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**SWAXS Analysis on some quasicrystal formations**

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Quasicrystals (QCs) show long-range order, but no translational periodicity and posses 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 CuKα 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.

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

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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.

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

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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 isostractural 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