FA3-MS21-P01

Complexity of aperiodic structures. Shelomo I. Ben-Abraham[a], Alexander Quandt[b]. [a]*Physics, Ben-Gurion University Beer-Sheba, Israel.* [b]*Physics, Ernst-Moritz-Arndt University Greifswald, Germany.*
E-mail: benabr@bgu.ac.il

Artificial aperiodic structures, such as quasiregular hetero-structures, photonic and phononic metamaterials, are an important and up-to-date research topic [1]. The fabrication of such structures is mostly governed by algorithms based on substitution sequences [2], [3].
The notions of "order" and "disorder" are context-dependent and subjective. For a deterministic structure "disorder" is a misnomer; the deviation from uniformity can be much better characterized and even quantified by symbolic complexity [2].
We have studied double-sided and two-dimensional versions of various standard substitution sequences.
Here we focus on the rectangle complexity [4] of a two-dimensional version of the Prouhet-Thue-Morse sequence and set an upper bound for its entropy. We also briefly hint at the complexity and entropy of lattice animals (polyominoes) living on an aperiodic structure.

[1] García-Moliner F., *Microelectronics J.*, 2005, 36, 870-876. [2] Allouche J.-P., Shallit J., A., *Automatic Sequences,* Cambridge UP, New York 2003. [3] *On-Line Encyclopedia of Integer Sequences,* http://www.research.att.com/~njas/sequences. [4] Berthé V., Vuillon L., *J. Théorie des Nombres de Bordeaux,* 2000, 12, 179-208.

Keywords: aperiodic structures, complexity, Prouhet-Thue-Morse sequence

FA3-MS21-P02

Positional Average Structure From an Incommensurately Modulated Crystal of Profilin:Actin. Gloria E. O. Borgstahl[a], Jason C. Porta[a], Jeff J. Lovelace[a], Antoine M. M. Schreurs[b]. [a]*The Eppley Institute for Research in Cancer and Allied Diseases, USA.* [b]*Bijvoet Center for Crystal and Structural Chemistry, Utrecht University, Utrecht, The Netherlands.*
E-mail: gborgstahl@unmc.edu

Modulation of protein crystals is seldom reported, mainly due to a lack of methods for solving these unique structures. We report here the incommensurately modulated average structure of profilin:actin and the methods that were used to carry out the analysis. Crystal modulation is characterized by a loss of short-range translational symmetry, where a single unit cell is no longer sufficient to accurately describe the structure. Such a loss of periodicity is often caused by dynamic processes within the crystal arising from, for example positional modulations. Experimentally, the incommensurately modulated state is characterized by the appearance of distinct satellite reflections surrounding the main Bragg reflections on the diffraction pattern that cannot be indexed with a supercell. In order to fully describe a modulated structure, and hence the dynamic processes within the crystal, one must explore higher-order space over multiple unit cells. By careful examination of atomic positions over higher dimensional space, a modulation function can be calculated that traces the atomic disorder. Such a function is periodic, but incommensurate with the crystal lattice. As a first step to solving this function for PA crystals, we have determined the average structure of the modulated state. Main and satellite reflections were integrated with *Eval15* and scaled with *SadAbs* to 3.0 Å. The average structure was then solved using the *Phenix* crystallographic software suite. Fourier electron density maps indicate the whole structure moves with major motion in actin subdomains 2 and 4. Superposition with the periodic profilin:actin structure and analysis by *DYNDOM* confirm these observations by showing the rotation of these domains. The modulation is in the **b** direction, which corresponds to the ribbon of actin molecules along this crystallographic axis. Analysis of these domain movements give insight into the long sought after globular (G) to fibrous (F) actin transition.

Keywords: incommensurate crystallography, modulated protein crystals, profilin, actin

FA3-MS21-P03

Incommensurate $BiMO_3$ Perovskites: $Bi_2Mn_{2/3}M_{2/3}Ni_{2/3}O_6$ and $Bi_2M'M''O_6$. John B. Claridge[a], Helen Hughes[a], Mathieu Allix[b], Sam Chong[a], Robert Szczecinski[a], Matthew Suchomel[a,c], Matthew Rosseinsky[a]. [a]*Department of Chemistry, University of Liverpool, Liverpool, U.K.* [b]*CRMHT, CNRS Orleans, Orleans, France.* [c]*Advanced Photon Source, Argonne National Laboratory, Argonne, USA.*
E-mail: j.b.claridge@liv.ac.uk

Materials in which dielectric and magnetic properties are coupled are of interest for multiple state memory and information storage applications, and fundamentally in terms of the mechanisms for coupling these properties. Single phase materials which display these properties are important as detailed studies of structural response are possible to permit the identification of the underlying mechanisms for this behaviour. In our search for ferromagnetic ferroelectrics based on Bi^{3+}, we have isolated new phases many of which are incommensurately modulated.
$Bi_2Mn_{4/3}Ni_{2/3}O_6$: This is a very unusual material as it adopts the perovskite structure with Bi^{3+} on the A site – there has only been one previous example of perovskite stable to ambient pressure synthesis, $BiFeO_3$. The material is spin-glass-like with a freezing temperature, T_f, of 35K due to competing exchange interactions on the B site of the perovskite structure and undergoes an incommensurate to "commensurate" transition above 410 K, which shows hysteresis. We have previously described the room temperature phase in 3+2 dimensional space group Ibmm(0-p0,q00)mm.ss ($\sqrt{2}a_p$ x $2a_p$ x $\sqrt{2}a_p$; p,q ~ ½).[1] Herein we will describe the temperature variation of the modulation vectors and the persistence of incommensurate cation order into the "commensurate" high temperature phase from combined synchrotron X-ray and time of flight neutron diffraction data.
$Bi_2Mn_{2/3}Ti_{2/3}Ni_{2/3}O_6$: This phases also crystallizes in the same superspace group as the manganese nickel analogue, in 3+2 dimensional space group Ibmm(0-p0,q00)mm.ss ($\sqrt{2}a_p$ x $2a_p$ x $\sqrt{2}a_p$; p,q ~ ½). It's room temperature structure based combined synchrotron X-ray and time of flight neutron diffraction will be discussed.
Bi_2CoTiO_6: This metastable high pressure double perovskite unusually shows no cation order but does show an incommensurate modulation, like several other similar phases. The combined refinements show that this material crystallizes in the polar superspace group I2cm(0p0)000 (p ~ -2/3).