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

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

Lukáš Palatinus,[a] Mariana Klementová,[a,b] Vladislav Dřínek,[c] Markéta Jarošová,[a] Václav Petříček,[a] *[a]Institute of Physics of the AS CR, v.v.i., Prague (Czechia). [b] Institute of Inorganic Chemistry of the AS CR, v.v.i., Husinec-Řež (Czechia). Institute of Chemical Process Fundamentals of the AS CR, v.v.i., Prague (Czechia).* E-mail: palat@fzu.cz

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.

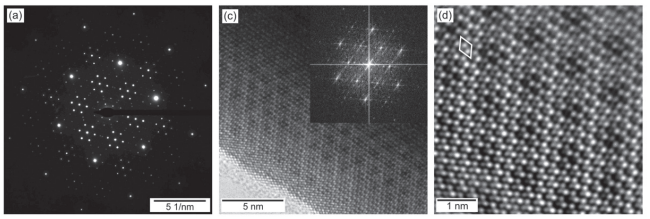

Figure 1: TEM observations. (a) Diffraction pattern of the zone [001]. (b) HRTEM image. (c) A Fourier-filtered scale-up of (c) showing clearly the non-periodic variation of the contrast. The basic unit cell is shown by the white rhombus.

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

M. de Boissieu,[a] H. Euchner,[b,a] T. Yamada,[c,a] S. Rols,[d] H. Schober,[d] R. Tamura,[c] M. Mihalkovic,[e] *[a]SIMaP, Grenoble-INP, CNRS, UJF, BP 75, 38402 Saint Martin d'Hères Cedex , (France). [b]ITAP, Universitat Stuttgart, Stuttgart 70550, (Germany). [c] Department of Materials Science & Technology, Tokyo Univ. of Science, Noda 278-8510, (Japan). [d] Institut Laue-Langevin, Grenoble, (France). [e]Institute of Physics, Slovak Academy of Sciences, 84511 Bratislava, (Slovakia).* E-mail: Marc.de-Boissieu@simap.grenoble-inp.fr

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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