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Abstract

ADVANCES IN THE APPLICATION OF DIRECT METHODS. By Fan Hai-fu*, Gu Yuan-xin, Zheng Chao-de, Hao Quan, Xiang Shi-bin & Li Fang-hua, Institute of Physics, Academia Sinica, Beijing 100080, China and Hengming Ke, Department of Chemistry, Harvard University, MA 02138, USA.

In spite of their great success, direct methods are still restricted mainly in the field of small molecular structures. Applications in other fields are now being explored. Encouraging results have been obtained.

1. Direct Phasing of One-wavelength Anomalous Scattering (OAS) Data from A Small Protein.

Multiple isomorphous replacement is now dominating the structure analysis of proteins with no structural precedent. It may occur that the derivatives are not isomorphous with the native protein. In this case multi-wavelength anomalous scattering (MAS) can in principle be used, if there are some suitable heavy atoms in the native protein or its non-isomorphous derivative. However MAS technique suffers from the difficulty of collecting and scaling data at different wavelengths accurately. OAS technique does not have this difficulty but it leads to the problem of phase ambiguity. A direct method has been proposed to solve this problem [Fan *et al.* (1984). *Acta Cryst.* A40, 489-495; 495-498.] The method has been tested with the Hg-derivative of a known protein, avian pancreatic polypeptide [Glover *et al*. (1985). *Adv. Biophys.*20,1-12]. It resulted in an interpretable Fourier map. A part of which together with the structure model plotted by FRODO is shown in Fig. 1.

Figure 1.

2. Resolution Enhancement of An Electron Micrograph

The high resolution electron micrograph of chlorinated copper phthalocyanine (Fig. 2a) [Uyeda et al. (1978-1979). *Chem. Scripta* 14, 47] though provides useful structural information, it is unable to resolve individual atoms. On the other hand the corresponding electron diffraction pattern offers much higher resolution but the phase problem has been proved difficult to solve by traditional direct methods. A phase extension technique with starting phases obtained from the electron micrograph at 2Å resolution has been used to derive the phases for reflections between 2Å-1 and 1Å-1 on the diffraction pattern. This led to an image (Fig. 2b) much closer to the true structure model (Fig. 2c).

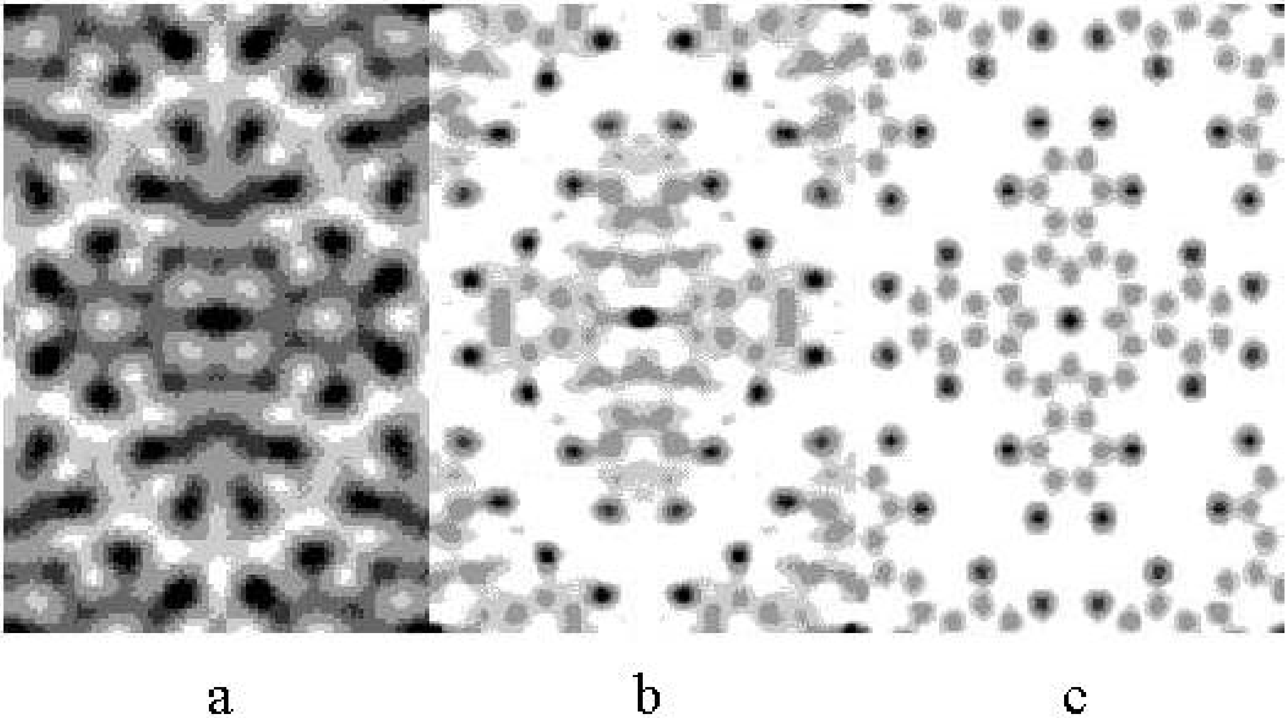

Figure 2.

3. Solving Incommensurate Modulated Structures

Incommensurate modulated phases exist in many important solid state materials. Up to the present, studies of incommensurate modulated structures were mostly based on preliminary assumption of the modulation function. Direct methods have been extended for solving incommensurate modulated structures in multi-dimensional space [Hao *et al*. (1987). *Acta Cryst*. A43, 820-824.]. Without making preliminary assumption, this method has succeeded in revealing the occupational and positional modulation of Ba atoms in an originally unknown mineral structure, ankangite. Use of the method to solve the incommensurate modulated structure of high Tc superconductors is in progress.