P23.03.02

Acta Cryst. (2008). A**64**, C624

Quasicrystals and approximants in the Ag-In-*M* and Au-Sn-*M*(*M*:Ca or rare earth metals) systems

Kengo Yamaguchi[1], Yoshiki Morita[1], An-Pang Tsai[2]
[1]Tohoku University, Engineering, Aoba-ku, Katahira2-1-1, Sendai, Miyagi, 980-8577, Japan, [2]Department of Materials Processing, Graduate school of Engineering, Tohoku University, Sendai 980-8579, Japan, E-mail：a7tm5629@mail.tagen.tohoku.ac.jp

Formation of 1/1 Yb-Cd type approximants has been verified in the Ag-In-RE system for RE=Tm, Tb, Er, Dy, Gd, Pr, Ce, Eu. The compositons of the 1/1 approximants determined by wavelength dispersive X-ray analysis (WDX). By employing the empirical rule of $e/a \approx 2.0$, where e/a is valence electron concentration, a number of approximants are newly found in the Au-Sn-RE systems for RE=Sm, Pr, Ce, Dy, Tb, Gd, Eu where the 1/1 approximants are formed in the range of 61≈64 at.% Au, 20≈23 at.% Sn and 14≈15 at.% REs. While the 2/1 approximants only form in $Ag_{43}In_{43}Eu_{14}$ and $Au_{60}Sn_{25}Ca_{15}$ for M=Eu, Yb, Ca, where atomic size for Eu, Yb and Ca is larger than that for other REs and they are all divalent. Quasicrystals are also oberved at $Au_{60}Sn_{25}Ca_{15}$ as a stable phase. Basically, the 2/1 and 1/1 approximants share the same e/a with the quasicrystals found in the In-Ag-*M* and the Cd-*M* groups. It is likely that the phase selection among the quasicrystalline, the 1/1 and the 2/1 approximants phases are dominated by a parameter, $R_{r.e}$, namely *effective atomic size factor*.

Keywords: quasicrystals, rare-earth compounds, valence charge density

P23.03.03

Acta Cryst. (2008). A**64**, C624

Formation of quasicrystal and approximant phases and their structures in Zn-Mg-(Ti, Zr, Hf) alloys

Satoshi Ohhashi[1], Cesar Pay Gomez[2], An-Pang Tsai[1,2]
[1]Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai, Miyagi, 980-8577, Japan, [2]National Institute for Materials Science (NIMS), Tsukuba 305-0047, Japan, E-mail：sohhashi@tagen.tohoku.ac.jp

Following the study of $Zn_{84}Mg_7Ti_6$ by Ishimasa et al [1], stable quasicrystals (Qc) and an 1/1 approximant in the Zn-Mg-Zr (Hf) system have been identified [2]. The Qcs reveal primitive (P) and face-centered (F) lattices which formed at different compositional regions. In this study, we investigate compositional regions for these two types of Qcs and 1/1 approximants (AP) for Zn-Mg-(Ti, Zr, Hf) systems and perform single-grained X-ray study for the 1/1 approxiamnts in order to get insights into the structure of icosahedral cluster. The compositional region of Qc was around $Zn_{83.5}Mg_{9.5}Zr_7$ for the P-ype Qc and around $Zn_{75}Mg_{18}Zr_6$ for the F type Qc. The 1/1 approximant is around $Zn_{77}Mg_{18}Zr_5$. The formation tendency is similar for the Zn-Mg-Hf system. It is noted that the concentration of Zr is almost the same for the two Qc phases but that of Mg is much higher for the F-type. This is an indication that the chemical order between Zn and Mg generates superlattice reflections which characterize the F-type structure. On the other hand, no Qc but only the 1/1 approximant was observed for the Zn-Mg-Ti system. The structures of the three 1/1 approximants have been analyzed by single crystal X-ray diffraction [3]. It is clear that these approximants contain two different types of clusters, which is different from that of Zn-Mg-Sc system.

[1] T. Ishimasa, Y. Kaneko and H. Kaneko, *J. Alloys Comp.* **342** (2002) 13.
[2] J. Hasegawa, S. Takeuchi, A.P. Tsai, *Phil. Mag. Lett.* **85** (2005) 289.
[3] C.P. Gomez et al., to be published.

Keywords: quasicrystals, superlattices, clusters

P23.03.04

Acta Cryst. (2008). A**64**, C624

The role of Mg in the stable Cd-Mg-RE (RE: rare earth metals) quasicrystals

Nozomu Kamiyama[1,2], Cesar Pay Gomez[3], An-Pang Tsai[2,3]
[1]Tohoku University, Engineering, Aoba-ku katahira 2-1-1, Sendai, Miyagi, 980-8577, Japan, [2]Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, [3]National Institute for Materials Science, Tsukuba 305-0047 Japan, E-mail：nozomu_k@mail.tagen.tohoku.ac.jp

Since discovery of a stable binary Cd-Yb quasicrystal [1)](Qc), the Qc with the same type of structure has been found in a large number of related alloys. Meanwhile, attention has also been drawn to Cd_6RE approximants since phase transitions at low temperatures[2)] have been observed for these approximants. Except the Cd-Yb system, no Qc was observed for other Cd-RE systems. However, it was found that replacement of a certain amount of Cd with Mg promotes formation of the Qc[3)]. In this study, we investigate formation of the Qc and approximants in relation to the content of Mg for the Cd-Mg-RE systems. Formation of the Qc was confirmed in the Cd-Mg-RE system with RE of Y, Dy, Gd and Tm. Phase transitions from approximants to Qcs facilitated by replacement of Cd with Mg were observed around 20 ~30 at.%. Mg. Further replacement, in contrast, stabilized crystalline phases. The role of Mg will be discussed on the basis of structures analyzed by single crystal X-ray diffraction.

1) A.P. Tsai, et al., Nature 408(2000)537.
2) R. Tamura et al., Jpn, J. Appl. Phys. 41(2002)L524.
3) J.Q. Guo, E. Abe and A.P. Tsai, Philo. Mag. Lett., 82(2002)27.

Keywords: quasicrystals, rare-earth compounds, transformation

P23.03.05

Acta Cryst. (2008). A**64**, C624−625

Surface studies on quasicrystals

Masahiko Shimoda[1], Hem Raji Sharma[2], An Pang Tsai[1,3]
[1]National Institute for Materials Science, Photocatalytic Materials Center, 1-2-1 Sengen, Tsukuba, Ibaraki, 305-0047, Japan, [2]Department of Physics, the University of Liverpool, England, [3]Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Japa, E-mail：SHIMODA.Masahiko@nims.go.jp

We have studied structure of quasiperiodic surfaces of various quasicrystals and epitaxial growth on quasicrystal surfaces. STM study on the clean fivefold surface of icosahedral Al-Cu-Fe reveals that the stable surface shows bulk termination at Al-rich planes without detectable reconstruction. A rule for the formation of stable surface is deduced from detailed analyses of the step-terrace morphology. By applying this rule to the refined structure model, the atomic arrangement observed in STM images is successfully explained (Figure 1). The motivation of the epitaxy study on quasicrystals is to evoke unknown phenomena by inducing quasiperiodic structure into various materials. In the case of Bi deposition on the fivefold surface of icosahedral Al-Cu-Fe, a wetting