and the phases of about 70 more were found in terms of a symbolic sign A. The value of A was then determined from 53 aberrant triples with about 85% consistency. A much higher level of consistency is not expected since the three E's in each aberrant triple are seldom very large (the negative regions in the benzene transform reach only one-third the height of the positive regions). One *MULTAN* cycle based on these 140 reflexions with fixed signs led to an E map in which we could easily identify all 30 non-hydrogen atoms in the two molecules.

In retrospect, the structure could probably have been determined from the initial *MULTAN* E map with a little more persistence on our part, since 20 of the 30 highest peaks turned out to be correct in the end. However, most of the atoms belonging to the ring substituents were missing and, moreover, the false peaks allowed three possible orientations of each naphthalene group. The eventual solution would not have been so straightforward.

We have seen here an example of planar, parallel, similarly oriented, six-membered rings giving rise to aberrant triples at a troublesome level. The question arises: are all these conditions (planar, parallel, similarly oriented, six-membered, ring) necessary for the same difficulty to arise? If we restrict our attention to planar rings it would appear that the only other essential feature is that the rings must be parallel. It is well known that the Fourier transform of a circle (*i.e.* the limit of an n-membered ring) is a zeroth-order Bessel function. This has a negative annulus of depth 0·4 times the magnitude of the origin peak, *i.e.* this trough is relatively even deeper than in the benzene transform and it will produce aberrant triples in just the same way. The arguments of Thiessen & Busing (1974), that pairs of such rings give rise to more complex transforms but to the same aberrant triples, still hold. If rings with equal numbers of atoms lie in parallel planes but in dissimilar orientations, the transform will be complex, in general, but the real part will be similar to the Bessel function, and aberrant triples will still occur. Hence aberrant triples can be a problem when a structure is dominated by similar, parallel, planar rings. Three- and four-membered rings are too far from circular for our argument to apply.

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A varying-step algorithm for the numerical integration of Takagi–Taupin equations.

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Abstract

A varying-step algorithm is presented which allows the automatic selection of the step for the integration of Takagi–Taupin equations.

Takagi–Taupin equations may be solved analytically only in a few cases. Various methods have been suggested for numerical integration (Taupin, 1964; Authier, Malgrange & Tournarie, 1968). More recently Petrashen (1976) has suggested a varying-step algorithm to take into account the fast oscillations of the amplitude of the wave fields near the edges of the Borrmann fan. The main difficulty is in finding a method of adapting the local integration step to its best value. We have developed an algorithm in which this step is automatically chosen throughout the numerical integration.

This new algorithm permits either faster calculations by a factor of two to three without increasing the precision of the integration or a much better accuracy in all details of simulated images of Lang section topographs.

It is based upon the following three considerations:

(1) Choosing of integration step is dependent upon the local value of the extinction distance (Epelboin, 1977).

(2) The interaction of a defect with the wave fields is weaker near the reflected edge of the Borrmann fan.

(3) The amplitude of the wave fields increases tremendously in the direction of the direct image of a defect whenever it exists.

Firstly, the integration network is established according to the above ideas.

For this purpose the zeros of the J_0 Bessel functions are calculated and the horizontal integration step is chosen in such a way that between two zeros at least five steps are calculated (Fig. 1). It is thus possible to calculate the amplitudes of the wave fields near the edges of the Borrmann fan without losing any oscillation.

To decrease the computation time the integration step may be increased wherever the amplitudes of the wave fields vary more slowly. Moreover, the integration step may be larger near $\mathbf{S}_n$ than near $\mathbf{S}_0$, due to the weak interaction of any defect with the wave fields.

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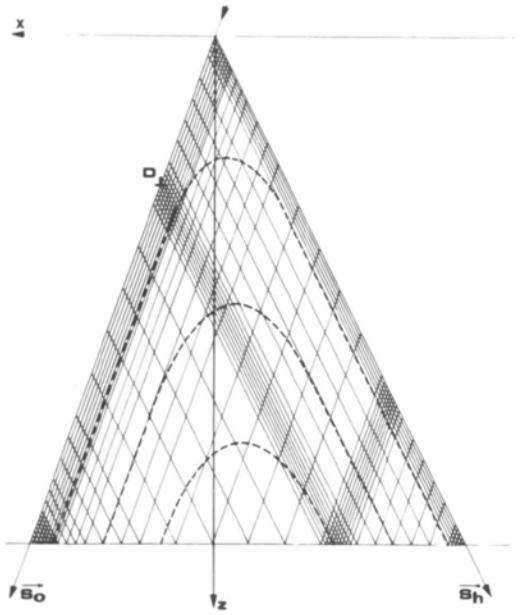

Fig. 1. Principles of the integration network.

When the defect possesses a direct image, its shape is roughly calculated according to the kinematical theory (Authier, 1967) and the length of the integration step is decreased in the corresponding area (Fig. 1).

The Takagi–Taupin equations are then integrated. The program automatically switches from an integration network taking into account the direct image to another one without it, when it is needed. This automatic adaptation of the program to the diffraction conditions permits the simulation of the section topograph of a dislocation with high accuracy. We have been able, for example, to determine the direction of the Burgers vector of a dislocation through the features of its direct image (Fig. 2).

Thus it is now possible to simulate section topographs with good accuracy in all parts of the image. More details about this new routine *DEFV* will be given in a further paper.

Topograph shown in Fig. 2 is from Dr M. Lefeld-Sosnowska (University of Warsaw). Its contrast will be discussed in a work currently in progress in collaboration with A. Authier.

Fig. 2. Section topograph of a silicon wafer, Mo $K\alpha$, $33\bar{3}$.

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A general rule for origin specification in any space group.

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Abstract

A general and simple rule for the derivation of which reflections should be used for fixing the origin in any of the 230 space groups is given.

The number of reflections needed to specify the origin is identical to the number of elements in the seminvariant vector of that space group. For example, in $P2_12_12_1$, the seminvariant vector is (hkl) modulo (2 2 2). Thus three reflections are needed to specify the origin. In $P4$ the seminvariant vector is $(h + k, l)$ modulo (2,0) and two

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