another setting while SETSTRU converts alternative settings structure description to a standard setting and vice versa. EQUIVSTRU applies the space-group normalizers to derive the equivalent descriptions of the same structure.

The structure utilities are not restricted only to transformations: for a given pair of structure descriptions, STRAIN is used to calculate the linear and finite strain tensors as well as the degree of the lattice deformation and COMPSTRU tries to find the normalizer transformation that best matches the transformation between different descriptions. The program is also helpful for the recognition of identical or nearly identical atomic arrangements of different compounds which is essential for the crystal-structure classification problem. WPASSIGN identifies the Wyckoff positions to which the occupied atomic orbits of a structure belong.

The structures can be visualized in an interactive 3D environment via the VISUALIZE tool, using the Jmol script [2].

Where applicable, the tools support the CIF file format both for input and output, making it easy to exchange information between various related software packages.

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Keywords: crystal-structure description, structural similarity, Bilbao crystallographic server

MS.97.5

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Jpowder: a Web/Java based program for the display of powder diffraction data

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Jpowder [1,2] is a Java/Web based program which purposes are:

- Display and inspect powder diffraction data quickly and efficiently
- Use it to create web based crystallographic teaching content by allowing users to create interactive plots of data in addition to static plots [3]

Jpowder is written in Java and uses its associated JavaWeb Start and Java applet technologies. Java Web Start provides the ability to launch fully featured Java applications with a single click and without the need to go through operating system installation procedures. Based on the same code-base, a version of Jpowder has been exposed in the form of a Java applet – a self-contained Java component that can be embedded within a standard HTML web page. This means a user may initially use Jpowder to highlight regions of interest in datasets and then save such data not just as static images, such as jpgs, but also as 'Jpowder-applet format' files. These can subsequently be used as teaching material allowing students not only to learn from static images but also from interacting with the images directly.

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Keywords: teaching, powder, Web

MS.98.1

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Solving the incommensurately modulated structure in profilin: actin crystals

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Cellular motility, critical for neuronal development, cellular immunity, and intracellular bacterial locomotion, etc., is regulated through cytoplasmic actin/profilin interactions. In these interactions, profilin sequesters actin monomers for delivery to actin filament assembly sites. Detailed structural information on monomeric actin has been provided by X-ray crystallography, but it is not known how actin is delivered by profilin to the end of a growing actin filament. To study the structural rearrangements of actin and the associated changes in protein-protein interactions in filament formation, profilin:actin (PA) crystals provide an excellent model because they retain the dynamic nature of actin. Twenty five years ago it was found that when PA crystals were exposed to conditions known to promote actin filament formation, they transformed into a modulated state characterized by unusual off-lattice satellite reflections. The satellites are caused by the formation of an actin superstructure within the crystal. Methods for solving such modulated crystal structures are known to aperiodic small-molecule crystallographers, yet macromolecular crystallographers have not yet solved one. Several crystals of macromolecular complexes have modulations and cannot be solved. The biologically-important, modulated PA crystals will be solved as a first case and bring the 25 year old mystery of what is happening in these crystals to a close. The crystallographic tools we are developing for this PA case will provide the platform needed to tackle similar, rare, but important, structural conundrums.

These PA crystals contain an incommensurate modulation in one direction, a so-called (3+1) dimensional modulation. We can reproducibly produce isomorphously modulated crystals of PA and collect complete cryocooled data to 2 Å resolution. These data can be indexed with the q vector approach and the main and satellite reflections integrated using EVAL15 software. We have reindexed these data with an approximate super cell and solved a superstructure approximation of the modulated structure. Routes for solving the incommensurate crystal structure using the full super space theory will be discussed.

Keywords: aperiodic, incommensurate, protein

MS.98.2

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Soft Quasicrystals Thermodynamic stability of complex structures

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There is growing interest in recent years in the ability to grow quasicrystals and other complex structures, whose building blocks are on a mesoscopic scale of tens to thousands of nanometers. These range from artificially constructed metamaterials, such as photonic quasicrystals, to self-assembled soft-matter quasicrystals [1-3]. In addition to having promising applications, especially in the optical domain, these materials give us the opportunity to study quasicrystals in ways that were impossible before. As time permits, I will discuss a few aspects of our ongoing work on these systems, ranging from our recent explanation of the stability of quasicrystals composed of soft isotropic

particles [4,5], to the design of nonlinear photonic quasicrystals for optical frequency conversion [6].

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Keywords: quasicrystals, soft matter, self assembly

MS.98.3

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Incommensurate Tiling in η'-Cu_{3+x}(Si,Ge) Determined by Electron Diffraction

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Despite its technological importance *e.g.* as a catalyst for the production of chlorosilanes used in semiconductor industry, η'-$Cu_{3+x}Si$ has eluded correct structural description for decades due to the combination of a complex, two-dimensional incommensurately modulated structure, and difficulty to obtain large samples suitable for single crystal analysis.

We prepared small isolated platelets about 40 nanometres thick with composition $Cu_{76.1}Si_{11.7}Ge_{12.2}$ by deposition of organometallic precursors (hexamethyldigermane $Ge_2(CH_3)_6$ and ethyl silane $SiH_3C_2H_5$) on Cu substrate by the CVD method at the temperature of 500 °C.

Initial investigation of the samples revealed complex diffraction pattern with satellite reflections at incommensurate positions (Fig. 1a). The complex diffraction pattern is not a consequence of twinning, but it stems from one phase. This is evidenced by high-resolution TEM images (Fig. 1b,c). The data for structural investigation were collected by quantitative electron diffraction tomography coupled with precession electron diffraction on a Philips CM120 with LaB_6 cathode operating at 120kV, equipped with a precession device SpinningStar (NanoMegas). The structure was solved by the charge-flipping algorithm in superspace [2].

The structure is trigonal, and it is incommensurately modulated with two modulation vectors $q_1 = (\alpha,\alpha,1/3)$ and $q_2 = (-2\alpha,\alpha,1/3)$, superspace group $P\bar{3}1m$ $(\alpha,\alpha,1/3)000(-2\alpha,\alpha,1/3)000$ (number 162.2.76.3 in the recently published tables [3]). The structure of η'-Cu_{3+x}(Si,Ge) can be described as a stacking of slabs of face- and edge-sharing Cu clusters, and honeycomb layers formed by Si and Ge. The Cu slabs are strongly modulated, leading to a predominant icosahedral coordination of the central atoms of the clusters. The two-dimensional modulation functions describing the shifts of the atoms show an unprecedented complexity and large amplitude. The conflict between the striving for locally favorable icosahedral coordination of the Cu atoms and the need for a long-period arrangement is the most likely reason for the modulation.

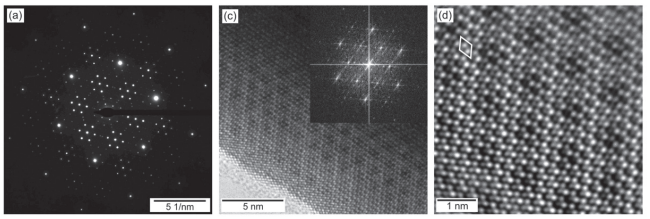

Figure 1: TEM observations. (a) Diffraction pattern of the zone [001]. (b) HRTEM image. (c) A Fourier-filtered scale-up of (c) showing clearly the non-periodic variation of the contrast. The basic unit cell is shown by the white rhombus.

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Keywords: electron diffraction tomography, 5D structure, charge flipping

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Dynamics of the inner tetrahedron in the ZnSc 1/1 quasicrystal approximant: experiment and simulation

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We present a combined experimental and theoretical study of the dynamic of the inner tetrahedron in the ZnSc 1/1 periodic approximant to the quasicrystal. The structure of the approximant is described by a body centre cubic packing of the so-called Tsai type cluster [1]. The central part of this cluster is a tetrahedron, whose orientation is randomly distributed at room temperature [2]. At about 150 K, there is an order-disorder phase transition accompanied by a lattice distortion towards a phase of monoclinic symmetry [3]. In the low temperature phase, the tetrahedra are oriented in an anti-parallel manner along the (110) direction [4].

We will present a detailed quasielastic neutron scattering study of the ZnSc approximant as a function of the temperature. The experiment un-ambiguously shows that the tetrahedra are dynamically moving above Tc, whereas they are locked-in below Tc. This will be compared to atomistic simulations using oscillating pair potentials [5] which shows the importance of the cluster distortion and resulting frustration in the dynamics of this complex systems.

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Keywords: quasicrystals, dynamics, neutron scattering