

Structure Analysis of Modulated Crystals: Trends and Tendencies

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The superspace theory as developed by DeWolff, Jansen & Janner [1] gave to crystallographers a unique tool for generalization of structural analytical methods to be especially applicable to modulated structures. In many cases the structure analysis can now be performed almost routinely [2]. The superspace approach can also be used to find a systematic way of describing whole families of related structures [3]. The use of CCD and imaging plate systems changed considerably sensitivity of data collection for modulated structures and therefore a need for further improvement of the methods is obvious. The modulation of more complicated systems cannot be efficiently described as series of harmonic functions. Special discontinuous functions already introduced for 3+1 dimensions [4] are to be generalized to 3+2 and 3+3 superspace.

Recently modulations have been found in complicated organic structures including proteins. This opens a various new problems concerning efficiency of methods used for solution and refinement of modulated structures. New techniques such as maximum entropy [5] and charge flipping methods [6] give us a good chance to make such a generalization.

[1] Wolff de P.M., Janssen T., Janner A., *Acta Cryst.*, 1981, **A37**, 625. [2] Petříček V., Dušek M. Z., *Kristallogr.*, **219**, 692. [3] Perez-Mato J.M., Zakhour-Nakhl M., Weill F., Darriet J. J., *Mat. Sci.*, 1999, **9**, 2795. [4] Petříček V., van der Lee A., Evain M., *Acta Cryst.*, 1995, **A51**, 529. [5] Smaalen van S., Palatinus L., Schneider M., *Acta Cryst.*, 2003, **A59**, 459. [6] Palatinus L., *Acta Cryst.*, 2004, **A60**, 604.

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