Poster Presentation

MS100.P02

How phase measurements can change X-ray crystallography

S. Morelhao[1], Z. Amirkhanyan[1], C. Remedios[2], C. Guzzo

[1]*Universidade de São Paulo, Instituto de Física, Sao Paulo, Brazil,* [2]*Universidade Federal do Pará, Faculdade de Física, Belem, Brazil,* [3]*Universidade de São Paulo, Instituto de Ciências Biomédicas, São Paulo, Brazil*

From inorganic crystals to macromolecular crystals, structure determination with atomic resolution is based on diffraction techniques (electrons, X-rays and neutrons). However, since the coherent scattering cross-section for X-rays by atoms have intermediate values between those for electrons and neutrons, experimental measurements of the phases of structure factors are feasible only for X-rays. Unprecedented results [1-3] have show how phase measurements can reveal important information of the crystalline structure of doped crystals, which are inaccessible by other techniques: "differently from any other method in X-ray crystallography based on structure refinement of intensity data, the presented method pinpoint a specific feature of the structure and directly prove its existence beyond of any reliability parameter or of goodness-of-fitting value." Although there are instrumental and computational challenges, the method can be extended to protein crystallography for improving resolution of poorly solved features of the structures. As depicted in Fig. 1, the structure factor of a given reflection has contributions of distinct groups of atoms. Low resolution at one group can result in phase deviation of Fickle, without significantly affecting its amplitude. For instance, small differences in the symmetry of charge balance at group B can cause great difference in the phase angle of this group, which increases the phase angle of Fickle, Fig. 1 (b). On the other hand, reduction in the scattering amplitude of group E due to atomic disordering decreases the phase angle, Fig. 1 (c). In this presentation, we discuss the current understanding of this method, its perspectives, and importance of providing a tool for structural analysis of macromolecules that is able to go beyond the resolution achieved by the techniques actually in use.

[1] *S.L. Morelhao, C.M.R. Remedios, R.O. Freitas, et al., J. Appl. Cryst., 2011, 44, 93-101.,* ***[2]*** *Z.G. Amirkhanyan, C.M.R. Remedios, Y.P. Mascarenhas, et al., J. Appl. Cryst., 2014, 47, 160-165.,* ***[3]*** *Z.G. Amirkhanyan, C.M. R. Remédios, S.L. Morelhão, et al., Appl. Phys. Lett. Mat., submitted.*

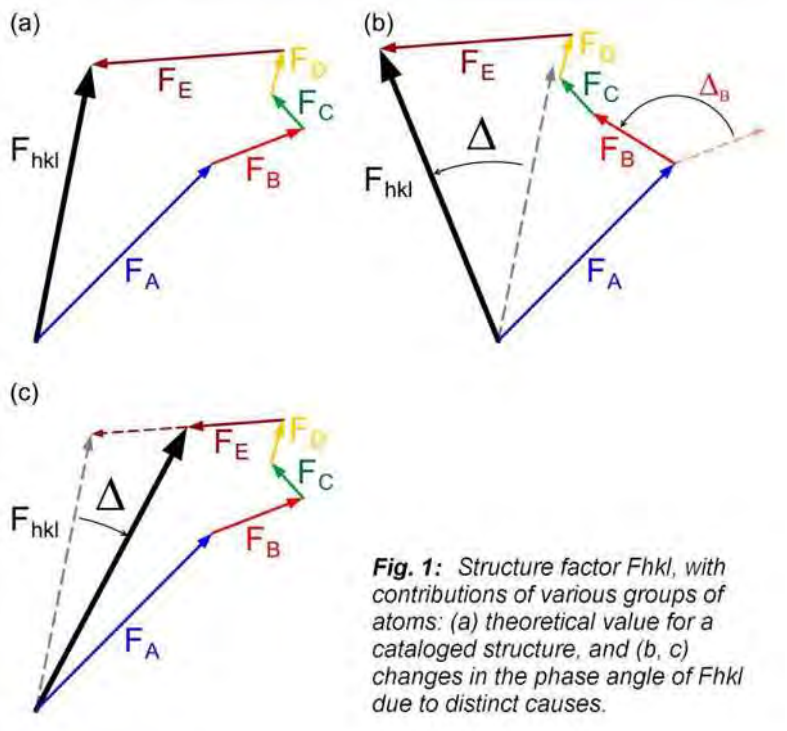

Fig. 1: *Structure factor Fhkl, with contributions of various groups of atoms: (a) theoretical value for a cataloged structure, and (b, c) changes in the phase angle of Fhkl due to distinct causes.*

Keywords: invariant triplet phase, X-ray crystallography, multi-beam diffraction