There are several criteria that may be used to evaluate the relative merits of the two forms of calculation. First there is the question of calculation time. A fast-Fourier transform will only require $n \,.\, \log_2 n$ operations for $n$ reflexions. However, there is still the necessity to evaluate $\sin[\sigma\varphi(x,y)\Delta z]$ and $\cos[\sigma\varphi(x,y)\Delta z]$ at $n$ sampling points. Thus, although there are required $r \,.\, n^2$ operations for the convolution method, the calculation times remain remarkably close together for a range of values of $n$ (29 to 435). Thus there is no particular advantage in either method on this point.

Second, there are the questions of convenience and amount of memory storage required. In this case, the convolution method is far better as it requires far less storage and the procedure is identical with that used in the kernel of the multislice method, and thus a considerable economy in computer code is achieved. In terms of non-specialist investigators requiring their own routines for calculation, the convolution method is felt to be simpler to set up in the computer.

Finally, there are questions of physical insight gained from intermediate steps in the calculation. In this respect, it is felt that the potential distribution that is calculated in the course of the usual method is a great help, particularly in symmetry considerations and hence the convolution method is at a disadvantage in this case.

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*Acta Cryst.* (1974). A**30**, 102

## A comment on Tiwari, Prasad & Srivastava's paper *The arcing of X-ray diffracion spots in X-ray photographs of cadmium iodide crystals.*

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It is shown that the arcing in X-ray photographs of $CdI_2$ crystals cannot be attributed to paracrystalline distortions in crystals.

In the paper quoted (Tiwari, Prasad & Srivastava, 1973) the authors attempted to explain the arcing on *a*-axis oscillation photographs of $CdI_2$ crystals in terms of paracrystalline distortions. Earlier Prasad & Srivastava (1971) had explained the arcing observed on X-ray *c*-axis oscillation photographs as crystal shape and size effects; this has already been shown to be wrong (Agrawal, 1973). The latter explained it in terms of tilt boundaries consisting of unit and partial edge dislocations created during crystal growth, as Agrawal & Trigunayat (1969*a*,*b*; 1970) and Agrawal, Chadha & Trigunayat (1970) had already suggested in the cases of arcing in X-ray *a*-axis oscillation and Laue photographs of $CdI_2$, $CdBr_2$ and $PbI_2$ crystals. Agrawal (1970, 1971) had also established the correlation between the phenomena of arcing and polytypism on the basis of experimental results. However, it is not necessary that the compounds displaying polytypism should also exhibit arcing, whereas the opposite may be true.

The diffraction patterns observed in $CdI_2$ crystals are quite different from those observed in chain molecules or fibrous crystals. In general, the patterns for natural fibres do not yield the reciprocal lattice of the crystal because, instead of a single crystal, one has a 'two-dimensional powder' resulting from the grouping of crystallites of random orientation along the axis of the fibre. The pattern therefore gives the figure of revolution obtained by rotating the reciprocal lattice for a single crystal around the fibre axis (Guinier, 1963). The crystals of cadmium iodide exhibit arcs of various shapes, *e.g.* fork, cross, square, semi-elliptical, *etc.*, each consisting of two or more spots, corresponding to each reciprocal lattice point (Agrawal & Trigunayat, 1969*a*), whereas in chain molecules or fibrous crystals each reciprocal lattice point gives rise to its own elongated and broadened spot. The intensity and broadening of the spots are a maximum near or at the centre and decrease towards their ends. The $CdI_2$ crystals also exhibit closed rings on Laue photographs each corresponding to a reciprocal lattice point, whereas in the latter case the spots are bridged by intensity ridges forming a ring because various reciprocal-lattice points or nodes at equal distances from the centre of the net are connected to form a ring due to paracrystalline distortions (Vainshtein, 1966). Besides, in the latter case the geometry of the diffraction pattern would not change if the crystal is irradiated either wholly or partially by the X-ray beam because the lattice cells which are different from one another are randomly distributed, whereas in the crystal exhibiting arcing or rings on the photographs, the diffraction pattern does change (Agrawal & Trigunayat, 1969*a*, Figs. 4 and 5; 1969*b*, Figs. 12 and 13).

In the paper quoted the paracrystallinity in $CdI_2$ crystals had been introduced during growth in two possible ways. Firstly, the fluctuations in axial parameters due to water molecules adsorbed on the surface of layers forming the crystal during growth, which itself is unrealistic, would give rise to (i) streaking joining the reflexions on the layer lines due to the *c*-axis fluctuations and (ii) extra spots occurring

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above and below the normal positions of the layer lines because of *a*-axis fluctuations on the *a*-axis oscillation photographs. This explanation of arcing phenomena is contrary to the experimental observations of Lal & Trigunayat (1970, 1971) which showed an increase in arcing or the formation of new arcs on heating the solution-grown $CdI_2$ crystals at about 270°C. Besides, crystals of lead iodide grown by the gel method also exhibit arcing (Agrawal, Chadha & Trigunayat, 1970). Secondly, the growth of incoherent nuclei on top of a flat surface, resulting in small gaps between different domains of the crystal, would affect the shape and the size of the spots. The arcs might be formed but the spots on them would not be resolved because of random growth of incoherent nuclei. Besides, on irradiating the crystal partially by the X-ray beam, the shape of the diffraction pattern would not change; however, the size of the arcs might be affected; this again is contrary to experimental observations (Agrawal & Trigunayat, 1969*a*). Furthermore, the arcing is not a surface phenomenon. It is also observed after cleaving off layers from the surface and it is, in general, found that the arcing decreases in a regular fashion from the lower to upper basal surfaces (Gyaneshwar & Trigunayat, 1972). The latter have also found that the closed rings on Laue photographs do change into arcs when crystals are peeled layer by layer. Under no circumstances can the formation of regular hexagonal, trigonal, *etc.* types of rings corresponding to each reflexion be understood on the basis of paracrystalline distortions randomly distributed in the crystals. When a few $CdI_2$ crystals, grown from solution at room temperature, were re-examined after nearly four years, changes in arcing, streaking and polytypism were observed (Agrawal, 1972); this cannot be explained on the basis of paracrystalline distortions induced during crystal growth. It may be pointed out that the model of a paracrystal is more acceptable for fibrous crystals, which are in fact built up on a two-dimensional lattice, one of the vectors being parallel to the axis of the fibre, and the other perpendicular. The fluctuations of these vectors arise from essentially different sources, *viz.* the interactions along and between the chains.

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*Acta Cryst.* (1974). A **30**, 103

## On the form of the fundamental equations of the dynamical theory of X-ray diffraction.

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Property of the fundamental equations of the dynamical theory of X-ray diffraction given in terms of the electric field **E**(**r**), instead of **D**(**r**), is discussed, and some merits of the equations in terms of **E**(**r**) are pointed out.

The fundamental equations of the dynamical theory of X-ray diffraction according to Laue's formulation are usually given by the form

$$\frac{\mathbf{k}_\mathbf{h}^2 - K^2}{\mathbf{k}_\mathbf{h}^2}\mathbf{D}_\mathbf{h} = \sum_\mathbf{g} \chi_{\mathbf{h}-\mathbf{g}} \mathbf{D}_{\mathbf{g}[\perp \mathbf{k}_\mathbf{h}]} \qquad (1)$$

(Laue, 1960), where $K(=\nu/c)$ is the wave number of X-rays in the vacuum space, $\mathbf{k}_\mathbf{h} = \mathbf{k}_0 + \mathbf{h}$, $\mathbf{k}_0$ being the wave vector of the primary beam in the Ewald (or Bloch) wave field in the crystal, and **h** or **g** is the reciprocal-lattice vector; $\mathbf{D}_\mathbf{h}$ is the Fourier component of the field **D**(**r**) which is defined by

$$\mathbf{D}(\mathbf{r}) = \varepsilon(\mathbf{r})\mathbf{E}(\mathbf{r}) \qquad (2)$$

where **E**(**r**) is the electric field of the X-ray wave, and $\chi_\mathbf{h}$ is the Fourier component of $\chi(\mathbf{r})$, which is a quantity corresponding to $4\pi$ times the 'electric susceptibility' and related to the 'dielectric constant' $\varepsilon(\mathbf{r})$ as

$$\varepsilon(\mathbf{r}) = 1 - \frac{1}{\pi}\left(\frac{e^2}{mc^2}\right)\frac{\varrho(\mathbf{r})}{K^2} = 1 + \chi(\mathbf{r}) \qquad (3)$$

where $\varrho(\mathbf{r})$ is the electron density in the crystal. The notation $\mathbf{D}_{\mathbf{g}[\perp \mathbf{k}_\mathbf{h}]}$ means the component vector of $\mathbf{D}_\mathbf{g}$ parallel to a plane perpendicular to $\mathbf{k}_\mathbf{h}$.

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