

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

Yeong-Gi So,<sup>a</sup> Fukuaki Saruhashi,<sup>b</sup> Keiichi Edagawa,<sup>a</sup> and Ryuji Tamura,<sup>b</sup> <sup>a</sup>*Institute of Industrial Science, The University of Tokyo, Komaba, Meguro-ku, Tokyo, (Japan).* <sup>b</sup>*Department of Materials Science and Technology, Tokyo University of Science, Yamazaki, Noda-shi, Chiba, (Japan).* E-mail: so@iis.u-tokyo.ac.jp

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)<sub>54</sub>Pd<sub>30</sub>RE<sub>16</sub> 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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### Adsorption of pentacene on quasi-periodic surfaces

Kirsty Young,<sup>a</sup> Joseph Smerdon,<sup>b</sup> Hem Raj Sharma,<sup>a</sup> Ronan McGrath <sup>a</sup>*Department of Physics, University of Liverpool, Oxford Street, L69 7ZE (UK)* <sup>b</sup>*Center for Nanoscale Materials, Argonne National Laboratory, Cass Avenue, 60439 (USA).* E-mail: k.m.young@liv.ac.uk

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