IAP Seminar

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Structure analysis of two-dimensional oxide quasicrystal in physical and internal space

Recently the formation of $BaTiO_3$-derived and $SrTiO_3$-derived two-dimensional oxide quasicrystals (OQC) with 12-fold symmetry have been discovered on Pt(111) substrates [1,2]. The characteristic Niizeki-Gähler tiling formed by these OQCs consists of quadratic, triangular, and rhombic elements of equal side length with Ti atoms at the vertices. This tiling can be derived from cutting a periodic hyperhexagonal structure in the four-dimensional space and projecting it back into two dimensions. This main projection leads to the so-called physical space of the tiling which is embedded in the atomic lattice. An alternative projection of the four-dimensional lattice leads to a limited region in two dimensions, the so-called acceptance region in the internal space. Both projections of the ideal Niizeki-Gähler tiling with 128 vertices are shown in Fig. 1.

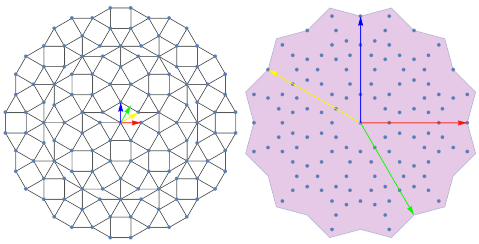

Fig. 1 Niizeki-Gähler tiling in physical space (left) and internal space (right), together with the four 4D unit vectors color coded in red, yellow, green and blue. The acceptance region is marked on the right in light red.

Here we present an analysis of atomically-resolved STM images of the OQC making use of the tools of higher-dimensional crystallography as described above. This allows to determine the deviations of the real OQC structure as observed by STM from the ideal Niizeki-Gähler tiling. This deviations come along as atomic flips in the tiling. By color coding all vertices in the STM image which are located outside of the acceptance domain upon lifting into the internal space, these atomic flips can be identified in the STM images. An additional statistical evaluation of the frequency and the orientational distribution of various building blocks of the OQC tiling is used to systematically study the way how the OQC tiling adopts to the underlying periodic lattice. This type of analysis is essential for elucidating the way how this spontaneous quasicrystal-crystal heteroepitaxy is realized.

[1] S. Förster, K. Meinel, R. Hammer, M. Trautmann, and W. Widdra, Nature **502**, 215 (2013)

[2] S. Schenk, S. Förster, K. Meinel, R. Hammer, B. Leibundgut, M. Paleschke, J. Pantzer, C. Dresler, F.O. Schumann, and W. Widdra, J. Phys.: Condens. Matter **29**, 134002 (2017)

All interested colleagues are welcome to this seminar lecture (45 min. presentation followed by discussion)

Friedrich Aumayr
(LVA-Leiter)

M. Setvin
(Seminar Chair)