DIMS - Direct methods In Multidimensional Space

Hai-fu Fan & Yuan-xin Gu
Institute of Physics, Chinese Academy of Sciences, Beijing 100190, P.R. China. E-mail: fanhf@cryst.iphy.ac.cn

1. Introduction

DIMS (Direct methods In Multidimensional Space) (Fu & Fan, 1994; Fan, 2005a,b) is a direct-methods program for solving one-dimensionally modulated incommensurate structures and composite structures consists of two subsystems with two axes of the unit cell coincided to each other. Actually DIMS can also deal with three-dimensional periodic structures including commensurate modulated structures. The latter is also known as superstructures. The theoretical basic behind DIMS is the direct-method treatment of the phase ambiguity due to pseudo-translational symmetry. This originated from solving the crystal structure of a natural amino acid [Fan, 1975 (in Chinese); see also Fan, 1984]. The crystal structure in that study possesses a two-fold pseudo-translational symmetry leading to phase ambiguities for one half of the total reflections. The Sayre equation (Sayre, 1952) was modified and successfully used to break the phase ambiguity. Later, a direct method of solving commensurate modulated structures (superstructures) was proposed [Fan, He, Qian and Liu, 1978 (in Chinese); see also Fan, Yao, Main & Woolfson, 1983]. The method was subsequently extended to multidimensional space for dealing with incommensurate modulated structures (Hao, Liu & Fan, 1987). Further developments were made on extending the method in solving composite structures (Fan, Smaalen, Lam & Beurskens, 1993; Sha *et al.*, 1994; Mo *et al.*, 1996). DIMS has been integrated with the program VEC (Visual computing in Electron Crystallography) (Wan *et al.* 2003). Implementation and application of DIMS/VEC have been described in detail previously (Fan, 2005a, b). In this paper a summary of the theory behind DIMS and some details inside DIMS will be given.

2. Theory behind DIMS

2.1 Modulated structures

Modulated structures can be regarded as the result of applying a periodic modulation to a basic structure, which possesses exact 3-dimensional periodicity. Figure 1 shows two examples. The modulation wave in Fig.1a represents the fluctuation of atomic occupancy. When it is applied to a basic structure (atoms of which are represented by black vertical rods), the 'heights' of the atoms are modified. A commensurate modulated structure (superstructure) will result (Fig.1b), if the period **T** of the modulation function matches the period **t** of the basic structure, i.e. **T/t** = n, where n is a simple integer. The resulting superstructure now has a true period **T** and a pseudo period **t**, which respectively correspond to a true unit cell and a pseudo unit cell. On the other hand, if **T** does not match **t** (Fig.1c), i.e. **T/t** = r, where r is not a simple integer, we obtain an incommensurate modulated structure, which possesses no exact 3-dimensional periodicity although **t** remains a pseudo period. A modulation function can also represent the fluctuation of atomic position or thermal motion. In practice a modulated structure may simultaneously include different kinds of modulation.

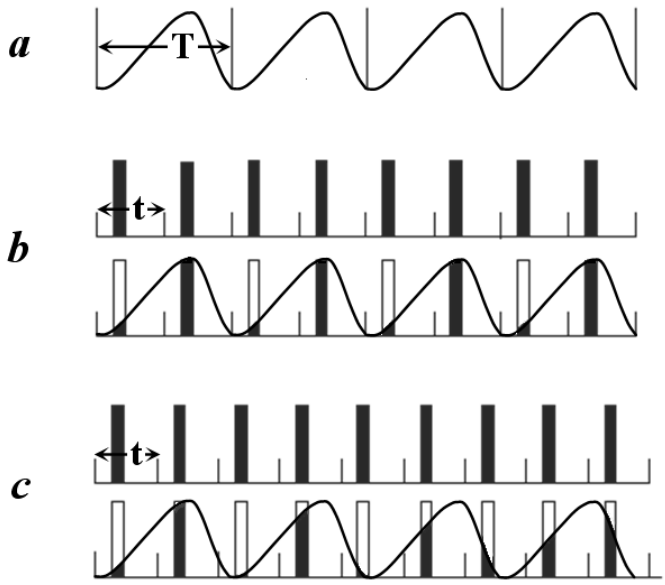

Figure 1. Occupational modulation of a one-dimensional structure

Incommensurate modulated crystals yield 3-dimensional diffraction patterns, which contains satellites round the main reflections. An example of a section of such a 3-dimensional diffraction pattern is shown schematically in Fig.2. The main reflections are consistent with a regular 3-dimensional reciprocal lattice but the satellites do not fit the same lattice. On the other hand, while the satellites do not match the main lattice, they have their own periodicity (see the vertical line segments in Fig.2). Hence, it can be imagined that the 3-dimensional diffraction pattern is the projection of a 4-dimensional reciprocal lattice, in which the main and the satellite reflections are all regularly situated at the lattice nodes. From the properties of the Fourier transform the incommensurate modulated structure here considered can be regarded as a 3-dimensional "section" of a 4-dimensional periodic structure. The above example corresponds to a one-dimensional modulation. In the case of n-dimensional (n=1, 2, …) modulation, it needs a (3+n)-dimensional description.

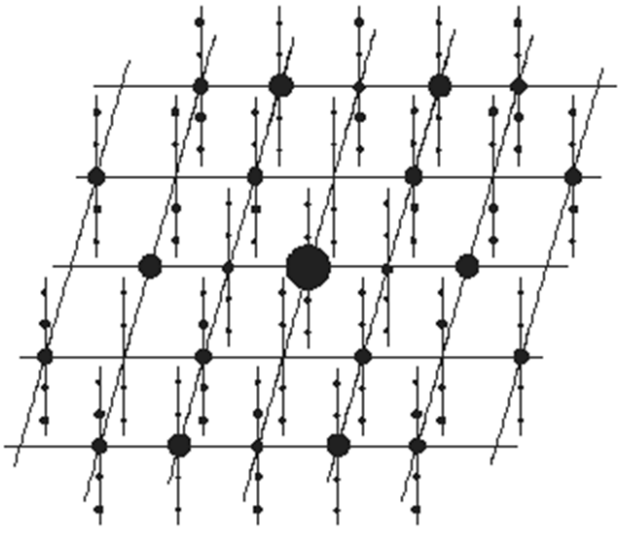

Figure 2. Schematic diffraction pattern of an incommensurate modulated structure

There is a special kind of incommensurate modulated structures called composite structures. The characteristic of which is the coexistence of two or more mutually incommensurate 3-dimensional lattices. Owing to the interaction of coexisting lattices, composite structures are also incommensurate modulated structures. Unlike ordinary incommensurate modulated structures, composite structures do not have a 3-dimensional basic structure. Instead, they will have a 4- or higher-dimensional basic structure.

For details of superspace representation of modulated crystal structures the reader is referred to Janssen *et al*. (2006), Smaalen (1995) and Yamamoto (1996).

2.2 4-diemnsional representation of one-dimensionally modulated structures

As is described above, one-dimensionally incommensurate modulated structures can be regarded as a 4-dimensional periodic structure cut with a 3-dimensional hyperplane parallel to the 3-dimensional physical space. A position vector **x** within the 4-dimensional unit cell is expressed as

$$\mathbf{x} = x_1\mathbf{a}_1 + x_2\mathbf{a}_2 + x_3\mathbf{a}_3 + x_4\mathbf{a}_4 . \qquad (1)$$

In equation (1), x_1, x_2, x_3 and x_4 are fractional coordinates; $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ and $\mathbf{a}_4$ are basic vectors defining the 4-dimensional unit cell. A reciprocal lattice vector **h** is expressed as

$$\mathbf{h} = h_1\mathbf{b}_1 + h_2\mathbf{b}_2 + h_3\mathbf{b}_3 + h_4\mathbf{b}_4 . \qquad (2)$$

In equation (2), h_1, h_2, h_3 and h_4 are diffraction indices, which are components of **h** with respect to the basic vectors $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$ and $\mathbf{b}_4$ of the 4-dimensional reciprocal lattice. Vectors $\mathbf{a}_i$ and $\mathbf{b}_j$ satisfy the reciprocal relationships

$$\mathbf{a}_i \cdot \mathbf{b}_j = \delta_{ij} \quad (i, j = 1,2,3,4), \ \delta_{ij} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases} . \qquad (3)$$

The 4-dimensional unit cell of the modulated structure is related to the 3-dimensional unit cell of the basic structure through the following relationships.

$$\begin{aligned} \mathbf{a}_1 &= \mathbf{a} - q_1\mathbf{d} & \mathbf{b}_1 &= (\mathbf{a}^*, 0) \\ \mathbf{a}_2 &= \mathbf{b} - q_2\mathbf{d}, & \mathbf{b}_2 &= (\mathbf{b}^*, 0). \\ \mathbf{a}_3 &= \mathbf{c} - q_3\mathbf{d} & \mathbf{b}_3 &= (\mathbf{c}^*, 0) \\ \mathbf{a}_4 &= (0, \mathbf{d}) & \mathbf{b}_4 &= (\mathbf{q}, \mathbf{d}) \end{aligned} \qquad (4)$$

Where **a**, **b**, and **c** are the basic vectors defining the unit cell of the 3-dimensional basic structure, while **a***, **b***, and **c*** are the basic vectors defining the corresponding reciprocal lattice. The unit vector **d** is perpendicular to the 3-dimensional physical space. The modulation wave vector **q** is expressed as

$$\mathbf{q} = q_1\mathbf{a}^* + q_2\mathbf{b}^* + q_3\mathbf{c}^* . \qquad (5)$$

In the case of incommensurate modulation, at least one of the components q_1, q_2 and q_3 on the right-hand side of (5) should be irrational.

The structure-factor formula for a one-dimensionally modulated structure is written as

$$F(\mathbf{h}) = \sum_{j=1}^{N} f_j(\mathbf{h}) \exp\left[i2\pi \left(h_1\bar{x}_{j1} + h_2\bar{x}_{j2} + h_3\bar{x}_{j3} \right) \right] . \qquad (6)$$

Where

$$f_j(\mathbf{h}) = f_j^o(h)\int_0^1 P_j(\bar{x}_4)\exp\left[i2\pi\left(h_1U_{j1} + h_2U_{j2} + h_3U_{j3} + h_4x_{j4}\right)\right]d\bar{x}_4 \cdot \qquad (7)$$

On the right-hand side of (7) $f_j^o(h)$ is the ordinary atomic scattering factor, P_j is the compositional modulation function and U_j describes the deviation of the j^{th} atom from its average position ($\bar{x}_{j1}$, $\bar{x}_{j2}$, $\bar{x}_{j3}$). For more details on (6) and (7) the reader is referred to the papers by de Wolff (1974), Yamamoto (1982) and Hao, Liu & Fan (1987). What should be emphasized here is that, according to (6) and (7) a modulated structure can be regarded as a set of 'modulated atoms' situated at their average positions in 3-dimensional space. While the 'modulated atom' in turn is defined by the 'modulated atomic scattering factor' $f_j(\mathbf{h})$.

2.3 Sayre's equation in multidimensional space

It has been proved by Hao, Liu & Fan (1987) that the Sayre equation (Sayre, 1952) can easily be extended into multidimensional space. We have

$$F(\mathbf{h}) \approx \frac{\theta}{V}\sum_{\mathbf{h'}} F(\mathbf{h'})F(\mathbf{h}-\mathbf{h'}) \cdot \qquad (8)$$

Where θ is an atomic form factor; V is the unit-cell volume of the basic structure. The reciprocal-lattice vector **h** is now a multidimensional vector defined as

$$\mathbf{h} = \sum_{i=1}^{3+n} h_i\mathbf{b}_i \qquad , \qquad n = 1, 2, 3, \cdots \cdot \qquad (9)$$

Where h_i are components of the vector **h**; $\mathbf{b}_i$ are basic vectors defining a multidimensional reciprocal unit cell. The right-hand side of (8) can be split into three parts, i.e.

$$F(\mathbf{h}) = \frac{\theta}{V}\left\{\sum_{\mathbf{h'}} F_m(\mathbf{h'})F_m(\mathbf{h}-\mathbf{h'}) + 2\sum_{\mathbf{h'}} F_m(\mathbf{h'})F_s(\mathbf{h}-\mathbf{h'}) + \sum_{\mathbf{h'}} F_s(\mathbf{h'})F_s(\mathbf{h}-\mathbf{h'})\right\} \cdot \qquad (10)$$

In equation (10), the subscript *m* stands for main reflections, while the subscript *s* stands for satellites. Since the intensities of satellites are on average much weaker than those of main reflections, the last summation on the right-hand side of (10) is negligible in comparison with the second, while the last two summations on the right-hand side of (10) are negligible in comparison with the first. If F(**h**) on the left-hand side of (10) represents structure factors of main reflections, we have to first approximation

$$F_m(\mathbf{h}) \approx \frac{\theta}{V}\sum_{\mathbf{h'}} F_m(\mathbf{h'})F_m(\mathbf{h}-\mathbf{h'}) \cdot \qquad (11)$$

This implies that the basic structure can be solved by conventional methods (direct methods or other methods) in 3-dimensional space neglecting all satellite reflections. On the other hand, if F(**h**) on the left-hand side of (10) corresponds to satellite reflections, it follows that

$$F_s(\mathbf{h}) \approx \frac{\theta}{V}\sum_{\mathbf{h'}} F_m(\mathbf{h'})F_m(\mathbf{h}-\mathbf{h'}) + \frac{2\theta}{V}\sum_{\mathbf{h'}} F_m(\mathbf{h'})F_s(\mathbf{h}-\mathbf{h'}) \cdot \qquad (12)$$

For ordinary incommensurate modulated structures the first summation on the right-hand side of (12) has vanished. Because any three-dimensional reciprocal lattice vector corresponding to a main reflection will

have zero components in the extra dimensions so that the sum of two such lattice vectors could never give rise to a lattice vector corresponding to a satellite. We then have

$$F_s(\mathbf{h}) \approx \frac{2\theta}{V}\sum_{\mathbf{h'}} F_m(\mathbf{h'})F_s(\mathbf{h}-\mathbf{h'})\cdot \qquad (13)$$

For composite structures (Fan *et al.* 1993; Sha *et al.*, 1994; Mo *et al.*, 1996) on the other hand, since the average structure itself is a 4- or higher-dimensional periodic structure, the first summation on the right-hand side of (12) does not vanish. We have instead of (13) the following equation:

$$F_{\mathrm{s}}(\mathbf{h}) \approx \frac{\theta}{V}\sum_{\mathbf{h'}} F_{\mathrm{m}}(\mathbf{h'})F_{\mathrm{m}}(\mathbf{h}-\mathbf{h'})\cdot \qquad (14)$$

Equation (13) or (14) imply that, once the phases of main reflections are known, it is straight forward to derive phases of satellites by using (13) and (14) respectively for ordinary incommensurate modulated structures and composite structures. The whole procedure will be in the following stages:

i) Derive the phases of main reflections using Equation (11) or other methods in 3-dimensional space;
ii) Derive the phases of satellite reflections using Equation (13) or (14);
iii) Calculate a multidimensional Fourier map using the observed structure-factor magnitudes and the phases from i) and ii);
iv) Cut the resulting Fourier map with a 3-dimensional 'hyperplane' to obtain a 'structure image' of the incommensurate modulated structure in the 3-dimensional physical space;
v) Parameters of the modulation functions are measured directly on the multidimensional Fourier map resulting from iii).

3. (3+1)-dimensional symmetry generators from superspace-group symbols

In the first edition of DIMS (Fu & Fan, 1994; source code in Appendix I) the superspace symmetry generators should be manually input to the program. Later, the subroutine SPGR4D (Fu & Fan, 1997; source code in Appendix II) was written and incorporated into DIMS enabling automatic derivation of superspace symmetry generators from the input two-line superspace-group symbol (Wolff, Janssen & Janner, 1981). Recently, the subroutine SYMBOL1to2 was written for converting one-line symbols to two-line symbols of (3+1)-dimensional superspace groups (Li, Li & Fan, 2009; source codes in Appendix III). The subroutine has been incorporated into the program VEC (Wan *et al.*, 2003). Now, the program DIMS (source code of MS Windows version in Appendix IV) invoking from VEC, accepts symmetry generators, two-line superspace-group symbols or one-line superspace-group symbols.

4. Phasing formula

The phasing formula used in DIMS looks like the tangent formula of Karle & Hauptman (1956)

$$\tan\varphi(\mathbf{h}) = \frac{\sum_{\mathbf{h'}}\left|E(\mathbf{h'})E(\mathbf{h}-\mathbf{h'})\right|\sin\left[\varphi(\mathbf{h'})+\varphi(\mathbf{h}-\mathbf{h'})\right]}{\sum_{\mathbf{h'}}\left|E(\mathbf{h'})E(\mathbf{h}-\mathbf{h'})\right|\cos\left[\varphi(\mathbf{h'})+\varphi(\mathbf{h}-\mathbf{h'})\right]}, \qquad (15)$$

with

$$\left|E(\mathbf{h})\right| \propto \left|F(\mathbf{h})\right| \Big/ \left\langle \left|F(\mathbf{h})\right|^2 \right\rangle^{1/2}. \qquad (16)$$

Here the vector **h** is a 4-dimensional reciprocal lattice vector. Strictly speaking, equation (15) is not a tangent formula. The tangent formula for 3-dimensional periodic structures may be regarded as the result of maximizing the phase probability density function given by Cochran (1955):

$$P(\varphi_{\mathbf{h}}) = \left[2\pi I_0(\alpha)\right]^{-1} \exp[\alpha \cos(\varphi_{\mathbf{h}} - \langle\varphi_{\mathbf{h}}\rangle)] \qquad (17)$$

with

$$\alpha = \left[\left(\sum_{\mathbf{h}} \kappa_{\mathbf{h},\mathbf{h}'} \sin(\varphi_{\mathbf{h}} + \varphi_{\mathbf{h}-\mathbf{h}})\right)^2 + \left(\sum_{\mathbf{h}} \kappa_{\mathbf{h},\mathbf{h}'} \cos(\varphi_{\mathbf{h}} + \varphi_{\mathbf{h}-\mathbf{h}})\right)^2\right]^{1/2} \qquad (18)$$

and

$$\kappa_{\mathbf{h},\mathbf{h}'} = 2\sigma_3\sigma_2^{-3/2}\left|E_{\mathbf{h}}E_{\mathbf{h}'}E_{\mathbf{h}-\mathbf{h}'}\right|. \qquad (19)$$

However this phase probability density function is not necessarily valid for incommensurate modulated structures. Besides, in practice all observable reflections [with the restriction of equation (11), (13) or (14)] are used in the calculation of equation (15). In view of these, equation (15) would better be regarded as the angular portion of the Sayre equation rather than the tangent formula (see the discussion by Fan, 1998). On the other hand, as is shown by Gelder *et al.* (1996) that the probability distribution associated with the structure invariants $E(-\mathbf{h})E(\mathbf{h}')E(\mathbf{h}-\mathbf{h}')$, where **h** and **h'** are reciprocal vectors of main and/or satellite reflections, approximately has the same functional form as the Cochran distribution. Hence, equation (15) can still be approximately regarded as the tangent formula and, the associated equations (16) to (19) can still be used in dealing with incommensurate modulated structures. The $|E(\mathbf{h})|$ values calculated from equation (16) are not exactly the normalized structure-factor amplitudes but just specially scaled structure-factor amplitudes, which contain an empirical scaling factor to balance between main and satellite reflections. The use of equation (16) implies also that the calculation is independent of atomic scattering factors. Hence for ordinary incommensurate modulated structures DIMS can be used in phasing X-ray, electron and even neutron diffraction data. Equation (18) is used empirically for the calculation of figures of merit. However it should be aware that such figures of merit are not as reliable as that used for 3-dimensional periodic structures.

5. Phasing strategy

The phasing strategy used in DIMS is the 'random-starting-phases multisolution algorithm' developed in M.M. Woolfson's group in York University, UK. The reader is referred to the paper by Yao (1981) for details. For ordinary incommensurate modulated structures, it is assumed that phases of main reflections are already known before running DIMS. These phases are treated as 'known phases' and are kept fixed during the phasing process. Phases of all satellite reflections are 'unknown phases', which are given random starting values and will be refined during the phasing process. For composite structures, phases of main reflections can either be input as known phases or derived by DIMS it self before phasing satellite reflections. All unknown phases are given random starting values and then refined using the phasing formula.

5.1 Phasing satellites of ordinary incommensurate modulated structures

Here, the most important part is to phase the first-order satellites, since higher-order satellites are usually much weaker. The phasing is based on phase relationships existing in equation (13). Since phases of the main reflections are known in advance, the phasing process is straightforward. After deriving phases of the first-order satellites, phases of higher-order satellites (if any) will be derived also based on phase relationships existing in equation (13). In addition, phase relationships involving three satellites with at least one first order satellite will also be used. The goal of using this kind of phase relationships is to link phases between the first-order and higher order satellites.

5.2 Phasing main reflections of composite structures

The phasing is based on phase relationships existing in equation (11). The process is nearly the same as that for 3-dimensional periodic structures. Here the normalized structure-factor amplitudes are calculated as

$$|E(\mathbf{h})| = |F(\mathbf{h})| \Big/ \left(\varepsilon \sum_{j=1}^{N} f_j^2 \right)^{1/2} \qquad (20)$$

with atomic scattering factors for X-rays. In this case DIMS can deal with only X-ray diffraction data. For details of the procedure, the reader is referred to the paper by Mo *et al.* (1996).

5.3 Phasing satellite reflections of composite structures

The phasing is based on phase relationships existing in equation (14). Phases of the main reflections are known and kept fixed during the phasing process. For details of the procedure, the reader is referred to the paper by Fan et al. (1993).

Acknowledgement

The project was supported in part by the National Natural Science Foundation of China.

References

Cochran, W. (1955). Relations between the Phases of Structure Factors. *Acta Cryst.* **8**, 473-478.

Fan, H.F. (1975). The phase ambiguity in heavy-atom method treated by structure-factor relationships. *Acta Phys. Sin.* **24**, 57-60. (In Chinese)

Fan, H.F. (1984). The problem of phase ambiguity in single crystal structure analysis. *The Rigaku Journal*, **1**, *No.* 2, 15-21.

Fan, H.F. (1998). Sayre equation, tangent formula and SAYTAN. in *Direct Methods for Solving Macromolecular Structures*. Ed. by S. Fortier, Kluwer Academic Publishes, The Netherlands. Pp. 79-85.

Fan, H.F. (2005a). DIMS on the VEC platform. *IUCr Computing Commission Newsletter* No.5, 16-23.

Fan, H.F. (2005b). DIMS/VEC applications. *IUCr Computing Commission Newsletter* No.5, 24-27.

Fan, H.F., He, L., Qian, J.Z. & Liu, S.X. (1978). Solving crystal superstructures by the direct method. *Acta Phys Sin.* **27**, 554-558. (In Chinese)

Fan, H.F., van Smaalen, S., Lam, E.J.W. & Beurskens, P.T. (1993). Direct methods for incommensurate intergrowth compounds I. Determination of the modulation. *Acta Cryst*. A**49**, 704-708.

Fan, H.F., Yao, J.X., Main, P. & Woolfson, M.M. (1983). On the application of phase relationships to complex structures. XXIII. Automatic determination of crystal structures having pseudo-translational symmetry by a modified MULTAN procedure. *Acta Cryst.* A**39**, 566-569.

Fu, Z.Q. & Fan, H.F. (1994). DIMS --- a direct method program for incommensurate modulated structures. *J. Appl. Cryst.,* **27**, 124-127.

Fu, Z.Q. & Fan, H.F. (1997). A computer program to derive (3+1)-dimensional symmetry operations from two-line symbols. *J. Appl. Cryst.,* **30**, 73-78.

Gelder, R. de, Randy, I., Lam, E.J.W., Beurskens, P.T., Smaalen, S. van, Fu, Z.Q. & Fan, H.F. (1996). Direct methods for incommensurately modulated structures. On the applicability of normalized structure factors. *Acta Cryst.* A**52**, 947-954.

Hao, Q., Liu, Y.W. & Fan, H.F. (1987). Direct methods in superspace I. Preliminary theory and test on the determination of incommensurate modulated structures. *Acta Cryst.* A**43**, 820-824.

Hauptman, H. & Karle, J. (1953). Solution of the phase problem. I. The centrosymmetric crystal. ACA Monograph No. 3. Dayton, Ohio: Polycrystal Book Service.

Janssen, T., Janner, A., Looijenga-Vos, A. & de Wolff, P. M. (2006). Incommensurate and commensurate modulated structures. *International tables for crystallography*, Vol. C, ch. 9.8. pp. 907-955, edited by E. Prince, Springer.
Karle, J. & Hauptman, H. (1956). A theory of phase determination for the four types of non-centrosymmetric space groups 1P222, 2P22, 3P12, 3P22. *Acta Cryst.* **9**, 635–651.
Li, X.M., Li, F.H. & Fan, H.F. (2009). A revised version of the Program VEC. *Chinese Physics B* **18**, 2459-2463.
Mo, Y.D., Fu, Z.Q., Fan, H.F., van Smaalen, S. Lam, E.J.W. & Beurskens, P.T. (1996). Direct methods for incommensurate intergrowth compounds III. Solving the average structure in multidimensional space. *Acta Cryst*. A**52**, 640-644.
Sayre, D. (1952). The squaring method: a new method for phase determination. *Acta Cryst.* **5**, 60-65.
Sha, B.D., Fan, H.F., van Smaalen, S., Lam, E.J.W. & Beurskens, P.T. (1994). Direct methods for incommensurate intergrowth compounds II. Determination of the modulation using only main reflections. *Acta Cryst*. A**50**, 511-515.
Smaalen, S. van (1995). Incommensurate crystal structures. *Crystallogr. Rev.* **4**, 79–202.
Wan, Z.H., Liu, Y.D. Fu, Z.Q., Li, Y., Cheng, T.Z., Li, F.H. & Fan, H.F. (2003). Visual computing in electron crystallography. *Z. Krist.* **218**, 308-315.
Wolff, P. M. de (1974). The pseudo-symmetry of modulated crystal structures, *Acta Cryst*. A**30**, 777-785.
Wolff, P. M. de, Janssen, T. & Janner (1981). The superspace groups for incommensurate crystal structures with a one-dimensional modulation. *Acta Cryst*. A**37**, 625-636.
Yamamoto, A. (1982). Structure factor of modulated crystal structures, *Acta Cryst.* A**38**, 87-92.
Yamamoto, A. (1996). Crystallography of quasiperiodic crystals. *Acta Cryst*. A**52**, 509–560.
Yao, J. X. (1981). On the application of phase relationships to complex structures XVIII. RANTAN—Random MULTAN. *Acta Cryst.*, A**37**, 642-644.

Editor's note: following appendices deposited as a separate zip file with this newsletter.

Appendix I. Source codes of the first edition of DIMS (1994)

Appendix II. Source codes of SPGR4D

Appendix III. Source codes of SYMBOL1to2

Appendix IV. Source codes of DIMS (2000) for MS Windows

Appendix V. Source codes of DIMS (2009) for Linux