Poster Presentations

[MS17-P01] Solving molecular structures with TALP from diffraction data of limited quality. Oriol Vallcorba,[a] Jordi Rius[a] Stavros Nicolopoulus.[b]

[a]*Institut de Ciència de Materials de Barcelona, CSIC, Catalunya (Spain).*
[b]*NanoMEGAS SPRL, Blvd Edmond Machtens 79 , B-1080 Brussels, Belgium*
E-mail: ovallcorba@icmab.es

The optimum strategy for solving the crystal structure of a molecular compound largely depends on the quality of the measured diffraction data (accuracy, completeness, resolution range and also peak overlap in the case of powder diffraction). In difficult situations, direct-space methods offer a valid alternative to direct methods. Several recent applications of the direct-space multisolution strategy TALP [1] to laboratory x-ray diffraction and to oblique textured electron diffraction are studied. Each structure solution trial comprises a preliminary exploration of the conformation and the position of the molecular model in the unit cell (taking into account molecular overlap), followed by local refinements around the best solution obtained in the exploration. Intermediate and final models are checked against measured diffraction data. In the case of powder diffraction, peak overlap is specifically handled. Regarding the application of TALP to laboratory diffraction data, two crystal structures (with Z'=2 and 3) have been recently determined using the measurement strategy based on 2D detectors described in [2]. With respect to electron diffraction (ED) in transmission electron microscope (TEM), there is an increasing interest to solve molecular structures of nanocrystals. However, the obtention of reliable ED intensities from nanocrystals is challenging because of radiation damage (dynamic scattering effects are less important here). Several techniques have been developed in order to obtain reliable ED intensities for structure determination such as Precession Electron Diffraction (PED) from selected Zone Axis Patterns, Automated 3D Diffraction Tomography (ADT 3D) coupled with PED or Oblique Textured Electron Diffraction (OTED). To check the combination of OTED technique with TALP, data taken from bibliography [3] have been used. Despite the reduced number of observations, the crystal structures of the four organic polymers tested have been recovered.

[1] Vallcorba, O., Rius, J., Frontera, C. & Miravitlles, C. (2012). *J. Appl. Crystallogr.*, **45**, 1270–1277.
[2] Vallcorba, O., Crespi, A., Rius, J. & Miravitlles, C. (2013). *Powder Diffr. EPDIC13 proceedings*., in press.
[3] Dorset, D.L. (1995) *Structural Electron Crystallography* . Plenum, New York; London.

Keywords: direct-space methods; powder diffraction; electron diffraction