

MS63.P19

Acta Cryst. (2011) A67, C629

SWAXS Analysis on some quasicrystal formations

Caner Tükel,^a Elif Şen,^b Semra İde,^c Mehmet Erbudak,^d Abdullah Vercin^e ^aHacettepe Univ. Dept. of Nanotechnology and Nanomedicine, Ankara, (Turkey). ^bKaradeniz Technical Univ., Dept. of Physics, Trabzon, (Turkey). ^cHacettepe Univ., Dept. of Physics Eng., Beytepe, Ankara, (Turkey). ^dETH Swiss Federal Inst. of Technology, Zürich Area, (Switzerland). ^eAnkara Univ. Dept. of Physics, Ankara (Turkey). E-mail: ctukel@gmail.com

Quasicrystals (QCs) show long-range order, but no translational periodicity and possess rotational symmetries forbidden in crystallography (i.e., 5-fold and 10-fold symmetries) [1]. They have unusual periodic and quasiperiodic atomic structures beside of crystal-glass inner phases which have great importance in solid state physics, metallurgy and new technological applications. These intermetallic compounds not only have original structure, but also have unique properties that display unusual hardness and brittleness, low coefficients of friction, and high thermal and electrical resistance [2]. As known, X-rays and microscopic methods (such as XRD, SWAXS, XPS, AFM, SEM, and TEM [3-6]) have been widely used to access structural information and understand the relationship between their structures and properties.

As a part of our researches related with a TUBITAK Project, SAXS and WAXS methods have been used to characterize three novel synthesized (Al-Ni-Co, Al-Cu-Co, and Al-Pd-Mn) quasicrystals, and the nanosized similar/different electron density regions in long range order of the samples in the form of thin sections (5 µm) have been investigated. Size, shape and pair distance distributions of these regions have been also examined by using scattered X-rays. So the local environments and long range orders of these samples have been tried to explain by using simultaneous SAXS and WAXS measurements and the evaluated data. Scattering profiles were measured by an HECUS-SWAXS system using CuK α radiation during 40, 80 and 120 min. The first structural parameters have been obtained from Guinier and Porod regions of the scattering patterns. And then, three dimensional suitable structural models were developed and applied to experimental data.

[1] D. Shechtman, et al. *Phys. Rev. Lett.* **1984**, 53, 1951. [2] J.M. Dubois, **2005**, *Useful Quasicrystals*, World Sci. Publis. Co. Pte. Ltd. [3] P.J. Pinhero et al. *Phil. Mag. B* **1999**, 79, 91-110. [4] S.-L. Chang, et al. *J. Non-cryst. Solids* **1996**, 195, 95-101. [5] J.Y. Park et al. *Physical Review B* **2005**, 72, 220201. [6] H. Okuda et al. *J. Physics: Conf. Series* **247**, **2010**, 012037.

Keywords: quasicrystals, SAXS, WAXS

MS63.P20

Acta Cryst. (2011) A67, C629

Theoretical study for pseudomorphic growth on Ag-In-Yb quasicrystal surface

Kazuki Nozawa, Yasushi Ishii, Department of Physics, Chuo University, Tokyo, (Japan). E-mail: nozawa@phys.chuo-u.ac.jp

Quasicrystals (QCs) are long-range ordered materials with rotational symmetry incompatible with translational symmetry. Recent experimental studies reveal that the quasiperiodic atomic arrangement remains even on the surface, and moreover succeed in observing pseudomorphic monoatomic layers deposited by evaporation method. In this study, we report adsorbed structures of Pb atoms on the fivefold surface of icosahedral (*i*-) QC Ag-In-Yb, which is obtained by a substitution of Ag and In for Cd of the binary QC *i*-Cd-Yb [1], calculated by density functional method with the quasiperiodic surface treated in a cluster model. Sharma *et al.* [2] studied the fivefold surface of *i*-QC Ag-

In-Yb by scanning tunneling microscopy (STM), and reported that the surface are formed at bulk planes intersecting the center of the rhombic triacontahedral cluster, which is the structural building block of *i*-Cd-Yb. According to the STM observation, we construct a cluster model, the topmost layer of which is an Yb-rich fivefold plane intersecting the cluster center. Atomic positions are extracted from the QC model proposed by Takakura *et al.* [3]. Since chemical order in *i*-Ag-In-Yb has not known completely, the ordering of Ag and In is determined according to a study for Ag-In-Yb approximant phase by Gomez [4]. We have checked the effect of chemical disorder for some particular sites, but essential difference was not observed. As a preliminary result, we reported energetically preferred Pb adsorption sites using a thin cluster, the diameter and thickness of which are 40 and 0.5 Å, respectively [4]. The calculated potential energy surfaces indicate that at very low coverage the adsorbed Pd atoms form a pentagon 1.0 Å above the topmost layer of the substrate with the edge length about 9.9 Å, which seems consistent with recent experimental results [5]. After the formation of the Pb pentagon, we found two possible adsorption sites at same adsorption height, but those are not consistent with the experimental observation, indicating that further deposition leads second Pb layer 2.0 Å above the substrate.

To examine the possible adsorption sites after the Pb pentagon formation, further calculations have been done with various diameters and thickness of the cluster. New energetically preferred adsorption site is found using a cluster with 50 Å diameter and 4.0 Å thickness, and including 363 atoms in the super cell. The adsorption height of this newly predicted site is same as the first Pb layer (1.0 Å). However, Pb atom sitting on this site may not prevent the next adsorption on the experimentally observed site with height of 2.0 Å, because the distance between these site is about 3.3 Å, not very short compared with the nearest neighbor distance in the fcc Pb (3.5 Å). Two In atoms locating 2.5 Å below the topmost surface layer seem to play an important role to stabilize this new adsorption site.

[1] H.R. Sharma, M. Shimoda, K. Sagisaka, H. Takakura, J.A. Smerdon, P.J. Nugent, R. McGrath, D. Fujita, S. Ohhashi, A. P. Tsai, *Physical Review B* **2009**, 80, 121401(R). [2] A.P. Tsai, J.Q. Guo, E. Abe, H. Takakura, T.J. Sato, *Nature* **2000**, 408, 537-538. [3] H. Takakura, C.P. Gómez, A. Yamamoto, M. de Boissieu, A.P. Tsai, *Nature Materials*, **2007**, 6, 58-63. [4] C.P. Gómez, *private communication*. [5] K. Nozawa, Y. Ishii, Phil. Mag. (to be published) [6] H.R. Sharma, P.J. Nugent, G. Simutis, J. Smerdon, V.R. Dhanak, R. McGrath, M. Shimoda, C. Cui, Y. Ishii, A.P. Tsai, *Abstract book of 11th International Conference on Quasicrystals*, **2010**, 43.

Keywords: quasicrystal, surface, theory

MS63.P21

Acta Cryst. (2011) A67, C629-C630

Simulated STM images for surface of Ag-In-Yb cubic approximant

Naoki Tanaka, Kazuki Nozawa, Masahiko Shimoda, Yasushi Ishii, Department of Physics, Chuo University, Tokyo, (Japan). ^bNational Institute for Materials Science, Tsukuba, (Japan). E-mail: ishii@phys.chuo-u.ac.jp

Recent extensive studies on surface structure of quasicrystals (QCs) reveal that the quasiperiodic arrangement remains even on the surface, and it is expected that the unique atomic arrangement exhibit a novel surface property. Sharma *et al.* performed scanning tunneling microscopy (STM) measurements for icosahedral Ag-In-Yb fivefold surface [1], which is isostructural to binary Cd-based QC family [2]. They reported that surface are formed at Yb-rich bulk plane intersecting the center of the rhombic triacontahedral cluster, which is a building block of this family of QCs [3]. We carried out a density functional

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].

[1] H.R. Sharma, M. Shimoda, K. Sagisaka, H. Takakura, J.A. Smerdon, P.J. Nugent, R. McGrath, D. Fujita, S. Ohhashi, A.P. Tsai, *Physical Review B* **2004**, *80*, 120401(R). [2] A.P. Tsai, J.Q. Guo, E. Abe, H. Takakura, T.J. Sato, *Nature* **2000**, *408*, 537-538. [3] H. Takakura, C.P. Gómez, A. Yamamoto, M. de Boissieu, A.P. Tsai, *Nature Materials*, **2007**, *6*, 58-63. [4] K. Nozawa, Y. Ishii, *Journal of Physics: Conference Series* **2010**, *226*, 012030. [5] C.P. Gómez and S. Lidin, *Physical Review B* **2003**, *68*, 024203. [6] Y. Ishii, T. Fujiwara, *Physical Review Letters*, **2001**, *87*, 206408.

Keywords: quasicrystal, surface, STM

MS63.P22

Acta Cryst. (2011) A67, C630

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

Yeong-Gi So,^a Fukuaki Saruhashi,^b Keiichi Edagawa,^a and Ryuji Tamura,^b ^a*Institute of Industrial Science, The University of Tokyo, Komaba, Meguro-ku, Tokyo, (Japan).* ^b*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)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.

[1] Y.G. So, K. Edagawa, *Materials Transactions, JIM* **2009**, *50*, 948-951. [2] A.P. Tsai, in *Quasicrystals*, ed. by T. Fujiwara, Y. Ishii (Elsevier Science B.V., Oxford), **2007**, 75-106. [3] T. Ishimasa, in *Quasicrystals*, ed. by T. Fujiwara and Y. Ishii (Elsevier Science B.V., Oxford), **2007**, 49-74.

Keywords: quasicrystal, formation, alloy

MS63.P23

Acta Cryst. (2011) A67, C630-C631

Adsorption of pentacene on quasi-periodic surfaces

Kirsty Young,^a Joseph Smerdon,^b Hem Raj Sharma,^a Ronan McGrath ^a*Department of Physics, University of Liverpool, Oxford Street, L69 7ZE (UK)* ^b*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