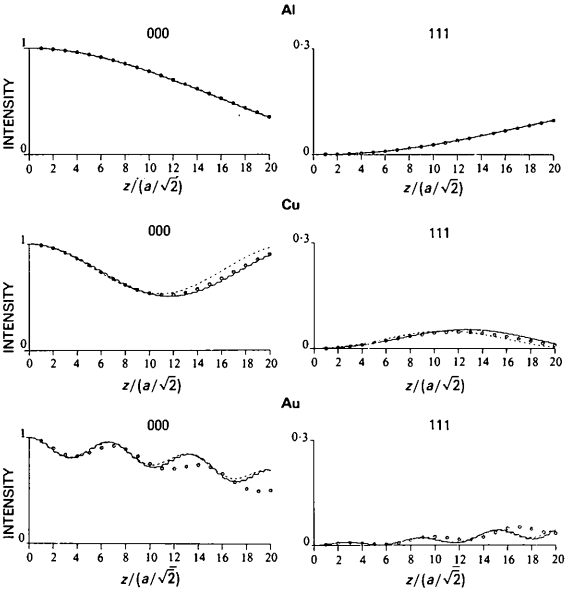

Fig. 3. Beam intensities of the 000 and 111 reflections for (110) n-beam dynamical calculations at 100 kV: multi-slice (circles), Bethe (dashed line) and new method (solid line).

multi-slice method. These parameters made the calculation of these methods converge. The parameters in Table 1 were used for the calculation by the present method. In Figs. 3 and 4, the intensities of the 000 and 111 beams calculated by the three methods are plotted against thickness. The present method is in good agreement with Bethe's for all atomic scattering powers whether the accelerating voltage is 100 or 300 kV. While the multi-slice method is identical with the present one for aluminium, the deviation increases with atomic scattering power. Compared with the (100) n-beam dynamical calculation, the deviation is not so large, and is not drastically diminished with increasing accelerating voltage. This small deviation may be caused by a smaller slice thickness than the (100) one. However, the effect of accelerating voltage cannot be interpreted simply by a sudden perturbed approximation, unlike (100).

4. Concluding remarks

An improved n-beam dynamical equation is derived using modulated plane waves on the basis of a two-dimensional periodic Schrödinger equation. Reductions of calculation time and required memory are achieved, and this method can be applied to various orientations and accelerating voltages. The slice thickness is so small that the calculation has little effect on slice position, unlike the multi-slice method. Thus, it may be expanded not only to complex systems but also to defects using the periodic continuation approximation. The Fourier transform to real space may correspond to the real-space method. In our treatment, two-dimensional periodicity was used in deriving an equation to avoid troublesome two-dimensional Laplacian calculations, whereas the real-space method extracts this problem using a three-point Laplacian approximation. From the results of practical numerical calculations, it becomes evident that maximum slice thickness is a function of atomic scattering power and minimum beam number depends on orientation. Furthermore, the present method turns out to be competitive with respect not only to accuracy but also to speed from the comparison with the multi-slice and Bethe's eigenvalue methods. However, computing time is still about four times as long as for the multi-slice method, although such a calculation time is not a very serious problem with today's advanced computers.

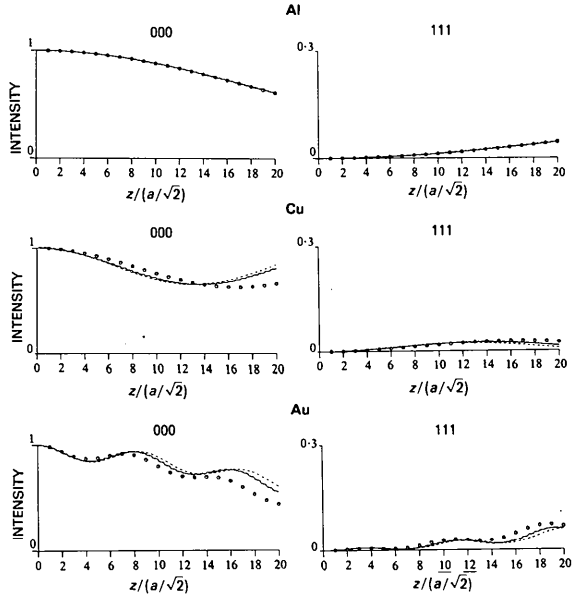

Fig. 4. Beam intensities of the 000 and 111 reflections for (110) n-beam dynamical calculations at 300 kV: multi-slice (circles), Bethe (dashed line) and new method (solid line).

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