study for cubic Ag-In-Ca [4], which is an approximant phase of the QC, to investigate the crystal and electronic structure including bias voltage dependence of STM images reported in the experiments [1]. We found that the bright contrast on different subsets of the In sites are obtained from charge distributions of occupied and unoccupied states. However, the simulated images cannot be directly compared with QC surface, because the surface used in the calculation is the twofold (001) surface of the approximant phase.

For direct comparison of crystal and electronic structures, we perform STM analyses for the (001) surface of the approximant. However, STM images with atomic resolutions obtained in QC surface are not observed in the approximant phase. For the approximant surface, observed bright spots are larger than that of observed in QC surface, implying that the spot obtained in the approximant surface represents an atomic cluster. The obtained images are not consistent not only with that of the QC surface, but also calculated images. In the above-mentioned calculation [4], we used a slab model, and according to the analysis of QC surface an Yb-rich flat layer intersecting the cluster center is selected as the topmost surface layer. We suppose that the incompatibility between experiment and theory is originated in the flat surface used in the calculation.

To examine this possibility, we construct an alternative model surface with non-flat Yb-rich topmost layer based on the bulk structure [5] and re-calculate the STM images. After the structural relaxation by the self-consistently estimated atomic force, the corrugation of topmost Yb-rich plane is enhanced. On the contrary, In atoms located about 1.8 Å below the topmost layer move toward the vacuum area. The obtained charge distribution shows a large bright spot with about 7 Å in diameter for negative bias voltage. The bright contrast is made from the charge distribution around Yb and In sites near the surface layer, supposedly originated in the hybridization of In-sp states and low-lying Yb-d states [6].

We present an experimental study, utilising the scanning tunnelling microscopy (STM) technique, of pentacene adsorption on one- and two-dimensionally quasi-periodic surfaces. There have been numerous studies on the growth of overlayers on quasicrystal surfaces with the aspiration to further the understanding of epitaxial interactions at surfaces with complex order, reduce the chemical complexity inherent to bulk quasicrystals and produce thin-films and nano-scale features with novel electronic properties. To date, several epitaxial systems have been found [1]. However, no epitaxial quasi-periodic ordering of molecules has been observed experimentally.

The pentacene molecule is an organic semiconductor with a tendency to form ordered flat films on metallic surfaces [2]. STM is useful to image such complex, non-periodic surface structures on a local scale and determine molecular adsorption sites. When deposited upon bulk-terminated, high symmetry quasicrystal surfaces a degree of orientation order is observed in the adsorbed linear molecules at sub-monolayer coverage. The completed layer on the respective surfaces is disordered and loosely bound.

The adsorption and growth of the molecules is also observed on the one-dimensionally quasi-periodic, vicinal surface of Cu formed with novel electronic properties. To date, several epitaxial systems have been found [1]. However, no epitaxial quasi-periodic ordering of molecules has been observed experimentally.

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Poster Sessions

MS63.P24

Structure solution of decagonal ZnMgDy quasicrystal
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Here we report the first structure solution of decagonal ZnMgDy quasicrystal (d-ZnMgDy) based on single crystal X-ray diffraction data. Samples with the composition (Zn_{0.57}Mg_{0.43}Dy_{0.33}) were prepared by induction melting followed by annealing at 375°C for 10 months. The alloys were then quenched to room temperature. The resulting samples consist mainly of a hexagonal phase with the d-ZnMgDy existing as the secondary phase. The morphology of the decagonal phase is typically needle-like. These grains are of 50 μm in length and approximately 15 μm in other dimensions. X-ray diffraction experiments were carried out both in-house (Oxford Xcalibur PX diffractometer, CCD detector, Mo Kα radiation) and at the Synchrotron facility in Swiss-Norwegian beam line, ESRF, Grenoble (λ=0.6980 Å).

The Laue group was specified to be 10/mm with a periodicity of 5.22 Å along the periodic direction. No systematic extinctions were observed. SUPERFLIP program package [1] (based on charge flipping and low density elimination algorithms) was used for structure solution.


Keywords: quasicrystal, decagonal

MS63.P26

Ab-initio calculations on the stability of heptagonal ordering in Gallium
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Sevenfold symmetry is the lowest rotational symmetry not yet observed in quasicrystals. However, there are several strong hints that indicate the existence of heptagonal quasicrystals (QCs) [1]. In a previous ab-initio study [2] it was shown that theoretical sevenfold approximants, designed from promising known boride and borocarbide structure types by using a supertile approach, were acceptably stable within the range of error. Due to the fact that these structures and their associated tilings are ternary, the weak matching rules automatically imposed on the edges of the tiles only allow for a limited number of possible structural arrangements.

The configurational degrees of freedom can be increased by investigating the structure of monatomic γ-Ga, a metastable low temperature phase that forms when undercooling liquid Ga to below -35.6°C. Its structure consists of regular sevenfold antiprisms centered at the γ-Ga atoms. As only periodic structures can be imposed on the edges of the tiles only allow for a limited number of possible structural arrangements.

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For the missing two unit tiles (with acute angles π/7 and 2π/7), decorations were be designed by using similar atomic arrangements as for the fat tile (i.e. γ-Ga). As only periodic structures can be accessed by means of ab-initio total energy calculations, the unit tiles were subsequently used to decorate approximants. Therefore various theoretical structure types were generated, either by periodic arrangement of single tiles or hexagon supertiles of the rhomb tiles, or by creating rational heptagonal approximants using the cut-and-project method.

The first-principles DFT calculations were performed with the VASP code [3], using a plane-wave basis set, the GGA algorithm and PAW-PBE pseudopotentials. Total energies were calculated for all theoretical Ga structure types, as well as the electron localization function (ELF), and the atom relaxation movements were investigated.

The possibility of stabilizing the designed structures by dopant atoms was also explored: the rational approximant structures mentioned above exhibit a small number of voids or holes too large for Ga-atoms,