PREFACE

Direct methods are so successful in crystal structure analysis, their important contribution to science has been recognized by the award of the Nobel Prize for Chemistry to two pioneers of direct methods, H. Hauptman and J. Karle. On the other hand direct methods are still limited to crystal structure analysis of moderate complexity. New application fields for direct methods remain to be explored.

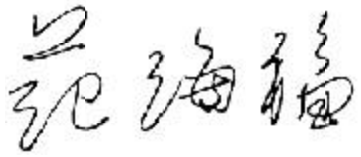
In spite of their great success in the determination of small molecular structures, direct methods have had little influence on protein crystallography. However, the combination of direct methods with single isomorphous replacement or one-wavelength anomalous scattering will be important in solving protein structures. Such a combination can reduce the number of heavy-atom derivatives, save time for data collection and simplify the process of structure determination. Test results on experimental protein data showed that it is possible to solve the phase problem without the necessity of preparing isomorphous heavy-atom derivatives. Recently study showed that even a pure direct-method procedure is probably useful for ab-initio phasing of small proteins.

Modulated structures belong to that kind of crystal structure in which the atoms suffer from certain occupational and/or positional fluctuation. If the period of fluctuation is commensurate with that of the three-dimensional unit cell then a superstructure results, otherwise an incommensurate modulated structure is obtained. Incommensurate modulated phases can be found in many important solid state materials. In many cases, the transition to the incommensurate modulated structure corresponds to a change of certain physical properties. Hence it is essential to know the structure of incommensurate modulated phases in order to understand the mechanism of the transition and properties in the modulated state. Direct methods have now been extended from three-dimensional to multi-dimensional space and used successfully in phasing the main as well as the satellite reflections of incommensurate modulated structures. Unlike the traditional methods for solving incommensurate modulated structures, direct methods solve the structure in a straightforward way without relying on the preliminary knowledge of either the modulation property or the average structure. Recently an important type of condensed matter called the quasicrystal has been discovered and extensively investigated. There exists certain similarity between quasicrystals and incommensurate modulated structures. Both of them can be regarded as the three-dimensional hyper-section of a regular periodic structure in multi-dimensional space. Direct methods may also be useful for structure analysis of quasicrystals.

Apart from X-ray methods, high resolution electron microscopy (HREM) is another important technique for structure analysis. Many solid state materials important in science and technology are composed of very small and imperfect crystals. They are not suitable for X-ray diffraction analysis but are suitable for electron microscopic observation. However, HREM suffers from two difficulties: Firstly, an electron microscopic image is not a true structural image of the object but just a convolution of the true image with the Fourier transform of the contrast transfer function. Secondly, the point to point resolution of an electron microscopic image is about 2 Angstrom at present time, which is not enough to reveal individual atoms in

most cases. Hence it is essential to have some image processing technique for both image deconvolution and resolution enhancement. On the other hand, direct methods are, in fact, a special kind of image processing technique: a three-dimensional X-ray diffraction pattern without phase information can be regarded as the Fourier transform of a blurred image, i.e. a Patterson function, of the crystal structure. Now direct methods can solve the phase problem in reciprocal space and thus restore the true structure image from the blurred one in real space. Such a process is in fact a kind of image deblurring. Hence direct methods might help with the image processing of HREM. Procedures have been proposed using direct methods in both image deconvolution and resolution enhancement of electron microscopic images. The efficiency of the methods has been proved to be satisfactory with an experimental image of copper chlorinated phthalocyanine.

Looking forward to the 1990's it can be expected that direct methods will be as successful in many new fields as they have been in the traditional field.



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