spectrometry (RBS). In addition, supplementary compositional analysis was performed by energy dispersive X-ray (EDX) analysis, X-ray photoelectron spectroscopy (XPS) in combination with sputter depth profiling, and secondary ion mass spectrometry (ToF-SIMS) in dynamic mode.

It was found that the as-deposited Al/Cu/Fe layers on Si clearly has a multilayered structure. After annealing the individual layers diffused together creating a homogeneous film with an ~50 nm thick Al_2O_3 surface oxide. Si started to diffuse into the film below 390 °C, during a substrate-film reaction. This caused a change in film composition preventing the quasicrystalline phase region to be reached, and instead the approximant $Al_{55}Si_7Cu_{25.5}Fe_{12.5}$ together with other crystalline phases was formed in the temperature range 400 to 670 °C. The single approximant phase was obtained at 600 °C.

After 4 h annealing at 600 °C the film contained ~9 at% Si, corresponding well to the expected value of the approximant phase [2]. Even though the amount of Si in the films is found to slowly increase to ~13 at% during extended annealing (>100 h) the approximant phase was retained.

[1] D.S. Shaitura, A.A. Enaleeva, *Cryst. Rep.* **2007**, *52*, 945-952. [2] A. Quivy, M. Quiquandon, Y. Calvayrac, F. Faudot, D. Gratias, C. Berger, R.A. Brand, V. Simonet and F. Hippert, *J. Phys. Condens. Matter* **1996**, *8*, 4223-4234.

Keywords: thin film, approximant, ion beam analysis

MS63.P04

Acta Cryst. (2011) A**67,** C623

Structural transformation in Al-Fe-Cu-Mn one dimensional quasicrystals

T. P. Yadav,[a] N.K. Mukhopadhyay [b] and O. N. Srivastava [a] *[a]Department of Physics, Banaras Hindu University, Varanasi-221 005 (India). [b]Department of Metallurgical Engineering, Institute of Technology, Banaras Hindu University, Varanasi-221 005, (India).* E-mail:yadavtp@gmail.com

The main objective of the proposed work would be to investigate into the transformation mechanism in one dimensional quasicrystal. The one dimensional quasicrystalline phases in $Al_{70}Cu_{20}Fe_7Mn_8$ alloy have been synthesized by melting the individual elements using radio frequency induction furnace (18 kW) under continuous flow of argon gas into the silica tube. During melting process, water is circulated in the outer jacket around the silica tube to reduce the contamination of the alloy. The transformation behaviors of one dimensional quasicrystalline have been investigated during annealing (up to 900 °C) and mechanical milling (up to 100 hours). The transformation of one dimensional quasicrystalline phase to icosahedral as well as various disordered states have been observed in Al-Fe-Cu-Mn alloys during milling. The milling of pre-alloyed material was carried out a high-energy ball mill by varying milling time up to 100 h under liquid hexane medium and at various milling intensity. X-ray diffraction and transmission electron microscope were carried out for evaluating the lattice strain, lattice parameters and crystallite sizes of the mechanically milled samples. The evolution of nano icosahedral phases as well as crystalline phases was found to occur. The subsequent thermal treatment led to the structural ordering in the concerned phases. The implication of the evolution of various phases, their structural correlations and their relative stability will be discussed.

Keywords: quasicrystal, phase transformation, mechanical milling

MS63.P05

Acta Cryst. (2011) A**67,** C623

Structural characterization of highly defective Al-Pd-Fe crystalline approximant

W. Sun, J. P. Wang, Z. Y. Liu, *Institute of Microstructure and Property of Advanced Materials, Beijing University of Technology 100 Pingle Yuan, Chao Yang District, Beijing 100124, (China).* E-mail: weisun@bjut.edu.cn

Crystalline approximants, which are structurally related to their corresponding quasicrystals, belong to a class of structurally complex alloy phase. A crystalline approximant can have a quite large unit cell consisting of hundreds or even thousands of atoms. Due to its structural complexity, the structural defects in the crystalline approximant can be quite different in comparison with those in an ordinary crystalline phase with a small unit cell [1]. In general, a crystalline approximant contains the characteristic atom clusters which are of the same type as those in its corresponding quasicrystal. Therefore, in order to understand the intrinsic structure of the crystalline approximant and special structural defects in it, the characteristic arrangement of atom clusters has to be taken into account rather than a usual structural description in terms of unit cell. Existence of various special structural defects associated with wrong arrangements of atom clusters in hexagonal tiling structures of the ξ- and ξ'-phases in Al-Pd-Mn [2] and Al-Ni-Rh [3] systems has been reported. In the Al-Pd-Fe system, the crystalline approximant, corresponding to an Al-Pd-Fe decagonal quasicrystal with 1.6 nm periodicity, can have a kind of pentagonal tiling structure of atom clusters, which is more complex than the tiling structures of the ξ- and ξ'-phases. It is still an open question about whether any new defect can exist in the non-hexagonal tiling structure of atom clusters. In this study, a highly defective Al-Pd-Fe crystalline approximant which can accommodate new type of special structural defect (H-type) has been found in the as-cast and heat-treated $Al_{75}Pd_{15}Fe_{10}$ alloys. By means of high resolution electron microscopy (HREM), the highly complex defective structure in the Al-Pd-Fe crystalline approximant has been characterized.

Electron diffraction examinations show that the principal diffraction patterns of the Al-Pd-Fe crystalline approximant (E-phase) can be indexed as a ε_{16}-phase. However the actual structure of the E-phase is far from an ideal ε_{16}-structure, because of the extensive existence of wrong arrangement and series absence of atom clusters. The significant deterioration of long-range crystallinity for the as-cast E-phase can be attributed to the coexistence of microtwins and underdeveloped H-defects without regular shape. Strap-shaped H-defects have been observed in the $Al_{75}Pd_{15}Fe_{10}$ alloys subjected to high-temperature heat treatments (>900°C). HREM observations and imaging simulations reveal that those atom clusters observed in the H-defect area are of the same type as the atom clusters in the E-phase structure. The arrangement of atom clusters in the strap of H-defect is characterized by a ξ-phase-like hexagonal tiling whose edge length is τ time larger than that of the hexagonal tiling of an Al-Pd-Fe ξ-phase. The formation of strap-shaped H-defects in the highly defective E-phase is associated with the rearrangement of atom clusters during high-temperature heat treatment. For the ill-formed atom clusters identified to exist in the E-phase, the possible atomic structural model has been proposed and discussed.

[1] H. Klein, M. Feuerbacher, P.. Schall, K. Urban, *Phys.Rev.Lett,* **1999**, *82*,3468-3471. [2] H. Klein, M. Audier, M. Boudard, M. De.Boissieu, *Phil. Mag. A,* **1996**, *73*, 309-331. [3] Y.H. Chen, W. Sun, Z. Zhang, *Phil. Mag. Lett.,* **2006**, *86*, 817-827.

Keywords: complex_ structure, defect, electron_microscopy