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INDEXING AND DATA PROCESSING OF MODULATED STRUCTURES ON CCD DETECTORS

F. van Meurs[1] L.H. Straver[1] A.J.M. Duisenberg[2] A.M.M. Schreurs[2] R.W.W. Hooft[1]
[1]Bruker Nonius BV PO Box 811 DELFT 2600 AV NETHERLANDS [2]University of Utrecht, Padualaan 8, 3584 CH Utrecht, The Netherlands

Indexing and Data processing of incommensurately modulated structures is often troubled by overlapping reflection integration areas. By introduction of a model that describes the crystal shape and crystal scattering properties, a more accurately shaped integration area can be predicted by X-ray tracing employing EvalCCD.
Visual feedback of predicted integration areas on reflection planes, facilitate fine tuning of the model parameters. The processed data, with four indices, are formatted to be read by JANA2000. Direction cosines and status flags describe the X-ray path through the crystal and the overlap conditions. Thanks to the modular setup of the software, the method is capable to also handle crystals which show signs of twinning as well.

Keywords: MODULATED STRUCTURES INDEXING CCD

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THE MAXIMUM ENTROPY METHOD IN SUPERSPACE

S. Van Smaalen L. Palatinus
University of Bayreuth Laboratory of Crystallography Universitaetsstrasse 30 BAYREUTH 95440 GERMANY

One application of the Maximum Entropy Method (MEM) in crystallography is the computation of a model-free electron density map from a set of phased structure factors. Up to now, the use of the MEM instead of multipole refinements for the computation of so-called accurate electron densities has appeared problematic. However, the MEM is an excellent method to replace noisy Fourier maps, and it has been successfully used to study disorder in crystal structures.
Here we present the application of the MEM to aperiodic crystals. Maximum Entropy (MaxEnt) optimizations in superspace give an electron density map, that allows the study of the true shapes of modulation functions. A computer program, BAYMEM, for the MEM in superspace has been written that takes into account the full superspace symmetry. It can be applied to aperiodic crystals of arbitrary dimensions, including modulated crystals, composite crystals and quasicrystals. Furthermore, it can handle periodic crystals. Applications of MaxEnt calculations to the study of the shapes of the modulation functions in different incommensurate crystals will be given.

Keywords: **APERIODIC CRYSTALS, MAXIMUM ENTROPY METHOD, ELECTRON DENSITY**

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MAGNETIC PROPERTIES OF $ThFe_xAl_{12-x}$ POWDER SAMPLES

L. Dobrzynski[1,2] K. Recko[1] K. Szymanski[1] D. Satula[1] K. Perzynska[1] M. Biernacka[1] P. Zaleski[1] J. Waliszewski[1] W. Suski[3, 4] K. Wochowski[3] M. Hofmann[5] D. Hohlwein[5]
[1]Institute of Experimental Physics University of Bialystok Lipowa 41 BIALYSTOK 15-424 POLAND [2]The Soltan Institute for Nuclear Studies, 05-400 Otwock-'Swierk, Poland [3]Polish Academy of Sciences, W. Trzebiatowski Institute of Low Temperatures and Structures Research. P.O. Box 1410, 50-950 Wroclaw 2, Poland [4]International Laboratory of High Magnetic Fields and Low Temperatures, ul. Gajowicka 95, 53-421 Wroclaw, Poland [5]Hahn-Meitner-Institut, BENSC, Glienicker Strasse 100, D-14109 Berlin, Germany

The investigations of magnetic properties of $ThFe_xAl_{12-x}$ powder samples with the iron concentration x = 4, 4.5 and 5 have been studied by means of X-ray and neutron diffraction techniques as well as the Mössbauer spectroscopy with the monochromatic circularly polarized source (MCPMS) and magnetization measurements. The structure refinement in the paramagnetic state of the ternary thorium compounds confirms body centered tetragonal (*I*4/*mmm*) structures. Unpolarized neutron diffraction pattern leaves no doubts that the modulated magnetic structure is observed in $ThFe_4Al_8$ compound with iron magnetic moment equal to 1.5(3) μB at 1.5 K. The Mössbauer investigations reveal no ferromagnetism of $ThFe_4Al_8$ sample. Knowing that this technique senses the magnetic structure on the local scale, this result does not contradict the observation of the modulated structure by means of neutron diffraction. Moreover, the magnetization measurements indicate growing ferromagnetic character in the thorium samples with increasing iron content. The ferromagnetic structure is not, however, seen in the neutron diffraction patterns. The neutron diagrams, collected in the temperature range 1.5 – 200 K, exhibit non-collinear spin modulation in the basal tetragonal plane. The consistent description of our neutron data requires the propagation wave vector in form: q = (0.267(7), 0.267(7), 0). The low-temperature patterns of $ThFe_4Al_8$ show pure magnetic satellites around the allowed nuclear reflections h + k + l = 2n, indicating the existence of incommensurately modulated magnetic structures in which the atoms related by the I operation scatter in phase. Acknowledgements This work was partly sponsored by the State Committee of Scientific Research through Grant No 2 PO3B 038 19.

Keywords: **ACTINIDES, POWDER DIFFRACTION, MODULATED STRUCTURES**

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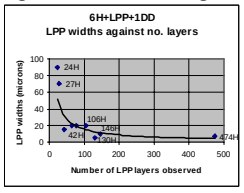
CORRELATION BETWEEN LAYER THICKNESS AND PERIODICITY OF LONG POLYTYPE COALESCENCE IN SILICON CARBIDE

J. Kelly P. Barnes
Industrial Materials Group School of Crystallography Birkbeck College, University of London Malet Street LONDON WC1E 7HX UK

The use of synchrotron radiation source edge diffraction topography (SRS-EDT) has been developed as a technique for investigating the spatial coalescence of polytypes in silicon carbide [1]. The problem has been of long-standing concern in materials science [2], while there is renewed interest in this burgeoning wide band gap semiconductor material. Current effort underlines the importance of understanding the role of defects and disorder in polytype formation and the novel application of SRS-EDT is well suited to this task. The use of SRS-EDT to obtain polytype profiles along with quantitative information on adjacent polytype neighbors and the regions between them has highlighted the ubiquitous nature of thin one-dimensionally disordered (1DD) layers [3]. A recent detailed study of long period polytype (LPP) coalescence [4] has enabled individual layer thickness measurements of periods up to 474H to be obtained for the first time (see Fig. 1). These results pose implications for the Lely growth of the crystals along with the comprehensive scope of the findings of this extensive survey into polytype neighborism in silicon carbide.
Figure1. The widths of LPP layers sandwiched between ordered and disordered regions in SiC shown against the layer stacking repeat.



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