

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].

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Keywords: quasicrystal, surface, STM

MS63.P22

Acta Cryst. (2011) A67, C630

Icosahedral and approximant phases in (Al,Ga,In)-Pd-(Rare Earth Metal) systems

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Tsai-type icosahedral quasicrystals have recently attracted a lot of interest for their formations, structural and physical properties. Recently, we have reported the formation of the i-phase and its 1/1-approximant phase in the Al-Pd-Sc alloy [1]. The i-phase satisfies well the formation conditions established for the Tsai-type i-phases [2, 3]. In the present study, we have done further demonstration of the formation conditions for the i-phases by the following substitutions of constituent elements in the Al-Pd-Sc alloy: Al for (Ga, In), and Sc for other rare earth metals. Note that the substitutions keep the *e/a* (valence electrons per atom ratio) = 2.10 where all the substitution elements are assumed

as trivalent except for Yb which is usually assumed as divalent in the quasicrystalline formations. Ternary alloys with various compositions around (Al, Ga, In)₅₄Pd₃₀RE₁₆ were prepared from elemental constituents with purity better than 99.9 mass% by arc-melting under an argon atmosphere. The Al-Pd-RE alloys were subsequently subjected to single-roller melt spinning in argon atmosphere. Some of the samples were sealed in evacuated silica tubes and annealed at various temperatures. All of samples were characterized by powder X-ray diffraction measurements. Electron diffraction measurements were performed for the i-phases newly found. Differential scanning calorimetry (DSC) measurements were carried out in the temperature range from room temperature to 1473K under an argon atmosphere. In the Al-Pd-RE(RE=Yb, Tm and Er) melt-quenched alloys, the 1/1-phase has been found to form. Moreover, the metastable i-phase has been found in the Al-Pd-Yb alloy. The 1/1-phase has also been found to form in the Ga-Pd-Sc and the In-Pd-RE((RE=Y, Sm and Gd) alloys. For the i- and the 1/1-phases found in this study, the ratio of the atomic radius of the rare earth element to that of the other base elements is in the range 1.15–1.24, which is within the range of the values reported for other Tsai-type i-phases [3]. Further searching for the i-phases in different alloy systems are now underway and the formation and the stability will be discussed in detail.

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Keywords: quasicrystal, formation, alloy

MS63.P23

Acta Cryst. (2011) A67, C630-C631

Adsorption of pentacene on quasi-periodic surfaces

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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 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 on the five-fold surface of AlPdMn [3, 4]. The pentacene aligns along the quasi-periodically sequenced rows. As the layer becomes more dense inter-molecular repulsion dominates leading to the formation of a periodic structure. This growth persists beyond the first layer and

it is evidenced that the second layer molecules are found to adsorb directly on top of the underlying layer.

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Keywords: quasicrystal, pentacene, adsorption

MS63.P24

Acta Cryst. (2011) A67, C631

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 ($\text{Zn}_{57.6}\text{Mg}_{40.8}\text{Dy}_{1.6}$) 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 K α radiation) and at the Synchrotron facility in Swiss-Norwegian beam line, ESRF, Grenoble ($\lambda=0.6980$ Å).

The Laue group was specified to be 10/mmm 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.

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Keywords: quasicrystal, decagonal

MS63.P25

Acta Cryst. (2011) A67, C631

Analysis of structure and chemical order in a ternary Yb₁₂Mg₅₂Cd₃₆ quasicrystal

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The atomic structure of the ternary Yb₁₂Mg₅₂Cd₃₆ quasicrystal has been refined from single crystal X-ray data. The ternary quasicrystal is related to the binary i-Yb₁₆Cd₈₄ parent phase, [1, 2] and suffers from chemical disorder mainly due to mixing between Mg and Cd. Studies on related ternary approximants however indicate that this chemical disorder is only partial, and that there are strong selection rules in

several ternary systems that govern the choice of a particular atom at a specific site. The purpose of this work is thus to elucidate the chemical order between the constituent elements in the ternary Yb₁₂Mg₅₂Cd₃₆ quasicrystal and its relation to ternary approximants in other RE-Mg-Cd (RE=Rare Earth) systems. The structure refinements performed on the Yb₁₂Mg₅₂Cd₃₆ quasicrystal clearly indicate that it is composed of similar atomic clusters as the binary i-Yb₁₆Cd₈₄ phase and that there is a strong selection rule that mainly determines the chemical order at the cluster level. Similar observations have also been made in other related ternary approximant phases. The structure refinement is the first of its kind performed on a ternary Yb-Cd-related quasicrystal, and the results indicate that the structures and chemical order of ternary quasicrystals can be understood by extracting and combining information from structure refinements on both quasicrystals and related approximants.

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Keywords: quasicrystal, approximant, chemical order

MS63.P26

Acta Cryst. (2011) A67, C631-C632

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 by a single Ga atom. Additionally it can be described as a periodic arrangement of one of the three heptagonal rhombic unit tiles, namely the "fat" tile with an ideal acute angle of $3\pi/7$ ($= 77.12^\circ$, in the structure 76.15°).

For the missing two unit tiles (with acute angles $\pi/7$ and $2\pi/7$), decorations were 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,