Program of Poster Presentations

Program of Poster Presentations

Monday, June 14, 2010

Poster Session 1: Formation (chair: K. Saitoh)

P01-01	M. Surowiec, W. Bogdanowicz, J. Krawczyk, B. Formanek and M. Sozańska Growth morphology of single grains obtained by directional crystallization of Al-Cu-Fe alloy
P01-02	T.A. Sviridova, A.P. Shevchukov, F.I. Falkovsky, V.V. Tcherdyntsev, S.D. Kaloshkin and D.L. Diakonov Formation of decagonal quasicrystalline phase in mechanically alloyed Al-Cu-Cr alloys
P01-03	N.K. Mukhopadhyay, F. Ali. V.C. Srivastava, M. Sakaliyska, K.B. Surreddi, S. Scudino, V. Uhlenwinkel and J. Eckert The effect of milling intensity on mechanical milling of spray-formed single-phase Al-Cu-Fe quasicrystals
P01-04	D.A. Shulyatev, M.A. Chernikov and A.S. Nigmatulin Solid-state synthesis of icosahedral Al-Cu-Fe
P01-05	R. Nicula, K. Ishizaki, M. Stir, Z.Shen and S. Vaucher Rapid synthesis of single-phase Al-Cu-Fe quasicrystals by spark plasma sintering and microwave heating
P01-06	S. Dasai and H. Takakura Solution growth of a decagonal quasicrystal and its related periodic crystals in the Al-Ni-Ru system
P01-07	T.P. Yadav, D. Singh, R.R. Shahi, M.A.Shaz, R.S. Tiwari and O.N. Srivastava Effect of Ga substitution on the stabilization of the quasicrystalline phase in Al-Pd-Mn system
P01-08	C. Cui and A.P. Tsai Sysnthesis of large single-grain 1/1 approximant crystal in the Ag-In-Eu system by self-flux method
P01-09	L. Lu, J.B. Wang and D.S. Zhao Spontaneous formation of filamentary Cd whiskers and degradation of CdMgYb icosahedral quasicrystal under ambient conditions
P01-10	Canceled
P01-11	T. Örs and W. Steurer Synthesis of decagonal Zn-Mg-RE compounds
P01-12	H. Iga, M. Mihalkovič and T. Ishimasa Approximant of the dodecagonal quasicrystal in Mn-Si-(Cr, V) alloys
P01-13	J.B. Qiang, Y.M. Wang, Q. Wang, C. Dong, W. Zhang and A. Inoue Formation of icosahedral phase in Zr-Ni-Sn glassy alloys
P01-14	H. Chen, Q. Wang, Y.M. Wang, J.B. Qiang and C. Dong Composition rule of binary quasicrystals

Monday, June 14, 2010

Poster Session 2: Structure and modeling (chair: K. Saitoh)

P02-01	C. Dong, J.X. Chen, Q. Wang, Y.M. Wang and J.B. Qiang Cluster formulas of alloy phases
P02-02	M. Mihalkovič, M. Widom and C.L. Henley Ni-rich versus Co-rich structures for d-AlCoNi via melt-quanch simulation
P02-03	C.L. Henley and M. Mihalkovič Energetic and dynamics of caged Zn$_4$ in i-ScZn
P02-04	M. Mihalkovič and C.L. Henley Atomic structure of decagonal Frank-Kasper Mg-Zn-RE quasicrystal

P02-05	Canceled
P02-06	K. Kato and A. Yamamoto A superstructural fluctuation of the rhombic Penrose tiling type decagonal quasicrystal
P02-07	A. Yamamoto and C.P. Gómez A Bergman-cluster-based model of face-centered icosahedral Zn-Mg-Ho quasicrystals
P02-08	H. Abe Anisotropic local structure of decagonal quasicrystals by DAFS
P02-09	H. Abe Medium-range order of decagonal quasicrystals
P02-10	H. Nakahara, K. Saitoh and N. Tanaka Determination of the electoron densiy distribution of the decagonal quasicrystal of $Al_{72}Ni_{20}Co_8$ by convergent-beam electron diffraction.
P02-11	K. Soda, M. Inukai, M. Kato, S. Yagi, Y. G. So and K. Edagawa Spectroscopic study of Ni-rich Al-Co-Ni quasicrystal
P02-12	T. Seki, E. Abe, H. Sawada, Y. Kondo and K. Takayanagi Modification of $Al_{70}Mn_{17}Pd_{13}$ decagonal structure by ultrahigh-resolution STEM
P02-13	Y. Miyazaki, T. Yoshida, J.T. Okada, E. Abe, Y. Yokoyama and K. Kimura Structure and stability of BTiRu approximant crystals to decagonal quasicrystal
P02-14	W. Sun, J.P. Wang and Z.Y. Liu Structural study of highly defective Al-Pd-Fe crystalline approximant
P02-15	S. Suzuki, R.Simura and K. Sugiyama Crystal structure of χ-AlPdRe.
P02-16	R. Simura, N. Kaji, K. Sugiyama and K. Hiraga Crystal structure of new orthorhombic approximant phase $Al_{72}Pd_{18}Mn_5Si_5$
P02-17	C. Fan, Th. Weber, S. Deloudi and W. Steurer Multiple diffraction in an icosahedral Al-Cu-Fe quasicrystal
P02-18	C.P. Gómez, H. Takakura, A. Yamamoto and A.P. Tsai Analysis of structure and chemical order in a ternary $Yb_{12}Mg_{52}Cd_{36}$ quasicrysta1
P02-19	T. Yamada, C.P. Gómez, R. Tamura, H. Euchner, A. Yamamoto and M. de Boissie Diffuse scattering in the Zn6Sc 1/1 cubic approximant
P02-20	K. Nishimoto, M. Muraki, T. Sato and R. Tamura Classification of low-temperature superstructures of Cd_6M 1/1 approximants
P02-21	T. Sato, M. Muraki, K. Nishimoto and R. Tamura Structural properties of $Cd_6M(M=Er,Ho,Lu)$ approximants
P02-22	T. Ishimasa, A. Hirao, T. Honma and M. Mihalkovič Crystal structure of 2/1 1/0 1/0 Cu-Al-Sc approximant
P02-23	Y. Ishibashi, H. Sugiura, K. Saitoh and N. Tanaka Three dimensional reconstruction method of icosahedral quasicrystals by binary discrete tomography

Monday, June 14, 2010

Poster Session 3: Mathematical aspects (chair: K. Saitoh)

P03-01	R. Lück Chiral pinwheel type tilings with singular centre
P03-02	R. Lück Tiling with global rotational symmetry based on Penrose rhombi
P03-03	G.R. Laigo, B.R. Gozo, Jr. and M.L.A.N. De Las Peñas Semi-perfect colorings of hyperbolic tilings
P03-04	Presented as S09-01
P03-05	Canceled
P03-06	M. Baake and U. Grimm Diffraction of limit periodic point sets
P03-07	S.I. Ben-Abraham and A. Quandt Aperiodic structures, order and disorder
P03-08	P. Kuczera, R. Strzałka and J. Wolny Application of the average unit cell concept to the 3D aperiodic Amman tiling
P03-09	R. Al Ajlouni A long-range order for growing perfect quasi-crystalline formations

Tuesday, June 15, 2010 (17:00-18:30)

Poster Session 4: Physical properties (chair: K. Edagawa)

P04-01	H. Suzuki, M. Saito, H. Kitahata, Y. Matsushita, I. Kanazawa T. Ohdaira, N. Oshima, R. Suzuki, Y. Takagiwa and K. Kimura Structural vacancies in 1/1-AlReSi approximant crystals probed by positron annihilation methods
P04-02	Y. Takagiwa, K. Kimura and I. Kanazawa Possibility of evaluation of bonding nature of Al-based icosahedral quasicrystals using positron annihilation rate
P04-03	D. Kawana, T. Watanuki, A. Machida, and A.P. Tsai Intermediate valence state in Cd-Mg-Yb quasicrystal
P04-04	Y.G. So, S. Sato, K. Edagawa and R. Tamura Internal friction study of icosahedral quasicrystals and their crystal approximants
P04-05	A.F. Prekul, N.I. Shchegolikhina and K. Edagawa On nature of the excess heat capacity in the icosahedral quasicrystals
P04-06	D. Singh, T.P. Yadav, R.K. Mandal, R.S. Tiwari and O.N. Srivastava Effect of Ti addition on the quasicrystalline phase formation and indentation characteristics of $Zr_{69.5}Al_{7.5}Cu_{12}Ni_{11}$ alloy
P04-07	S. Kashimoto Slow dynamics of spin glass phases in Tsai-type Zn-Fe-Sc and Zn-Mn-Sc quasicrystals
P04-08	S. Ibuka, K. Iida and T.J. Sato Magnetic properties of the Ag-In-rare-earth 1/1 approximants
P04-09	S. Koshiya, M. Terauchi, S. Ohhashi and A.P. Tsai EELS and SXES studies of electronic structures of Zn-Mg-Zr alloys
P04-10	Canceled
P04-11	I. Kanazawa, H. Suzuki and K. Yamada Anomalous conduction mechanisms of insulating Al-Pd-Re quasicrystals
P04-12	J. Ivkov, A. Smontara, P. Popčević, J. Dolinšek and P. Gille Anisotropic Hall effect in single crystals of $Al_{13}TM_4$ and $Al_{13}(Fe,Ni)_4$ decagonal approximants
P04-13	T. Mori, Y. Wakuda, R. Tamura, K. Nishio and K. Tokiwa Electrical properties of Al-Pd-Re quasicrystals prepared by spark plasma sintering method
P04-14	Y. Wakuda, T. Mori, K. Nishio and R. Tamura Influence of heat treatment on the electrical resistivity of Al-Pd-Re quasicrystal
P04-15	T. Hiroto and R. Tamura Structural and physical properties of single-grained Cd_6M 1/1 approximants
P04-16	Yu.Kh. Vekilov and M.A. Chernikov Variable-range hopping conductivity in icosahedral quasicrystals
P04-17	M.P. Belov, E.I. Isaev and Yu.Kh. Vekilov Hydrogen in the 1/1 approximant of the i-TiZrHf quasicrystal: energy, bond order and diffusion
P04-18	V. Sanchez and C. Wang Renormalization plus convolution approach to the quasiperiodic systems with defects
P04-19	C. Wang and J.C. Hernandez Small polaron approach to the electron-phonon interaction in quasiperiodic lattices
P04-20	N.E. Kaputkina, P.Yu. Korotaev, Yu.E. Lozovik and Yu.Kh. Vekilov The energy spectra and transport in aperiodic sequences of quantum dots in external electric and magnetic fields

P04-21	Canceled
P04-22	D.Y. Jung and W. Steurer First principles investigation of icosahedral quasicrystal approximants

Tuesday, June 15, 2010 (17:00-18:30)

Poster Session 5: Surfaces (chair: K. Edagawa)

P05-01	J. Yuhara, M. Sato, T. Matsui, and A.P. Tsai Multiple cluster model of Al-Co-Ni Co-rich quasicrystal
P05-02	R. Zenkyu, J. Yuhara, T. Matsui and A.P. Tsai The two nanometer cluster of the Al-Cu-Co quasicrystal surface observed by STM
P05-03	T. Duguet, B. Ünal, Y. Han, J.W. Evans, J. Ledieu, C.J. Jenks, J.M. Dubois, V. Fournée and P.A. Thiel The twofold surface of decagonal Al-Co-Cu: effect of nanodomains on adhesion and growth of Ag
P05-04	M. Shimoda, C. Cui, H.R. Sharma, P.J. Nugent, J.A. Smerdon, R. McGrath, K. Sagisaka, H. Takakura, S. Ohhashi, C.P. Gómez, Y. Ishii and A. P. Tsai Surfaces of In-Ag-Yb quasicrystal and 1/1 approximant
P05-05	I.M. McLeod, P. Nugent, J. Smerdon, V.R. Dhanak, C. Cui, A.P. Tsai and H.R. Sharma Characterisation of the growth of Pb and Bi thin films on Ag-In-Yb quasicrystal using XPS, UPS, STM and LEED
P05-06	P.J. Nugent, J.A. Smerdon, R. McGrath, M .Shimoda, C. Cui, A.P. Tsai and H.R. Sharma Growth of Sb on high symmetry surfaces of the icosahedral Ag-In-Yb quasicrystal
P05-07	K.M. Young, J.A. Smerdon, N. Cross, V. Dhanak, H.R. Sharma, T.A. Lograsso, A.R. Ross and R. McGrath Structure and stability of Bi thin film on the five-fold surface of the icohsahedral Al-Pd-Mn quasicrystal
P05-08	A.K. Shukla, J. Ledieu, B. Ünal, H.R. Sharma, E. Gaudry, M.-C. de Weerd, T. Duguet, J.-M Dubois, P. A. Thiel and V. Fournée Electron confinement in metal thin films on quasicrystalline substrates
P05-09	É. Gaudry, S. Alarcon, J. Ledieu, M.-C. de Weerd, Y. Grin, R. Diehl, H. Shin, K. Pussi, V. Fournée and J.-M. Dubois Surface termination of periodic complex metallic alloys: relative surface energy calculations
P05-10	S. Alarcón Villaseca, É. Gaudry, J. Ledieu, V. Fournée, P. Gille, M.-C. de Weerd and J.-M. Dubois Structure of the (001) surface of the Al_9Co_2 alloy
P05-11	K. Nozawa and Y. Ishii Theoretical studies on clean and adsorbed surfaces of Ag-In-Yb

Tuesday, June 15, 2010 (17:00-18:30)

Poster Session 6: Apllications (chair: K. Edagawa)

P06-01	A. Kocjan, S. Kovačič, J. Kovač, P.J. McGuiness and S. Kobe Selective hydrogenation of Ti-Zr-Ni alloys
P06-02	Canceled
P06-03	S.-B. Choi, S.-H. Lee and J.Y. Kim Pressure-composition-temperature curves and structure stability induced by hydrogen in TiZrNi quasicrystals

P06-04	W. Liu, X. Wang, Y. Kawabe and L. Wang Hydrogen storage characteristics of TiVNi-quasicrystal composite materials
P06-05	T. Tanabe, S. Kameoka and A.P. Tsai Al-Cu-Fe Quasicrystal as a catalyst precursor for hydrogen production reaction
P06-06	K. Kajiwara, Y. Matsui, T.P. Yadav, N.K. Mukhopadhyay and O.N. Srivastava Synthesis of carbon nanotubes by using mechanical-milled Al-Cu-Fe powders as catalysts
P06-07	S. Ohhashi, A. Kato and A.P. Tsai Annealing effects on quasicrystal reinforced Mg-Zn-Zr extrusions
P06-08	A.D. Kothalkar, G. Tripathy, K. Biswas and B. Basu A novel QC (Al-Co-Ni)-polymer composite for wear application

Tuesday, June 15, 2010 (17:00-18:30)

Poster Session 7: New systems (chair: K. Edagawa)

P07-01	J. Mikhael, G. Gera and C. Bechinger Structural phase transition of dense monolayers on quasiperiodic light potentials
P07-02	Canceled
P07-03	S. Thiem, M. Schreiber and U. Grimm Light transmission through metallic-mean quasiperiodic stacks with oblique incidence

Tuesday, June 15, 2010 (17:00-18:30)

Poster Session 8: Related topics (chair: K. Edagawa)

P08-01	Canceled
P08-02	A. Singh, J.M. Rosalie, H. Somekawa and T. Mukai Coexistence of Mg_4Zn_7 and $MgZn_2$ phases in Mg-Zn-Y alloys and their relationship to quasicrystals
P08-03	M. Duda and J. Wolny Stable configurations of atoms in Mg_2Al_3 phases
P08-04	D.S. Zhao, Y. Liu, J.P. Zhou, X. Nie, J.B. Wang, S.J. Zhu and Y. Shen In situ observation of ageing process and new orientation relationship of continuous precipitates in magnesium-aluminum based alloys
P08-05	J.M. Rosalie, H. Somekawa, A. Singh and T. Mukai Structural relationships between hexagonal $MgZn_2$, monoclinic Mg_4Zn_7 and related transition structures in Mg-Zn-Y alloys
P08-06	D.S. Zhao, Y. Liu, X. Nie, J.P. Zhou, J.B. Wang, S.J. Zhu and Y. Shen Microstructure and mechanical properties of a rapidly solidified Mg-9.0wt% Al-1.0wt%Zn-4.0wt%Sn alloy
P08-07	M. Inukai, K. Soda, H. Sato and U. Mizutani Electronic structure of Ag_9In_4, Ag_5Zn_8 and Mn_3In gamma-brasses studied by FLAPW band calculations
P08-08	J. Dshemuchadse, D.Y. Jung and W. Steurer Structural building principles of complex intermetallics
P08-09	K. Sugiyama, T. Muto and Y. Yokoyama Structural analysis of amorphous $Zr_{70}Pd_{30}$ alloy by anomalous X-ray scattering coupled with reverse Monte Carlo simulation
P08-10	D.G. Xiong, L. Lu, J.B. Wang, D.G. Zhao and Y.F. Sun Study of precipitations in Zr-Cu-Ni-Al-Nb bulk metallic glass matrix composites containg quasicrystals and crystals
P08-11	R. Murao, K. Sugiyama, Y. Kashiwagi, S. Kameoka, and A.P. Tsai Radial distribution function analysis of Raney Pd and Rh fine particles

P08-12	R. Berthold, E Dashjav, H. Borrmann, S. Hoffmann, U. Burkhardt and G. Kreiner Heterogenous equilibria and crystal structure of the Φ phase in the Al-Mg-Zn system

Poster Session 1

Formation

Monday, June 14, 2010

GROWTH MORPHOLOGY OF SINGLE GRAINS OBTAINED BY DIRECTIONAL CRYSTALLIZATION OF Al-Cu-Fe ALLOY

M. Surowiec[1], W. Bogdanowicz[1], J. Krawczyk[1], B. Formanek[2], M. Sozańska[2]

[1]*Institute of Material Science, Univ. of Silesia, 40 007 Katowice, Poland*
[2]*Faculty of Materials Engineering and Metallurgy, Silesian Univ. of Technology, 40-019 Katowice, Poland*

Quasicrystalline as well as crystalline faceted single grains have been obtained during directional crystallization of Al-Cu-Fe alloy by vertical Bridgman technique. Several phases can coexist in Al-Cu-Fe alloy. Among them four types of thermodynamically stable single crystal grains have apparently crystallized on the principle of the flux-growth mechanism and the grains were successfully observed inside cavities of the porous upper part of the ingot. Growth morphology of the stable phases have been investigated by scanning electron microscopy (SEM). Single quasicrystalline ψ phase Al_6Cu_2Fe exhibited icosahedral symmetry with pentagonal dodecahedral growth forms (fig. 1 left). Characteristic decorations appeared on facets, which has been already observed on Al-Pd-Mn single quasicrystal surfaces by C. Beeli and H.-U. Nissen (1993), *Phil. Mag*. B, **68**, 487. Polygonal single grains of ω phase Al_7Cu_2Fe (*P4/mnc* space group) exhibiting tetragonal symmetry formed the second type of thermodynamically stable growth forms. Single grains of the ω phase crystallized in a form of pellets with octagonal cross-section and lateral facets {100} and {110} type. The third attractive type of morphological forms exhibiting growth steps revealing two-fold, three-fold and four-fold symmetry axis have been observed on spherical single crystals of β phase Al(Fe,Cu) (*Pm3m* space group). Rectangular, hexagonal and octagonal shape of growth steps forms can be seen in the positions of two-fold, three-fold and four-fold symmetry axis respectively (fig. 1 right). Finally, the fourth type of faceted single crystals was formed inside of the ingot by dominant λ phase $Al_{13}Fe_4$ (*C2/m* space group). The {100} faceted monoclinic single crystals with characteristic angle $\beta = 108^o$ formed lamellas of 0.5mm to 1mm thickness. The lamellas were parallel to the direction of crystallization. The chemical composition of the described growth forms have been confirmed by X-ray microanalysis on scanning electron microscope whereas determination of the phase composition have been performed by X-ray powder diffraction.

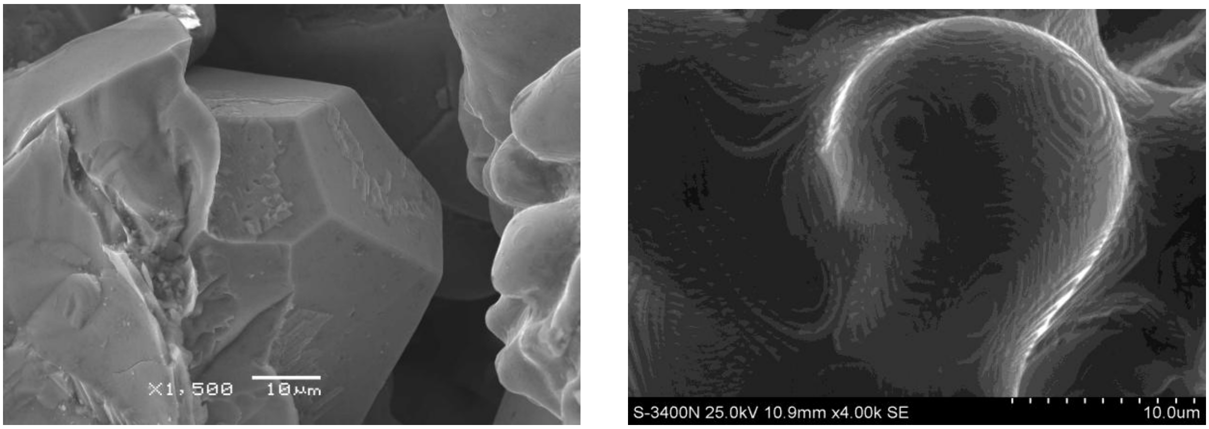

Fig. 1. Pentagonal dodecahedron of quasicrystalline ψ phase Al_6Cu_2Fe (left) and growth steps exhibiting 2-fold, 3-fold and 4-fold symmetry axis on the spherical like growth form of the cubic single crystal of β phase Al(Fe,Cu) (right).

P01-02

FORMATION OF DECAGONAL QUASICRYSTALLINE PHASE IN MECHANICALLY ALLOYED AL-CU-CR ALLOYS

T. A. Sviridova[1], A. P. Shevchukov[1], F. I. Falkovskiy[1], V. V. Tcherdyntsev[1],
S. D. Kaloshkin[1], D. L. Diakonov[2]

[1] *National University of Science and Technology "MISIS", Moscow, 119049, Russia*
[2] *Bardin Central Research Institute for the Iron and Steel Industry, Moscow, 105005, Russia*

The formation of decagonal quasicrystal was revealed after annealing of mechanically alloyed elemental Al-Cu-Cr mixtures. The high-energy planetary ball mill AGO-2M was employed for mechanical alloying. The intermixed powders were annealed under Ar atmosphere at different temperatures between 200 and 800 ° C for 1 h and then air cooled. Various phase transformations were monitored by X-ray diffraction and differential scanning calorimetry. The symmetry of quasicrystalline phase was characterized by TEM.

The mixtures $Al_{65}Cu_{24}Cr_{11}$, $Al_{69}Cu_{21}Cr_{10}$, $Al_{78}Cu_{10}Cr_{12}$, $Al_{65}Cu_{20}Cr_{15}$, $Al_{67}Cu_{23.5}Cr_{9.5}$, and $Al_{72.5}Cu_{16.5}Cr_{11}$ were mechanically alloyed and being annealed contain different amount of decagonal quasicrystal. The maximum content of quasicrystalline phase (~90-95 vol.%) was achieved in $Al_{69}Cu_{21}Cr_{10}$ and $Al_{72.5}Cu_{16.5}Cr_{11}$ alloys after annealing at 635 °C, that is the elevated and lowered temperatures of heat treatment reduce the quantity of quasicrystalline phase.

Transmission electron microscopy (JEM-200CX) study of almost single-phase $Al_{69}Cu_{21}Cr_{10}$ alloy confirms that the main phase is decagonal quasicrystal. Its electron diffraction pattern has tenfold axis with translation symmetry along it what is typical for decagonal symmetry.

THE EFFECT OF MILLING INTENSITY ON MECHANICAL MILLING OF SPRAY-FORMED SINGLE-PHASE AL-CU-FE QUASICRYSTALS

N.K. Mukhopadhyay[1], F. Ali[2], V.C. Srivastava[3,4], M. Sakaliyska[2], K.B. Surreddi[2], S. Scudino[2], V. Uhlenwinkel[4], J. Eckert[2,5]
[1] Centre of Advanced Study, Department of Metallurgical Engineering, Banaras Hindu University, Varanasi 221 005, India
[2] IFW Dresden, Institut für Komplexe Materialien, Postfach 27 01 16, D-01171 Dresden, Germany
[3] National Metallurgical Laboratory, Jamshedpur- 831 007, India
[4] Institut für Werkstofftechnik, Universität Bremen, D-28359 Bremen, Germany
[5] TU Dresden, Institut für Werkstoffwissenschaft, D-01062 Dresden, Germany

Earlier it was reported that decagonal and icosahedral quasicrystalline phases in Al-base alloys undergoes structural transformation to crystalline B2 phases. It should be pointed out that this type of structural transformation has also been observed in electron and ion beam irradiated, compression tested, scratched and fractured samples. However, the mechanisms and the origin of the structural transformation have yet been clearly not understood, though the geometrical transformation from quasilattice to cubic lattices has been understood. It is often argued that transformation is due to compositional changes or due to instability of the quasicrystalline phase under these driven conditions. The aim of the present investigation is to conduct careful and controlled experiments so that the compositional changes can be avoided. In the present experiment, a single-phase icosahedral quasicrystalline sample with composition $Al_{62.5}Cu_{25}Fe_{12.5}$ was produced by spray forming. These materials were employed for mechanical milling in Planetary ball mill under argon atmosphere so that the oxidation can be avoided. The effect of milling intensity on microstructure has been investigated by using different milling speeds (e.g. 150, 250 and 350 rpm) and with same ball to powder ratio. At the first stages of milling (within 5 h) a significant broadening of the diffraction peaks was observed indicating a decrease of the grain size and the introduction of lattice strain which is related to phason strain of the quasilattice. Line broadening was noticed to increase with increasing the milling time and in the material milled for longer time only few broad diffraction peaks, which can be identified as a nanoscale bcc phase (~a=2.9Å) are visible. The diffraction signals belonging to the quasicrystals were no longer observable, indicating a complete transformation of the quasicrystals into the bcc phase. It was found the time needed for such a phase transformation depends on the milling speed: for example, it required an extremely long milling period (> 200 h) for the sample milled at 150 rpm, whereas the transformation was completed within 100 h for the material milled at 250 and 350 rpm. The hardness measured on the milled powders decreased with increasing the milling time, most likely as a consequence of the increased volume fraction of the bcc phase. Finally, the bcc phase formed during milling transformed back to the quasicrystalline phase during the heat treatment. Attempts will be made to rationalize the structural transformation and the implications of these effects on possible applications as designing a composite materials.

P01-04

SOLID-STATE SYNTHESIS OF ICOSAHEDRAL Al-Cu-Fe

D. A. Shulyatev, M. A. Chernikov, A. S. Nigmatulin

Department of Theoretical Physics, Moscow State Institute of Steel and Alloys,
Moscow, 119049, Russia

Although the preparation of the icosahedral Al–Cu–Fe quasicrystals has been intensively studied for many years using techniques such as melt spinning, solidification from the melt, gas atomization and mechanical alloying, less attention has been given to solid-state synthesis, a simple method of preparing intermetallic materials in large quantities. The purpose of this study was to optimize the solid-state synthesis parameters including the initial composition and annealing regimes. Powders with nominal compositions $Al_{62}Cu_{25.5}Fe_{12.5}$, $Al_{63}Cu_{24}Fe_{13}$ and $Al_{65}Cu_{20}Fe_{15}$ were compacted and annealed at varying temperatures from 550 to 750 °C in a helium atmosphere between 2 and 20 hours. The annealed samples were characterized by X-ray diffraction and scanning electron microscopy. Some of the samples in addition to the icosahedral phase contained the cubic β-AlFe(Cu) phase and the monoclinic λ-$Al_{13}Fe_4$ phase. The X-ray diffraction study has revealed the absence the β and λ phases in the $Al_{63}Cu_{24}Fe_{13}$ sample annealed at 650 °C for 20 hours.

RAPID SYNTHESIS OF SINGLE-PHASE Al-Cu-Fe QUASICRYSTALS BY SPARK PLASMA SINTERING AND MICROWAVE HEATING

R. Nicula[1], K. Ishizaki[1], M. Stir[1], Z. Shen[2] and S. Vaucher[1]

[1] *Swiss Federal Laboratories for Materials Testing and Research – EMPA,*
Feuerwerkerstrasse 39, CH-3602 Thun, Switzerland
[2] *Department of Materials and Environmental Chemistry, Arrhenius Laboratory,*
Stockholm University, SE-10691 Stockholm, Sweden

Quasicrystalline QC phases are often stable only within narrow composition domains. For this reason, the synthesis of larger amounts of single-phase quasicrystalline powders meets some difficulties. Powder metallurgical approaches based on mechanical milling followed by conventional heating were therefore explored during the recent past. The manufacturing process leading to single-phase QCs - either in form of powders or bulk parts - can be accelerated by orders of magnitude upon the use of rapid heating methods that involve pulsed electric currents and/or high-frequency electromagnetic fields. Prior knowledge of the phase transformation sequence and transformation kinetics as revealed by *in situ* time-resolved synchrotron radiation experiments is instrumental in obtaining single-phase quasicrystals. We report on the simultaneous synthesis and densification of bulk single-phase Al-Cu-Fe QCs by spark plasma sintering (SPS) within *minutes* and on the ultrafast synthesis of single-phase Al-Cu-Fe QC powders by microwave heating within *seconds*. The effect of electric current application in the rapid processing of pre-alloyed powders is discussed to explain the faster diffusion and the enhancement of phase transformation kinetics.

P01-06

SOLUTION GROWTH OF A DECAGONAL QUASICRYSTAL AND ITS RELATED PERIODIC CRYSTALS IN THE Al-Ni-Ru SYSTEM

Shogo Dasai and Hiroyuki Takakura

Division of Applied Physics, Graduate School of Engineering,
Hokkaido University, Sapporo 060-8628, Japan

A decagonal phase (D-phase) with 1.6 nm periodicity was discovered in the Al-Ni-Ru system in 2000 by Sun *et al* [1]. The diffraction pattern of the D-phase shows fewer amounts of diffuse scattering than other stable D-phases [2]. This implies that the structure of the Al-Ni-Ru D-phase is highly ordered. Therefore, the D-phase is a good candidate for investigating the role of chemical order in a ternary decagonal quasicrytal. Structural investigations of the Al-Ni-Ru D-phase so far were done mainly by high-resolution electron microscopy, but not by X-ray diffraction. One of the reasons may be that there is a difficulty in growth of a crystal large enough for an X-ray diffraction, because of the high melting temperature of Ru. The aim of the present study is to grow single crystals of the Al-Ni-Ru D-phase and related crystalline phases with suitable sizes for X-ray diffraction by employing the solution-growth method. The chemical composition of the initial alloys was determined based on the reported isothermal sections of an Al-rich region of the Al-Ni-Ru system and the composition of the D-phase, $Al_{75}Ni_{15}Ru_{10}$ [3,4]. Alloy ingots with a weight of 5 g were prepared by melting high purity metals in an arc furnace under an argon atmosphere. These alloys were clashed and put in alumina crucibles, and sealed in evacuated quartz tubes, and then re-melted at 1100 ℃ in a muffle furnace. Subsequently, the melts were cooled down with 2 K/h. The grown crystals were separated from the remaining liquids at certain temperatures by centrifugation, and then the quartz tubes were quenched in water. We have succeeded to grow single crystals of the D-phase and its related crystalline phases with several millimeter sizes. The details of the growth conditions and the results of crystallographic characterizations are reported.

[1] W.Sun, K.Hiraga, Phil. Mag. Lett. **80,** 157 (2000).
[2] T.Scholpp, PhD thesis, ETH Zurich (2001).
[3] S.Mi, B.Grushko et al, Journal of Alloys and Compounds. **359,** 193-197 (2003).
[4] V.Raghavan, Journal of Phase Equilibria and Diffusion. **27**, 501-505 (2006).

EFFECT OF Ga SUBSTITUTION ON THE STABILIZATION OF THE QUASICRYSTALLINE PHASE IN Al-Pd-Mn SYSTEM

T.P. Yadav, Devinder Singh, Rohit R Shahi, M.A.Shaz, R.S.Tiwari and O.N.Srivastava

Department of Physics, Banaras Hindu University, Varanasi-221005, India

Abstract

Quasicrystalline $Al_{65}Ga_5Pd_{17}Mn_{13}$ icosahedral phase have been synthesized as shown in the previous papers [1]. It was shown that the formation of pure icosahedral phase is possible up to 5 at % of Ga substitution in $Al_{70-x}Ga_xPd_{17}Mn_{13}$ alloy composition. In the present investigation, the effect of Ga substitution on the formation and stabilization of icosahedral phase in $Al_{70-x}Ga_xPd_{17}Mn_{13}$ and $Al_{70-x}Ga_xPd_{20}Mn_{10}$ alloys have been investigated by employing X-ray diffraction, transmission electron microscopy and differential thermal analysis. The as-cast and rapidly quenched alloys with x = 0, 2.5, 5, 7.5, 10, 15 and 20 has been investigated. In both the cases, the alloys up to 5 at % Ga exhibit the formation of icosahedral phases and with higher concentration of Ga i-phase along with B2 type and ξ' crystalline (orthorhombic structure with unit cell a = 23.5Å, b= 16.6Å and c = 12.4 Å) and Al_3Pd_2 type hexagonal phase. The Energy dispersive X-ray analysis investigations suggest the presence of Ga in the elemental form on the quasicrystalline surface in $Al_{55}Ga_{15}Pd_{17}Mn_{13}$ alloy. The quasicrystalline Al-Ga-Pd–Mn provides a new opportunity to investigate the various characteristics including surface characteristics. Attempts will be made to discuss the micromechanisms for the formation of quasicrystalline phase in Al-Ga-Pd-Mn alloys.

[1] T.P. Yadav, M.A. Shaz, R.S. Tiwari and O.N. Srivastava Phil. Mag. 88, (2008) 1995

P01-08

SYNTHESIS OF LARGE SINGLE-GRAIN 1/1 APPROXIMANT CRYSTAL IN THE Ag-In-Eu SYSTEM BY SELF-FLUX METHOD

Can Cui, and An Pang Tsai

Institute of Multidisciplinary Research for Advanced Materials, Tohoku University,
Sendai 980-8577, Japan

For an icosahedral quasicrystal, an identical icosahedral cluster exists in both the quasicrystal and its related approximants, but it arrays in a quasi-periodic configuration for the former and in a periodic way for the later. Due to the quasi-periodicity in 3-dimensional space, it is difficult to solve the structure directly on the quasicrystalline sample by conventional X-ray diffraction methods. Thus, the approximants play a crucial role in understanding the structures of quasicrystals since the structures of approximants can be determined by conventional X-ray diffraction techniques. Additionally, due to similarity in chemical composition and structural units between approximants and their parent quasicrystal, the approximants are complementary in understanding the contribution of quasi-periodic atomic arrangement on the intrinsic physical properties and the surface properties. For the studies of crystal structure, intrinsic physical properties and surface properties, large single-grain quasicrystal and approximants are highly desirable. Recently, we reported the growth of centimeter sized single grain quasicrystal in the Ag-In-Yb system by Bridgman method; however, it is impossible to grow large single grain approximants with this method due to the peritectic reaction. In this study, we report the synthesis of large single grain of Ag-In-Eu 1/1 approximant in In-rich melt solution. Based on the binary phase diagram of Cd-Eu and DTA experimental result of powder Ag-In-Eu 1/1 approximant sample, the growth condition, including the nominal composition, cooling rate and decanted temperatures were optimized. A centimeter sized single-grained 1/1 approximant was obtained and characterized with powder XRD, SEM, EDS and back-reflection Laue X-ray diffraction, as shown in Figure 1. The experiment indicates a strategy to synthesize single grain approximants in other Ag-In-RE (RE=rare earth) system. Consequently, we were success in the Ag-In-Yb but failed in the Ag-In-RE (RE = Y, Ce, Gd and Ho) system.

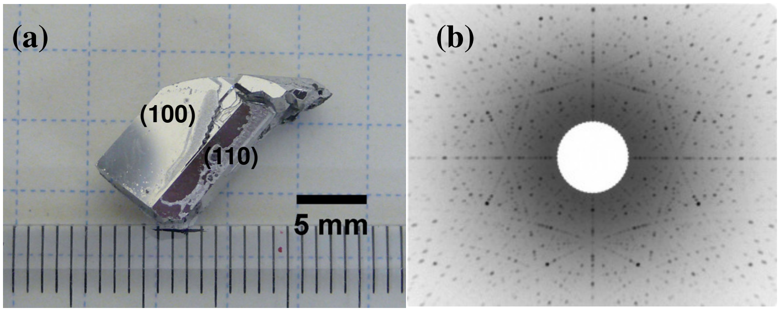

Figure1. Macrograph for the Ag-In-Eu 1/1 approximant sample (a) and back-reflection Laue X-ray diffraction pattern taken with incidence perpendicular to the (100) plane.

SPONTANEOUS FORMATION OF FILAMENTARY Cd WHISKERS AND DEGRADATION OF CdMgYb ICOSAHEDRAL QUASICRYSTAL UNDER AMBIENT CONDITIONS

Lu Lu, Jianbo Wang and Dongshan Zhao

School of Physics and Technology, Center for Electron Microscopy and MOE Key Laboratory of Artificial Micro- and Nano-structures, Wuhan University, Wuhan 430072, China

The spontaneously formed whiskers were systematically studied in the Cd-Mg-Yb icosahedral quasicrystal alloys with a primitive lattice by electron microscopy techniques. The whiskers were found to be Cd single crystals covered by CdO nano-crystallites by energy-dispersive X-ray spectroscopy and electron diffraction. The growth direction of Cd whiskers was determined to be along <11-20>. Four types of definite orientation relationship between Cd matrix and CdO were observed. The corresponding interfacial configurations were proposed using coincidence site lattice model, which was broadly used in studying of interface structure between metals and their oxides. The strain between Cd and CdO was analyzed based on double diffraction results. The mechanism of whisker formation and degradation of quasicrystal was discussed then. Selective oxidation of the sprouting metal Cd would lead to the volume expansion. The whiskers could nucleate and grow under the stress gradient induced by the resulting volume expansion. The gradual decreasing of Cd in quasicrystals resulted in the degradation and eventual collapse of the quasicrystal structure.

Acknowledgment: This research was supported by the National Natural Science Foundation of China (50571075) and the Program for New Century Excellent Talents in University (NCET-07-0640). The authors are grateful to Prof. Jianian Gui and late Prof. Renhui Wang for discussions and Dr. Junqing Guo for providing the samples.

P01-10

CANCELED

SYNTHESIS OF DECAGONAL Zn-Mg-*RE* COMPOUNDS

T. Örs and W. Steurer

Laboratory of Crystallography, Department of Materials, ETH Zurich,
CH-8093 Zurich, Switzerland

In this study, the formation of the decagonal (d-) quasicrystals in some Zn-Mg-*RE* systems (with *RE* = Dy, Er, Ho and Tm) was investigated. Samples having the reported composition of the decagonal phase ($Zn_{58}Mg_{40}RE_2$ [1]) were prepared by induction melting followed by annealing at different temperatures for various durations. The alloys were then quenched to room temperature. For the Zn-Mg-Dy system, it was found out by powder X-ray diffraction studies that annealing for 100 h at 350°C yields the d-phase as the single phase. Further annealing at this temperature causes the formation of a hexagonal phase.

Decagonal phase was also obtained in the systems with rare earth elements other than Dy (Er and Ho). The results further suggest that different elements require different annealing procedures for the formation of the d-phase.

For Dy and Er containing systems equilibrium cooling (instead of quenching) from higher temperatures also yields the d-phase. The d-phase occurs as the predominant phase in these samples. This could be a hint that the primary solidification range of the decagonal phase lies in the vicinity of its given composition.

[1] Sato, T. J., Abe, E., Tsai, A. P.: Phil. Mag. Letters, 77 (4) 213-219 (1998).

P01-12

APPROXIMANT OF THE DODECAGONAL QUASICRYSTAL IN Mn-Si-(Cr, V) ALLOYS

H.Iga[A], M. Mihalkovič[B], T.Ishimasa[A]

[A] *Graduate School of Engineering, Hokkaido University, Kita-ku, 060-8628 Sapporo, Japan*
[B] *Institute of Physics, Slovak Academy of Sciences, CS-842 28 Bratislava, Slovakia*

Ideal dodecagonal tiling in the 2-dimensional space has been proposed, which is a quasiperiodic triangle-square tiling [1]. Real dodecagonal phases in the 3-dimensional space have been reported, for example, in Ni-Cr and Ta-Te alloys in which triangular and tetragonal prisms are arranged. These 3-dimensional structures are classified into two groups according to the edge lengths of prisms which are 4.5Å in the former and 5.2Å in the latter. The difference is due to the inner structures of tiles (i.e. atomic arrangements in the triangular and tetragonal prisms). In order to search new dodecagonal quasicrystal of the Ni-Cr type, we focused on Mn-Si-(Cr,V) alloys because of the presence of the following three phases in these alloys; σ-, ν-, and A15 phases. Here we will present experimental results on an approximant of the dodecagonal quasicrystal formed in Mn-Si-(Cr,V).

Alloy ingots of $Mn_{60.0\text{-}81.5}Si_{16.0\text{-}30.0}Cr_{0.0\text{-}15.0}$ and $Mn_{70.0\text{-}81.5}Si_{14.5\text{-}22.0}V_{0.0\text{-}15.0}$ were made using an arc furnace. The pieces of ingots were further annealed at 923-1273K for 12-200 h, and then quenched in water. Powder X-ray diffraction and transmission electron microscopic studies indicated presence of a hexagonal crystal in both alloys, which can be interpreted as an approximant of the dodecagonal quasicrystal.

The experimental results are summarized as follows:

1. At 1073K this type of approximants is formed almost exclusively in the elongated region from $Mn_{81.5}Si_{16.5}Cr_{2.0}$ to $Mn_{70.0}Si_{20.0}Cr_{10.0}$ and from $Mn_{81.5}Si_{16.5}V_{2.0}$ to $Mn_{70.0}Si_{20.0}V_{10.0}$. The latter corresponds to unknown phase in the ternary phase diagram.
2. The probable space group of the approximant is P6/*mmm* that is consistent to the Laue class 6/*mmm* determined by electron diffraction experiments. The lattice parameters of $Mn_{70.0}Si_{20.0}Cr_{10.0}$ are measured to be a = 17.020Å and c = 4.636Å. Those of $Mn_{70.0}Si_{20.0}V_{10.0}$ are a = 17.057Å and c = 4.637 Å. The preliminary structural model includes 77.9 metal atoms 19.1 Si atoms in a unit cell in the case of $Mn_{70.0}Si_{20.0}V_{10.0}$. This approximant exhibits pseudo dodecagonal axis parallel to the *c*-axis.
3. A high resolution electron microscope image observed along the *c*-axis revealed the triangle-square tiling with the edge length 4.56 Å. The tiling consists of vertices (3^6) and $(3^2.4.3.4)$. A ratio of number of regular triangles to number of squares in the tiling is $14/6 \approx 2.333$ that approximates the ideal ratio $4/\sqrt{3} \approx 2.309$ in the dodecagonal triangle-square tiling [1].

[1] P. Stampli, Helvetica Phys. Acta, **59**, 1260 (1986).

FORMATION OF ICOSAHEDRAL PHASE IN ZR-NI-SN GLASSY ALLOYS

J. B. Qiang[1,2], Y. M. Wang[1,2], Q. Wang[1,2], C. Dong[1],
W. Zhang[2,3], and A. Inoue[4],

[1] *Key Laboratory for Materials Modification by Laser, Ion and Electron Beams (Ministry of Education), Dalian University of Technology (DUT), Dalian 116024, China*
[2] *DUT-IMR Joint Research Center, Dalian University of Technology, Dalian 116024, China*
[3] *Institute for Materials Research (IMR), Tohoku University, Sendai 980-8577, Japan*
[4] *Tohoku University, Sendai 980-8577, Japan*

Thermal stability and crystallization behavior of melt-spun Zr-Ni-Sn ternary glassy alloys were investigated by differential scanning calorimetry (DSC) coupled with X-ray diffraction (XRD), and transmission electron microscopy (TEM) as well. The addition of Sn in the Zr-Ni alloy was found to markedly alter crystallization process of the metallic glasses, and nano-scaled metastable icosahedral phase (I-phase) was observed in the first crystallization stage of the Zr-Ni-Sn ternary glassy alloys. Noticing that simple metallic alloying element Sn has negative heats of mixing with all the elemental constituents of Zr-Ni base alloy, the present experimental evidence reveals that zero or positive heats of mixing between the alloying elements and the base alloy elements is not an essential requirement for I-phase formation in the Zr-Ni-based alloy system, which appears to conflict with the current empirical criteria summarized from the compositional characterization of I-phase in the reported Zr-based glass-forming alloy systems*. To clarify the reason for this discrepancy, it is worth exploring the alloying effect of Sn on the formation and crystallization of Zr-Ni-Sn glassy alloys in detail.

---

*J. Saida and A. Inoue, *Journal of Non-Crystalline Solids* **317** (2003) 97-105; J. Saida, M. Matsushita and A. Inoue, *Mater. Trans.*, JIM **41** (2000) 543-545.

P01-14

Composition Rule of Binary Quasicrystals

Hua Chen, Qing Wang, Yingmin Wang, Jianbing Qiang, and Chuang Dong[*]

Key Laboratory of Materials Modification (Dalian University of Technology), Ministry of Education, Dalian 116024, China

Abstract

Quasicrystals (QCs) are widely present in Al-TM binary systems, TM being transition metals such as Cr, Mn, Fe, Co, Ni, Pd, etc. However their precise composition ranges have not been thoroughly clarified. A cluster-plus-glue-atom model has been proposed to explain the compositions of stable Al-based ternary QCs. In this model, QCs were described in terms of 1st-shell coordination polyhedra, or clusters in short, plus extra glue atoms expressed by a universal cluster formula $[\text{cluster}][\text{glue}]_x$. In this paper, the composition rules of Al-TM binary QCs is revisited using the cluster formulas. These metastable QCs all conform to a unified cluster formula $[\text{icosahedron}][\text{glue}]_1$. It is also shown that binary QCs fulfill the Hume-Rothery stabilization mechanism with *e/a* = 1.86-1.71. In general, icosahedral QCs have slightly larger *e/a* values (*e/a* close to 1.86) than the decagonal ones (*e/a* close to 1.71-1.79).

Keywords Quasicrystals, Al-transition metal alloys, electron concentration

---

[*] Corresponding author, dong@dlut.edu.cn.

Poster Session 2
Structure and modeling

Monday, June 14, 2010

P02-01

Cluster formulas of alloy phases

C. Dong [1,a)], J. X. Chen [1,2], Q. Wang [1],Y. M. Wang [1], J. B. Qiang [1],

[1] *Key Laboratory for Materials Modification by Laser, Ion and Electron Beams*
(Ministry of Education), Dalian University of Technology, Dalian 116024, China
[2] *Department of Physics, Dalian Maritime University, Dalian 116026, China*

Simple composition formulas for alloy phases are developed using 1st-neighbor coordination polyhedral cluster plus their connections. The resultant cluster formulas [cluster](glue atom)$_x$, similar to molecular formulas for chemicals, contain key structure and composition information of the alloy phases. Examples of quasicrystals, bulk metallic glasses and crystalline alloy phases are analyzed and two types of phases are classified, cluster phases with glue atoms and non-cluster phases without. The former type is also referred to complex metallic alloys. Each structure can be characterized by a close-packed principal cluster and the relevant principal cluster formula reflects the essential cluster structure feature. In such a way all alloy phases can be grouped according to the principal clusters, the cluster connections, and the glue atoms. For instance, the $Al_{11}Fe_2$ icosahedron serves the principal cluster for binary Al-Fe quasicrystal, ternary Al-Fe-containing quasicrystals, and the $Al_{13}Fe_4$ phase, and the respective cluster formulas are $[Fe_2Al_{11}]Al$, $[Fe_2Al_{11}]Cu_4$, and $[Fe_1Al_7](Fe_2Al_{2.75})$, the last one being the effective cluster after sharings (the cluster is interconnected to its neighbors so that the effective composition is reduced).

Ni-RICH VERSUS Co-RICH STRUCTURES FOR d-AlCoNi VIA MELT-QUENCH SIMULATION *

M.Mihalkovič[1], M. Widom[2] and C. L. Henley[3]

[1] *Institute of Physics, Slovak Academy of Sciences, 84511 Bratislava, Slovakia*
[2] *Dept. of Physics, Carnegie-Mellon Univ., Pittsburgh, PA 15213 USA*
[3] *Dept. of Physics, Cornell Univ., Ithaca, NY 14853-2501 USA*

Previous simulation studies, which discovered low-energy configurations by annealing an elaborated sort of lattice-gas on discrete sites, arrived at structure models for d-AlCoNi in the Ni-rich [1] and Co-rich [2] compositions. The models were closely related (based on hexagon/boat/star tiles, plus others in the Co-rich case) but qualitatively distinct: e.g., as found experimentally, the periodicity along the 10-fold axis is $4\AA$ for Ni-rich and $8\AA$ for Co-rich. Although both structures agree with experiment, their (ab-initio) energies are never computed to be stable with respect to the competing crystal phases – largely because the energy depends sensitively on how certain Al atoms pucker out of the main atom planes.

Using the same realistic pair potentials as before [1,2], we performed computer experiments quenching two compositions, Ni-rich $Al_{72}Co_8Ni_{20}$ and Co-rich $Al_{73}Co_{27}$, from the melt, using replica-exchange molecular dynamics. The key feature allowing an ordered result is the constraint that the unit cell parameters were chosen to fit decagonal phase approximants. The quasicrystal (approximant) structures thus obtained had the best energies seen to date for d-AlCoNi models (respectively +20 meV/atom and +9 meV/atom above the tie-plane of competing phases).

We find not only Co-rich but Ni-rich structures are *locally* 8 Å periodic. (Indeed, constraining the periodicity to be 4Å destabilizes the decagonal phase in favor of an unrelated one resembling X-AlCoNi.) The puckered motifs that break 4Å periodicity are rarer and less correlated in the Ni-rich case, giving it a *statistical* $4\AA$ periodicity. Furthermore, we found that, if we constrain the total atom density, we obtain the Ni-rich or Co-rich kinds of structures at lower and higher densities, respectively, no matter which composition is used.

[1] M. Mihalkovič *et al*, Phys. Rev. B 65, 104205 (2002).

[2] N. Gu, M. Mihalkovič, and C. L.Henley, Phil. Mag. Lett. 87, 923 (2007).

* Supported by U.S. Dept of Energy grant DE-FG02-89ER-45405 and by Slovak VEGA 2/0157/08.

ENERGETICS AND DYNAMICS OF CAGED Zn_4 IN i-ScZn *

C.L. Henley[1] and M. Mihalkovič[2]

[1] *Dept. of Physics, Cornell Univ., Ithaca NY 14853-2501, USA*
[2] *Inst. of Physics, Slovak Academy of Sciences, Dubravska cesta 9, 84511 Bratislava, Slovakia*

In *i*-ZnSc (like other quasicrystals of the *i*-CaCd class) the innermost shell of the icosahedral cluster is a Zn_4 tetrahedron which thus breaks the symmetry of the outer two cluster shells. We investigate theoretically the effective potential and the dynamics of individual tetrahedra, based on interatomic pair potentials (fitted from an ab-initio database) and molecular dynamics (MD).

The degrees of freedom for a tetrahedron can be labeled by a rigid-body rotation matrix $\mathbf{R}$, or equivalently three angles. The effective potential has three terms. The interaction $V_{\rm int}(\mathbf{R},\mathbf{R}')$ between tetrahedra of adjacent clusters, which drives structural ordering transitions in CaCd approximants, is already small in ZnSc. We construct model approximants containing the substitution $Zn_4 \rightarrow$RE in most clusters, where RE is a rare-earth atom – this is known to occur in the actual alloys (C. P. Gómez, personal communication). In this fashion we isolate the Zn_4 tetrahedra and can completely neglect $V_{\rm int}$.

We are left with the orientational potential $V_{\rm or} = V_{\rm ico} + V_{\rm env}$, where $V_{\rm ico}$ has icosahedral symmetry due to the caging atoms of the cluster, but $V_{\rm env}$ breaks icosahedral symmetry, due to the pattern of surrounding clusters. We parametrize these terms in simplified forms, based on simulations.

The low-frequency dynamics in *i*-ZnSc is dominated by cluster reorientations, which are thermally activated transitions over barriers in $V_{\rm or}(\mathbf{R})$. We have evaluated the velocity autocorrelations of tetrahedron atoms in MD simulations; the corresponding spectral density $S(\omega)$ is fairly well fitted using a simplified model in which each atom hops in a double well. We discuss what information can be obtained in a realistic model, in which tetrahedra undergo transitions among a set of discrete orientations which are minima of $V_{\rm or}(\mathbf{R})$.

* Supported by U.S. Dept of Energy grant DE-FG02-89ER-45405 and by Slovak VEGA 2/0157/08.

P02-04

ATOMIC STRUCTURE OF DECAGONAL FRANK–KASPER Mg-Zn-RE QUASICRYSTAL*

M. Mihalkovič[1], C. L. Henley[2]

[1] *Institute of Physics, Slovak Academy of Sciences, 84511 Bratislava, Slovakia*
[2] *Dept. of Physics, Cornell Univ., Ithaca NY, 14853-2501, USA*

Icosahedral quasicrystal structures of the Frank–Kasper (FK) class are well understood on a basic level, mainly thanks to refinements of large "1/1", "2/1" and even "(3/2,2/1,2/1)" approximants [1]. On the other hand, decagonal FK quasicrystals [2] are rarer and no refinements are reported. Long ago, a hypothetical FK decagonal structure was obtained by quenching a toy-potential binary alloy [3], and modeled by a simple decoration of the standard hexagon-boat-star (HBS) tiling.

Here we report a realistic study of structural stability and energetics of FK decagonals at low temperatures in two alloy compositions, binary Mg–Zn and ternary Mg–Zn–RE (where "RE" denotes "rare earth"). Our approach, following [4], is to select an ensemble of periodic tilings, and generate a family of decoration rules differing by small variations, and compute the total (relaxed) energy of every combination of a decoration and a tiling (using pair potentials, or ab-initio energies where feasible). By numerical fitting, we re-express the total energies in terms of a "tiling Hamiltonian" with single-tile energies and pairwise tile-tile interactions [4]. The aim is to produce a tile-decoration structural model of d-MgZnRE quasicrystal, more detailed than that of [3], in that it satisfies additional constraints: e.g. the actual tilings are better described by a "rectangle-triangle tiling". A key choice that must be made correctly in Mg–Zn–RE is which of the coordination-16 vertices are to receive the rare-earth atoms (which are even larger than Mg in this composition.)

[1] G. Kreiner, J. Alloys and Comp. 338, 261 (2002).
[2] E. Abe and A. P. Tsai, Phys. Rev. Lett. 83, 753 (1999)
[3] J. Roth and C. L. Henley, Philos. Mag. A 75, 861 (1997).
[4] M. Mihalkovič *et al*, Phys. Rev. B 53, 9002 (1996).

* Supported by U.S. Dept of Energy grant DE-FG02-89ER-45405 and by Slovak VEGA 2/0157/08.

P02-05

CANCELED

P02-06

A SUPERSTRUCTURAL FLUCTUATION OF THE RHOMBIC PENROSE TILING TYPE DECAGONAL QUASICRYSTAL

K. Kato[1] and A. Yamamoto[2]

[1] *Department of Physics Faculty of Science and Engineering Chuo University*
Kasuga 1-13-27 Bunkyo-ku, Tokyo 112 Japan
[2] *National Institute for Materials Science, Namiki 1, Tsukuba, Ibaraki, 305-0044, Japan*

The cluster arrangement of the regular decagonal occupation domain (OD) type decagonal quasicrystal may sometimes be disarranged from the ideal regular decagon OD, if actual observation was plotted to the internal-space. On the other hand, their satellite (superstructure) reflection does not appear in the diffraction was reported in spite of the disorder. This has the phason distortion adapted to a certain rule, and is considered to have average structure approximated to basic structure because this distributes on the average as a whole. It is supposed that this average structure is the regular decagon OD. (OD-10) When distribution of this internal-space occupation domain is observed, the center part does not have fluctuation mostly. The disorder has occurred in many cases within and without near the regular decagon perimeter line of average structure. One of the well known tiling in which OD occupies this center part is the rhombic Penrose tiling (RPT). This is the superstructure of the five-time period of OD-10. When the OD area is fully involves the RPT, the structure that had a certain additional cluster point including RPT can be considered. It may also be able to be treated that it has OD-10 type average structure as a whole, such a superstructure existing partially and fluctuating. We would like to express from the viewpoint of the 4D-section method about this superstructure fluctuation.

A BERGMAN-CLUSTER-BASED MODEL OF FACE-CENTERED ICOSAHEDRAL ZN-MG-HO QUASICRYSTALS

Akiji Yamamoto and Cesar P. Gomez

National Institute for Materials Science, Namiki 1, Tsukuba, Ibaraki, 305-0044, Japan

There are two types in icosahedral Zn-Mg-Ho quasicrystals (i-Zn-Mg-Ho QCs) which have primitive and face-centered icosahedral symmetry, respectively. The latter is a superstructure of the former with doubled unit cell volume. They are both considered to be composed of the Bergman cluster, since closely related Zn-Mg-TM systems with TM=Hf, Zr and Ti have both primitive and face-centered icosahedral QC and 1/1 approximants, although Zn-Mg-Ho system has no crystalline approximants.[2] Recently a model of the former, which is based on one kind of Bergman cluster, is proposed.[3] A model of the latter is shortly discussed using the subdivision of large ODs, which are used in the analysis of face-centered i-Al-Pd-Mn QCs.[5, 4] In the face-centered i-Zn-Mg-Ho QCs, 5 independent large occupation domains (ODs) are found in a unit cell of a six-dimensional (6D) face centered lattice using the low-density elimination method. In particular, it has ODs in both even and odd parity body centers, in contrast to i-Al-Pd-Mn QCs where only one of them exists. Its ODs will be more similar to those of primitive Zn-Mg-Ho QCs than face-centered Al-Pd-Mn ones. It is known that in Zn-Mg-TM QCs mentioned above, there exist 1/1 approximants consisting of two kinds of Bergman clusters.[1] Therefore a model with two kinds of Bergman clusters is conceivable in a face-centered i-Zn-Mg-Ho. In this paper, we build a 6D model of the face-centered Zn-Mg-Ho quasicrystals with two kinds of inter-penetrated rhombic-triacontahedral clusters, each of which includes a different Bergman cluster, and simulate its diffraction patterns. The similarity and difference of the structure with that of the primitive one will be discussed.

References

[1] P. C. Gomez, S. Ohhashi, A. Yamamoto, and A. P. Tsai. *Inorg. Chem.*, 47(18):8258, 2009.

[2] J. Hasegawa, S. Takeuchi, and A. P. Tsai. *Phil. Mag. Lett.*, 85:289, 2005.

[3] H. Takakura and A. Yamamoto. *Phil. Mag.*, 8:2713, 2007.

[4] A. Yamamoto and H. Takakura. *Ferroelectrics*, 305:223, 2004.

[5] A. Yamamoto, H. Takakura, and A. P. Tsai. *Phys. Rev.*, B68:094201, 2003.

P02-08

ANISOTROPIC LOCAL STRUCTURE OF DECAGONAL QUASICRYSTALS BY DAFS

H. Abe

Department of Materials Science and Engineering, National Defense Academy,
Yokosuka 239-8686, Japan

Al-Ni-Co (ANC) and Al-Ni-Fe (ANF) system is well known to be decagonal quasicrystals. An order-disorder phase transition takes place in the former ANC, while the latter ANF is characterized by approximant-quasicrystal phase transition. Relating each phase transitions, atomic short-range order (SRO) both in ANC and ANF is analyzed quantitatively [1].

In this study, local structures of quasicrystals are examined along the periodic direction compared with a quasiperiodic plane by X-ray diffraction anomalous fine structure (DAFS) technique. Here, DAFS possesses site selectivity and spatial selectivity. Along the periodic direction, zigzag correlation develops at high temperature.

[1] R. Barabash, G. E. Ice and P. E. A. Turchi, Ed., *Diffuse Scattering and the Fundamental Properties of Materials* (Momentum Press, New Jersey, 2009).

MEDIUM-RANGE ORDER OF DECAGONAL QUASICRYSTALS

H. Abe

Department of Materials Science and Engineering, National Defense Academy,
Yokosuka 239-8686, Japan

In order to analyze the medium-range order (MRO) in complex materials, MRO parameters are introduced by extending short-range order (SRO) parameters [1]. For the test case, $Al_{72}Ni_{20}Co_8$ is the best candidate to check the MRO. Here, $Al_{72}Ni_{20}Co_8$ is a decagonal quasicrystal, which obeys the ideal Penrose tiling.

In $Al_{72}Ni_{20}Co_8$, SRO diffuse scattering relating with an order-disorder phase transition is distributed at around the ideal positions of the superstructure reflections. Using the observed SRO diffuse scattering, MRO analysis is carried out. Monte Carlo method can optimized a combination between SRO and MRO parameters. In the cluster-based structure such as $Al_{72}Ni_{20}Co_8$, MRO is not ignored essentially.

[1] H. Abe, *J. Phys. Soc. Jpn.* **76** (2007) 094601.

P02-10

DETERMINATION OF THE ELECTRON DENSITY DISTRIBUTION OF THE DECAGONAL QUASICRYSTAL OF $Al_{72}Ni_{20}Co_8$ BY CONVERGENT-BEAM ELECTRON DIFFRACTION.

Hirotaka Nakahara[1] , Koh Saiton[2] and Nobuo Tanaka[2]

1 Department of Crystalline Materials Science Graduate School of Engineering
Nagoya University, Nagoya, 464-8603, Japan
2 EcoTopia Science Institute , Nagoya University, Nagoya, 464-8603, Japan

In this study, the convergent-beam electron diffraction(CBED) method is applied to decagonal quasicrystal of $Al_{72}Ni_{20}Co_8$ for the purpose of determination of the electoron densiy distribution. We performed the refinement of Debye-Waller factors and low-order structure factors for electron by using the structure model, whose atom positions were refined [1]. The structure refinement is carried out by comparing the experimental diffraction intensity due to elastic scattering electrons and the simulated diffraction intensity obtained by the many beam dynamical calculation.

CBED patterns were taken by using an energy filtering transmission electron microscope JEM-2010FEF at an accelerating voltage of 100 kV, with an acceptance energy width of 10 eV. The incident electron probe was set to be 1 nm in diameter with a convergence angle of approximately 10 mrad. Dynamical CBED calculation was carried out by using 250 waves including a strong reflections which are observed in the experiment pattern.

In this analysis we refined two Debye-Waller factors, one is for all Al atoms, and the other is for all transition metal atoms, using 5 reflections in zeroth-order-Laue zone (ZOLZ) and 10 reflections in higher-order Laue zone (HOLZ).

4 structure factors of the 00002, $11\bar{1}\bar{1}0$, $11\bar{1}\bar{1}2$ and $21\bar{1}\bar{2}0$ reflections were refined by using 5 ZOLZ reflections. The electron density distribution was obtained from the structure factors determined by the present study by using the Mott formula. We discuss the redistribution of charge from the deformation electron density which is the difference between electron density distribution obtained from indepedent atom model and that obtained from the present refinement.

[1]K.Saitoh, H.Murakami, N.Tanaka, Z.*Kristallogr.* 223(2008) 859.

P02-11

SPECTROSCOPIC STUDY OF Ni-RICH Al-Co-Ni QUASICRYSTAL

K. Soda[1], M. Inukai[2], M. Kato[1], S. Yagi[1], Y. G. So[3], and K. Edagawa[3]

[1] *Graduate School of Engineering, Nagoya University, Nagoya 464-8603, Japan*
[2] *Venture Business Laboratory, Nagoya University, Nagoya 464-8603, Japan*
[3] *Institute of Industrial Science, The University of Tokyo, Tokyo 153-8505, Japan*

Various structural modifications have been found as a function of the Co/Ni ratio in decagonal Al-Co-Ni quasicrystals (QC) by electron microscopy [1]. However, it is still hard to distinguish Co from Ni in the microscopic image. Thus, in order to clarify the chemical nature bringing the unique atomic arrangement with the various modifications, we have studied the transition metal arrangement by comparing the electronic structures obtained by spectroscopic observation and model cluster calculation [2,3]. In this study, we report the results of soft x-ray photoelectron spectroscopy (XPS) and discrete variational $X\alpha$ (DV-$X\alpha$) cluster calculation for a Ni-rich Al-Co-Ni QC.

In Fig.1, a typical XPS spectrum of the Ni-rich QC is compared with that of a Co-rich one and the electronic density of states (DOS) derived from a Ni-rich model cluster shown in Fig.2. Here, the model cluster is based on a theoretical prediction with use of the interatomic pair potential [4], which shows a Ni-Ni interaction as well as a strong Al-Co one. The present cluster calculation also predicts bimodal Ni partial DOS consisting of the Ni-Ni bonding and anti-bonding bands. However, the XPS spectrum of the Ni-rich QC is peaked at higher binding energy than the Co-rich one and seems not to show the predicted large anti-bonding component.

[1] K. Hiraga, Adv. Imaging and Electron Phys. **122** (2002) 1.
[2] M. Inukai *et al.*, Z. Krist. **223** (2008) 851.
[3] M. Inukai *et al.*, J. Phys.: Conf. Ser. *in press*.
[4] M. Mihalkovič *et al.*, Phys. Rev. B **65** (2002) 104205.

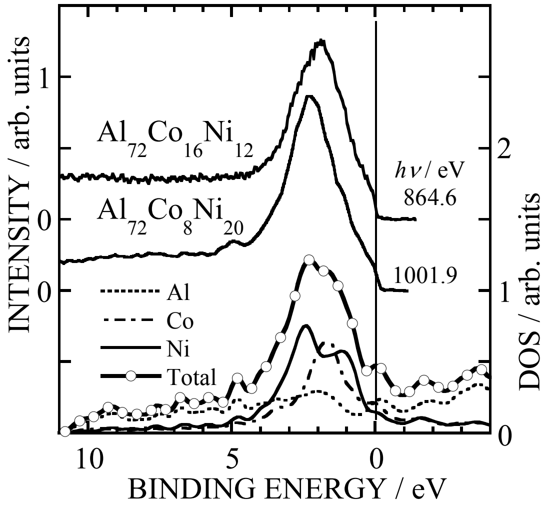

Fig.1 Photoelectron spectra and calculated density of states of Ni-rich Al-Co-Ni.

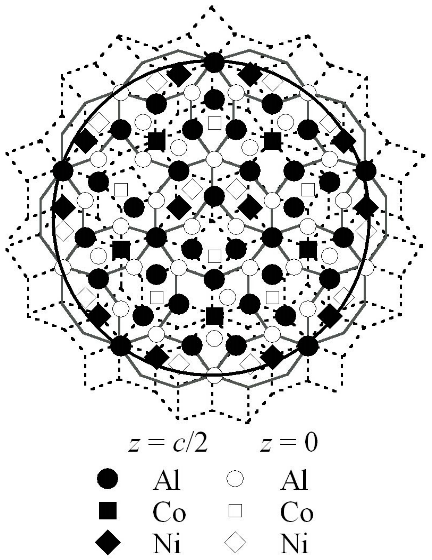

Fig.2 Cluster model of Ni-rich Al-Co-Ni.

P02-12

MODIFICATION OF $Al_{70}Mn_{17}Pd_{13}$ DECAGONAL STRUCTURE BY ULTRAHIGH-RESOLUTION STEM

T. Seki[1], E. Abe[1], H. Sawada[2, 4], Y. Kondo[2, 4], K. Takayanagi[3, 4]

[1]*Department of Materials Engineering, University of Tokyo, Tokyo 113-8656, Japan*
[2]*JEOL Ltd., Tokyo 196-8558, Japan*
[3]*Department of Condensed Matter Physics, Tokyo Institute of Technology, Tokyo 152-8551, Japan*
[4]*JST-CREST, Saitama 322-0012, Japan*

Al-Mn-Pd alloys form a stable decagonal quasicrystal with its periodic length about 12 Å, whose structure model was proposed based on a single-quasicrystal X-ray diffraction analysis [1,2] and high-resolution phase-contrast electron microscopy imaging [3,4]. In the present work, we have revisited the decagonal $Al_{70}Mn_{17}Pd_{13}$ by ultrahigh-resolution Z-contrast scanning transmission electron microscopy (STEM), and immediately find that the observed Z-contrast (Fig. 1(a)) is significantly different from that expected from the existing model structures. As exemplified by the decagonal clusters, the observed contrast (Fig. 1(b)) cannot be reproduced by the simulation (Fig. 1(c)) based on the model in ref. 2. Hence we modify the chemical order within the clusters, and the improved cluster structure (Fig. 2) now reproduces fairly well the observed contrast, as shown in Fig. 1(d). We will further modify the other clusters defined in ref. 2, in order to describe the entire atomic structure of the decagonal $Al_{70}Mn_{17}Pd_{13}$.

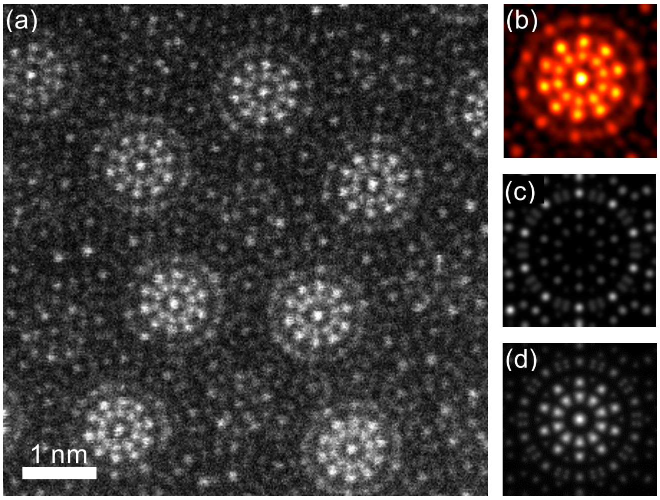

Fig. 1 (a) Z-contrast STEM image (300kV-STEM, JEOL-R005). (b) Averaged intensity map of the decagonal clusters. (c) Simulation image of the model in ref.1. (d) Simulation image of the modified structure shown in Fig. 2.

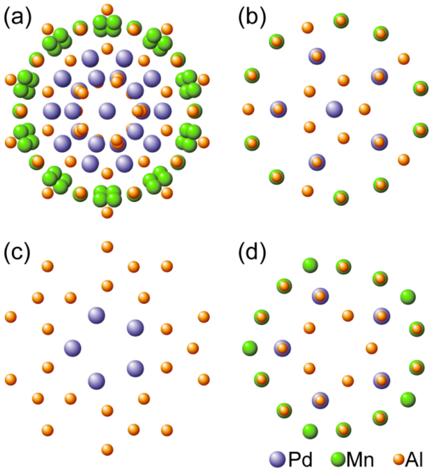

Fig. 2 Modified structure of the decagonal cluster. (a) Projection of all 6 layers. (b) - (d) Layers at z = 0.06, 0.25 and 0.43, which are related to the other 3 layers by the screw axis symmetry 10_5.

[1] W. Steurer *et al.* Journal of Physics, Condensed Matter, **6** (1994) 613.
[2] S. Weber and A. Yamamoto, Acta Crystallographica, **A54** (1998) 997.
[3] K. Hiraga and W. Sun, Phil. Mag. Lett., **67** (1993) 117.
[4] C. Beeli and S. Horiuchi, Phil. Mag. B **70** (1994) 215.

P02-13

Structure and Stability of BTiRu Approximant Crystals to Decagonal Quasicrystal

Y. Miyazaki[1], T. Yoshida[1], J. T. Okada[2], E. Abe[3], Y. Yokoyama[4], and K. Kimura[1]

1 *Department of Advanced Materials Science, The University of Tokyo,*
Kashiwa 277-8561, Japan
2 *Japan Aerospace Exploration Agency, Tsukuba, 305-8505, Japan*
3 *Department of Materials Science and Engineering, The University of Tokyo,*
Tokyo 113-8656, Japan
4 *Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan*

In 2004, BMgRu decagonal quasicrystal was predicted by M.Mihalkovic and M. Widom based on first-principle calculation [1]. The first quasicrystaline boride have been discovered by the authors in BTiRu rapidly quenched alloys, whose structure is interpreted as aperiodic tiling of three subunits: thin hexagon, boat, and star, with long range ten-fold symmetry [2]. However, the detailed atomic structure and stability of the quasicrystal have been unclear. We investigate approximant crystals in nearby compositions to help to understand the boride quasicrystal.

We have obtained nearly single-phase samples of three approximant crystals by means of SPS (spark plasma sintering). $B_{35}Ti_{19}Ru_{46}$ alloys formed α ($B_4Mg_2Ru_5$) type structure [2] at 1700K, $B_{38}Ti_{15.5}Ru_{46.5}$ and $B_{38}Ti_{14}Ru_{48}$ alloys formed similar structure to δ and ζ, which we have reported in BMgRu system [3][4] at 1650K. Neither quasicrystal nor other approximant (β, γ or ε) crystals have formed in homogenized alloys of surrounding compositions so that these phases are thought to be metastable in this ternary system. The lattice parameters of α, δ, and ζ correspond to approximant by rational ratio (1/1, 1/1), (1/1, 5/3) and (2/1, 1/1) to golden mean $\tau(=(1+\sqrt{5})/2)$, respectively. We build the structure models using 2 hexagons and 4 boats for δ, 2 boats for ζ. Rietveld's powder XRD pattern fitting confirm the reasonability of the models.

The quasicrystal and approximants in BMgRu have been expected to be "true ternary" system, whose each atomic site is unsubstitutable by the other element because of strong contrast in size and chemical property of the elements. However, nominal composition and SEM-EDX analysis shows δ– and ζ–BTiRu approsimants have smaller amount of Ti compared to that using the ideal tile set. Rietveld's powder XRD pattern fitting indicate that particular Ti sites in boat tiles are partially substituted by Ru. It means possibility of structural stabilization by adjusting Fermi level into a pseudo gap of the DOS.

[1]M. Mihalkovic and M. Widom, *Phys. Rev. Lett.*, **93**, 095507 (2004)
[2] Y. Miyazaki, J. T. Okada, E. Abe, Y. Yokoyama and K. Kimura, to be published (2010).
[3] K. Schweitzer and W. Jung, *Z. anorg. allg. Chem.* **530**, 127 (1985)
[4] Y. Miyazaki, J. T. Okada and K. Kimura, *Phil. Mag.*, **87**, 2701 (2007)
[5] Y. Miyazaki, J. T. Okada, E. Abe and K. Kimura, *Phil. Mag.*, **88** 1935 (2008)

P02-14

STRUCRUAL STUDY OF HIGHLY DEFECTIVE AL-PD-FE CREYSTALLINE APPROXIMANT

W. Sun, J. P. Wang and Z. Y. Liu

Institute of Microstructure and Property of Advanced Materials
Beijing University of Technology
100 Pingle Yuan, Chaoyang District, Beijing 100124, China

A kind of highly defective Al-Pd-Fe crystalline approximant phase (E-phase), which can be regarded as an intermediate structural state between a decagonal quasicrystal with 1.6 nm periodicity and an ideal Al-Pd-Fe ε_{16}-phase, has been observed in the as-cast $Al_{70}Pd_{15}Fe_{10}$ alloy. On the basis of HREM observations, the structures of as-cast and heat-treated E-phases are characterized and discussed in terms of different schemes in order to find out the intrinsic nature of their defective structural states. It has been found that the as-cast E-phase can form transitional and orientational nano-sized domains easily and this can destroy its long-range periodicity significantly. A kind of structural defect constructed with giant hexagonal unit (H type) has been found to exist in the E-phase; it has small size and dispersive distribution in the as-cast state, and turns to grow up significantly to form long strip-shaped domains when annealed at high temperatures. By means of HREM observations and imaging simulations, intrinsic structural units, which can interpret both the structure of the E-phase and formation of characteristic structural defects in it, have been proposed and their structural correlations with those in the other complex approximant structures will be discussed.

CRYSTAL STRUCTURE OF χ- AlPdRe.

Shota Suzuki, Rayko Simura and Kazumasa Sugiyama

Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

The structural information on the approximant crystals are frequently used for providing structural models of quasicrystals. Besides the icosahedral (i-) and dodecahedral (D-) phases of the Al-Pd-Re alloy system, a crystalline approximant of trigonal χ-AlPdRe phase have been found [1,2]. The purpose of this paper is to report the structure of χ-AlPdRe.

An alloy ingot with a composition Al80Pd15Re5 was prepared by arc melting in Ar atmosphere. Fragments of the solidified ingot were charged into a carbon crucible sealed in an evacuated silica tube and annealed at 750°C for 10 days. Single crystal samples were cut out from the annealed sample and used for the X-ray structural analysis (Mo$K\alpha$, Rigaku R-AXIS RAPID). The initial structure model was obtained by direct methods SIR97 [3] and refined by the least-squares software SHELXL-97 [4].

The structure of χ-AlPdRe ($P31c$ a=12.3744(4)Å and c=27.487(1)Å) is isotypic to that of Ir_9Al_{28} [5]. The heavy metal (Pd and Re) sites of χ-AlPdRe correspond to Ir sites of Ir_9Al_{28} by suggesting the typical pseudo-decagonal motifs together with the pseudo Mackay type icosahedron around a Re site. These structural features of χ-AlPdRe are well attributed to its chemical composition nearby the center of those for i- and D-phases in the Al-Pd-Re system.

[1]A.P.Tsai et al., (1990), Mater. Trans., JIM., **31**, 98.
[2]S.Balanetsky and B. Grushko (2008) J. Alloy. Comp., **456**, 105.
[3] A. Altomare et al., (1999) J. Appl. Cryst.. **32**, 115
[4] G.M. Sheldrick, (1997) SHELXL-97, University of Göttingen, Germany.
[5]S.Katrych et al., (2006), J. Alloy. Comp., **407**, 132.

CRYSTAL STRUCTURE OF NEW ORTHORHOMBIC APPROXIMANT PHASE $AL_{72}PD_{18}MN_5SI_5$

R.Simura, N.Kaji, K.Sugiyama and K.Hiraga

Institute for Materials Science, Tohoku University, Sendai 980-8577, Japan

The discovery of quasicrystals has encouraged a variety of structural studies on complex crystalline phases. In particular, Al-Pd-Mn(-Si) system indicates decagonal and icosahedral phases and corresponding approximant structures of orthorhombic-AlPdMn [1], 2/1-AlPdMnSi [2] and 1/1-AlPdMnSi [3] have been analyzed by single crystal X-ray diffraction. This paper demonstrates the structure of new orthorhombic approximant phase which coexists with 2/1- and 1/1-approximants in the Al-Pd-Mn-Si system.

An alloy ingot with a composition $Al_{69}Pd_{20}Mn_8Si_3$ was prepared by arc melting in Ar atmosphere. Needle-like crystals can be found in as-prepared ingot and EPMA (JEOL JXA-8621MX) showed that chemical composition of this unknown phase was Al71.7 Pd18.5 Mn5.0 Si4.8. Single crystal sample was cut out from the sample ingot and ground into a sphere of 140μm in diameter. Intensity data were collected on a AFC6S (Rigaku) four-circle diffractometer by using monochromated Mo $K\alpha$ radiation. The initial structure model was obtained by direct methods SIR97 [4] and refined by the least-squares software SHELXL-97 [5].

The structure of orthorhombic-AlPdMnSi (*Pnma; a*=14.396(3) Å, *b*=24.003(2)Å, *c*=7.603(2)Å) can be represented by the stacking of three types of layers (A,B,C) perpendicular to the *b*-axis. The flat layer (A) at *y*=1/4 is sandwiched by two puckered layers (B), by forming a pentagonal columnar structure similar to that found in the Al_3Pd structure [6]. The unique layer (C) can be ranked into three sub-layers and the pentagonal atomic arrangement similar to those found in the Al_3Mn structure can be realized in these sub-layers [7]. Therefore, the present orthorhombic-AlPdMnSi indicates structural features similar to both Al_3Mn and Al_3Pd approximants for the decagonal quasicrystals. It may be interesting to note that the orthorhombic-AlPdMnSi is similar to that of ϕ-AlCoSi.

[1]M.Audier, M.Durandcharre, and M.Deboissieu, Phil. Mag. B., **68** (1993) 607.
[2]K.Sugiyama, N.Kaji, K.Hiraga and T.Ishimasa, Z. Kristalogr., **213** (1998) 90.
[3]K.Sugiyama, N.Kaji, K.Hiraga and T.Ishimasa, Z. Kristalogr., **213** (1998) 168.
[4]A.Altomare, M.C.Burla, M.Camalli, G.L.Cascarano, C.Giacovazzo, A.Guagliardi, A.G.G.Moliterni, G.Polidori and R.Spagna, J. Appl. Cryst., **32** (1999) 115.
[5]G.M. Sheldrick, SHELXL-97, University of Göttingen, Germany (1997)
[6]K.Hiraga, E. Abe, and Y.Matsuo, Phil. Mag. Lett., **70** (1994) 163.
[7]K.Hiraga, M.Kaneko, Y.Matsuo and S.Hashimoto, Phil. Mag. B., **67** (1993) 193.

MULTIPLE DIFFRACTION IN AN ICOSAHEDRAL Al-Cu-Fe QUASICRYSTAL

C. Fan, Th. Weber, S. Deloudi and W. Steurer

Laboratory of Crystallography, ETH Zurich, CH-8093 Zurich, Switzerland

Multiple diffraction (*umweganregung*) effects in an icosahedral Al-Cu-Fe quasicrystal have been investigated in-house on an Oxford Diffraction four-circle diffractometer equipped with an Onyx™ CCD area detector and MoKα radiation. For that purpose, an automated approach for Renninger scans has been developed. Two weak reflections were chosen as the main reflections (called **P**) in the present measurements. For the first main reflection, the Renninger scans have been performed on three simultaneously excited reflections (called **H**) and three corresponding coupling reflections (**P**-**H**); For the second main reflection, only one multiple diffraction event has been checked. As well known for periodic crystals it is also observed for this quaicrystal that the intensity of the main reflection may significantly increase if the **H** and the **P**-**H** reflections are both strong, while there is no obvious multiple diffraction effect if one of them is weak. The occurrence of multiple diffraction events during data collection by 360 degree rotation has been studied based on an ideal structure model and a kinematical multiple diffraction theory. Simulations of ψ-scan diffraction experiments were done using three high-symmetric axes, *i.e.* 2-fold, 3-fold and 5-fold axes, and one arbitrary crystal direction as rotation axes. A protocol for minimizing and/or correcting multiple diffraction has been developed.

P02-18

ANALYSIS OF STRUCTURE AND CHEMICAL ORDER IN A TERNARY $Yb_{12}Mg_{52}Cd_{36}$ QUASICRYSTAL

Cesar Pay Gómez*[1], Hiroyuki Takakura[2], Akiji Yamamoto[3], An Pang Tsai[4]

[1]*Department of Materials Chemistry, Ångström Lab. Uppsala University, SE-751 21 Uppsala, SWEDEN*
[2]*Division of Applied Physics, Graduate School of Engeneering, Hokkaido University, Sapporo, 060-8628, JAPAN*
[3] *National Institute for Materials Science (NIMS), 1-1 Namiki, Tsukuba, Ibaraki, 305-0044, JAPAN*
[4]*Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, JAPAN*

The atomic structure of the ternary $Yb_{12}Mg_{52}Cd_{36}$ quasicrystal has been refined from single crystal X-ray data. The ternary quasicrystal is related to the binary i-$Yb_{16}Cd_{84}$ parent phase,[1, 2] and suffers from chemical disorder mainly due to mixing between Mg and Cd. Studies on related ternary approximants however indicate that this chemical disorder is only partial, and that there are strong selection rules in several ternary systems that govern the choice of a particular atom at a specific site. The purpose of this work is thus to elucidate the chemical order between the constituent elements in the ternary $Yb_{12}Mg_{52}Cd_{36}$ quasicrystal and its relation to ternary approximants in other *RE*-Mg-Cd (*RE*=Rare Earth) systems. The structure refinements performed on the $Yb_{12}Mg_{52}Cd_{36}$ quasicrystal clearly indicate that it is composed of similar atomic clusters as the binary i-$Yb_{16}Cd_{84}$ phase and that there is a strong selection rule that mainly determines the chemical order at the cluster level. Similar observations have also been made in related ternary approximant phases. The structure refinement is the first of its kind performed on a ternary Yb-Cd-related quasicrystal, and the results indicate that the structures and chemical order of ternary quasicrystals can be understood by extracting and combining information from structure refinements on both quasicrystals and related approximants.

[1] A. P. Tsai, J. Q. Guo, E. Abe, H. Takakura, T. J. Sato, *Nature* 408 (2000) 537.

[2] H. Takakura, C. P. Gómez, A. Yamamoto, M. d. Boissieu, A. P. Tsai, *Nat. Mater*. 6 (2007) 58.

DIFFUSE SCATTERING IN THE ZN6SC 1/1 CUBIC APPROXIMANT

T.Yamada[1,2], C.P.Gomez[3], R.Tamura[2], H.Euchner[4], A.Yamamoto[3] and M.de Boissieu[1]

[1]SIMaP, Grenoble-INP, CNRS,UJF ,BP 75, 38402 Saint Martin d'Hères Cedex, France
[2]Department of Material & Science., Tokyo Univ. of Science, Noda 278-8510, Japan
[3]National Institute for Materials Science, Tsukuba 305-0044, Japan
[4]ITAP, Universitat Stuttgart, Stuttgart 70550, Germany

The low-temperature phase transition of the Zn_6Sc cubic 1/1 approximant [1] has been investigated by X-ray diffraction. It is a crystalline approximant to a recently discovered quasicrystal $Zn_{88}Sc_{12}$ [2] and has a bcc lattice composed of a Tsai-type cluster with an orientationally disordered Zn tetrahedra at the centers [3]. The phase transition undergoes below 160K and has been attributed to the orientational ordering of the Zn tetrahedra along [110] direction of high-temperature phase [1, 4]. In order to obtain an insight into the orientational ordering occurring at the phase transition, diffuse scattering has been measured. Well above the phase transition at 220K (i.e. 60 K above) we observed a broad diffuse scattering intensity which sharpen and merges into a Bragg peak as the temperature decreases and reaches the transition temperature (T_c). This signature of short-range ordering above T_c will be discussed in details and compared to refined average structures obtained between T_c and room temperature by measuring Bragg peaks.

[1] R. Tamura *et al.*, Phys. Rev. B **71**, 092203, (2005).
[2] P. C. Canfield *et al.*, Phy. Rev. B **81**, 020201(R) (2010).
[3] Q. Lin and J. D. Corbett, Inorg. Chem., **43**, 1912, (2004).
[4] T. Ishimasa *et al.*, Phil. Mag., **87**, 2887, (2007).

Classification of low-temperature superstructures of Cd_6M 1/1 approximants

K. Nishimoto, M. Muraki, T. Sato and R. Tamura

Department Materials Science & Technology, Tokyo University of Science, Chiba 278-8510, Japan

Cd_6M (M=Ca, rare earth elements) crystalline approximants are cubic crystals made up of Tsai-type icosahedral clusters[1]. The Tsai-type icosahedral cluster is composed of 4 successive shells, which are, from the center, Cd4 tetrahedron, a Cd20 dodecahedron, a M12 icosahedron and a Cd30 icosidodecahedron. It is known that the Cd4 tetrahedron is orientationally disordered at room temperature except for Cd_6Eu and Cd_6Ce. An occurrence of a phase transition was first discovered for Cd_6Ca and Cd_6Yb at 100K and 110K, respectively[2,3], which has been attributed to orientational ordering of the Cd4 tetrahedron at the center of the Tsai-type cluster. Among them, Cd_6Ca has been extensively investigated and it has been found that it transforms into a $\sqrt{2}a\times a\times\sqrt{2}a$ *C*-centered monoclinic lattice with space group $C2/c$ below 100 K. In the present work, we have investigated phase transitions in a variety of Cd_6M(M= Y, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Yb, Lu) by transmission electron microscopy (TEM) in order to clarify their superstructures at low temperatures.

For most of the compounds, we observe superlattice reflections at middle points of the fundamental reflections at low temperatures. In the cases of Cd_6M(M=Y, Nd, Sm, Gd, Tb), the superlattices are explained by a $\sqrt{2}a\times a\times\sqrt{2}a$ *C*-centred monoclinic lattice with space group $C2/c$ or Cc. On the other hand, for Cd_6Dy, Cd_6Ho and Cd_6Lu, no superlattice reflection has been observed at low temperatures down to 20 K. The difference in the low T phases is well classified in terms of the atomic radius of M elements, which indicates that the space inside the M12 icosahedron plays dominant role in the superstructure formation.

1. C.P. Gomez *et al*., Phys. Rev. B, **68**, 024203 (2003).
2. R. Tamura *et al*., Jpn. J. Appl. Phys., **41** (2002) L524.
3. R. Tamura *et al*., J. Non-Cryst. Solids, **334**&**335** (2004) 173.

P02-21

Structural properties of Cd_6M(M=Er,Ho,Lu) approximants

T.Sato, M.Muraki, K.Nishimoto,and R.Tamura

Dept. of Mater. Sci. & Tech., Tokyo Univ. of Sci, Noda, Chiba, 278-8510, Japan

Cd_6M approximants (M = Ca, rare earth) are described as bcc packing of an icosahedral cluster called Tsai-type cluster [1]. In 2002, a low-temperature phase transition was discovered in Cd_6Yb and Cd_6Ca by Tamura et al[2]. The phase transition is interpreted to be due to orientational ordering of Cd_4 tetrahedron located at the center of the icosahedral cluster. Concerning with the transition mechanism, it is expected that the space inside the icosahedral cluster must be large enough in order for ordering of the Cd_4 tetrahedron to occur. Therefore, it is of interest what is the minimum size of the space required for the rotation of Cd_4 tetrahedron responsible for the phase transition. In the present work, we have focused on the Cd_6M (M=Er, Ho, Lu) approximants which have the smallest lattice constants among Cd_6M, having the smallest space inside the icosahedron cluster. The purpose of this study is to obtain insight into the low-temperature behavior of the Cd_4 tetrahedron in terms of the size of the space inside the icosahedral cluster.

Flakes of the constituent elements of Cd (6N), Er (3N), Ho (3N), Lu (3N), with nominal compositions of $Cd_{83.7}M_{16.3}$, were placed inside a stainless steel tube, sealed in a quartz tube under argon atmosphere. The elements were then melted at 1073K for 48h, and annealed at 823K for 100h, followed by quenching or slow cooling. Characterization of the samples was performed by powder X-ray diffraction (XRD) and transmission electron microscopy (TEM). Electrical resistivity measurements were performed by a four probe method in a temperature range between 15 and 300K.

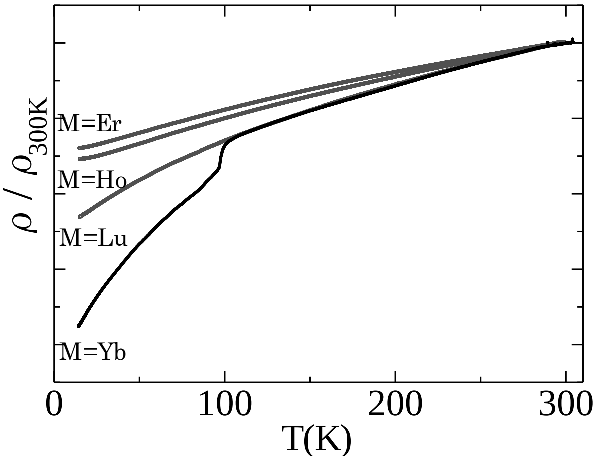

Figure 1 Temperature dependences of electrical resistivity for $Cd_{83.7}M_{16.3}$ (M = Er, Ho, Lu) approximants

Figure 1 shows temperature dependences of the electrical resistivity for $Cd_{83.7}M_{16.3}$ (M = Er, Ho, Lu) and Cd_6Yb. No anomaly is observed for $Cd_{83.7}M_{16.3}$ (M = Er, Ho, Lu) at low temperatures down to 15K, in contrast with the case of other Cd_6M compounds such as Cd_6Yb.

As mentioned above, the these compounds have smallest lattice constants among the Cd_6M type approximants. Therefore, no anomaly in the resistivity suggests that the rotation of the Cd_4 tetrahedron is suppressed due to the lack of the space for orientational ordering of the Cd_4 tetrahedron. [3] Results of other experiments including TEM observations will also be reported in the presentation.

1.Guo J. Q., Abe E.,Tsai A. P.,*Phys.Rev.*B,**62**,22,14605-14608(2000)

2. R. Tamura, *et al.*: *Jpn. J. Appl. Phys.* **41**, L524(2002)

3. K Nozawa *J. Phys.: Condens Matter* **20**,315206(2008)

P02-22

CRYSTAL STRUCTURE OF 2/1 1/0 1/0 Cu-Al-Sc APPROXIMANT

T. Ishimasa[1], A. Hirao[1], T. Honma[1] and M. Mihalkovič[2]

[1] *Graduate School of Engineering, Hokkaido University, 060-8628 Sapporo, Japan*
[2] *Institute of Physics, Slovak Academy of Sciences, 84228 Bratislava, Slovakia*

An approximant is a periodic structure consisting of the same local structural unit as in the corresponding quasicrystal. In the case of Tsai-type icosahedral quasicrystal such as Zn-Mg-Sc, two kinds of cubic approximants have been reported. They are 1/1 and 2/1 approximants. Both approximants include characteristic triple shell structure named Tsai-type cluster. In the case of Zn-Sc alloy, it consists of the first dodecahedron of Zn, the second icosahedron of Sc, and the third icosidodecahedron of Zn. The cluster further includes disordered four Zn atoms inside the first shell. In this presentation, crystal structure of a 2/1 1/0 1/0 approximant recently discovered in the Cu-Al-Sc system will be reported. In this system the presence of the icosahedral quasicrystal with $a_{6D} = 6.959$ Å was already reported at the alloy composition $Cu_{46}Al_{38}Sc_{16}$ [1].

An alloy specimen of $Cu_{47.0}Al_{37.5}Sc_{15.5}$ was made using an arc furnace. The specimen was re-melted at 1023 ºC and cooled to 340 ºC for 50 h. Powder X-ray diffraction experiment was performed at the beam line BL02B2 at SPring-8. The Rietveld analysis was carried out using the program RIETAN2000 developed by F. Izumi [2].

Since powder data themselves do not provide sufficient information to determine the structure without good starting model, we have performed search for optimal structure using solely cell parameters, and realistic pair interactions fitted to the ab-initio data, using so called "cell constrained melt-quenching technique" described in more detail in [3]. The resulting structure with the space group *Cm*2*m* has been then successfully used in final Rietveld refinement. The refinement indicated apparent presence of additional mirror plane normal to the *b*-axis.

The space group of the final model is *Cmmm*. The lattice parameters are $a = 8.3579$ Å, $b = 21.9855$ Å, $c = 8.3200$ Å, and the unit cell includes 51.6 Cu, 36.4 Al and 16.0 Sc atoms. The following characteristics of the structure indicate that it belongs to a new crystal type.

1. The lattice parameters both *a* and *c* can be related as 1/0 to the 6-dimensional lattice parameter of the icosahedral quasicrystal $a_{6D} = 6.959$ Å, and *c* as 2/1.
2. Framework of the structure is constructed by the arrangement of Sc atoms. Twelve Sc atoms form an icosahedron with the size just coincide to the lattice parameters *a* and *c*. This icosahedron corresponds to the second shell of the Tsai-type cluster.
3. In each Sc icosahedron, deformed dodecahedron of Cu and Al atoms is present. The dodecahdron further includes 6 atoms being mainly Cu, which form a small octahedron. This regular local structure is different from the disordered one in the 1/1 cubic approximant of the Tsai-type.
4. Along the *c*-axis a layer consisting of two kinds of polyhedra, namely an octahedron and a special polyhedron, is sandwiched between two layers of the icosahedra.

[1] T. Honma and T. Ishimasa, Phil. Mag. **87** 2721 (2007).
[2] F. Izumi and T. Ikeda, Mater. Sci. Forum **321**/**324** 198 (2000).
[3] M. Mihalkovič , M. Widom and C.L. Henley, in this abstract book.

THREE DIMENSIONAL RECONSTRUCTION METHOD OF ICOSAHEDRAL QUASICRYSTALS BY BINARY DISCRETE TOMOGRAPHY

Yukinori Ishibashi[1], Hiroto Sugiura[1], Koh Saitoh[2], and Nobuo Tanaka[2]
[1]*Department of Crystalline Materials Science, Nagoya University, Nagoya 464-8603, Japan*
[2]*EcoTopia Science Institute, Nagoya University, Nagoya, 464-8603, Japan*

Electron tomography is widely used as a technique for observing three-dimensional structures of materials. The method conventionally requires a large number of projection images with tilting a sample in steps of 1-2° around one or two tilt-axes to reconstruct the three-dimensional object function. A spatial resolution of this technique is 1 nm at most, which is insufficient for reconstructing three-dimensional structure with atomic resolution.

A noble method to reconstruct a three-dimensional atomic arrangement of crystals was reported by Van Aert. The method, *discrete tomography*, treats crystals as discrete sets of atoms and determines the existence of the atom on each lattice point using only zone-axis projections, where individual atoms are observed separately. The application to the gold nano-particles was reported1). Recently, a mathematical study of the discrete tomography for the quasiperiodic structures was reported2). The discrete tomography requires the correlation of the number of atoms in the projection direction and image intensity accurately. This requirement is not always maintained in actual experimental images, which contains statistical errors.

In the present study, we propose a new approach of a three dimension reconstruction of icosahedral quasicrystals on the basis of discrete tomography. In this technique, the presence of the lattice point is determined. First, experimental images are binarized by a certain threshold. Then, the voxels are filled by using back projection. A quasiperiodic system composed of 6311 atoms was used to test the present reconstruction method. It was found that by using 31 projection images, all the 6311 lattice points are reconstructed. The reconstructed lattice points are lifted up to six-dimensional space and projected to the internal space, which shows a characteristic feature of the phason.

1) S. Van Aert, P. Geuens, D. Van Dyck, C. Kisielowski, J.R. Jinschek, *Ultramicroscopy* 107(2007)551
2) Christian Huck, *Acta cryst*, A65(2009)240

Poster Session 3

Mathematical aspects

Monday, June 14, 2010

P03-01

CHIRAL PINWHEEL TYPE TILINGS WITH SINGULAR CENTRE

Reinhard Lück[1]

[1] *Weilstetter Weg 16, D-70567 Stuttgart, Germany*

Self-similar tilings with singular centre and rotational symmetry were designed for studies of colour groups [1]. Chiral pinwheel tilings were derived similarly. The pinwheel tiling is well known and discussed in the literature (see [2]). It is defined by a substitution process. The singularity is introduced as a global rotational centre and is represented by an 'unoccupied' central area. The vertex configurations and their change during the substitution process were studied in order to guarantee that no ‘forbidden’ vertex configurations are needed for the construction. The size of this central area of the singularity is shrinking during the substitution process. Several examples based on the pinwheel tiling will be presented and generalized pinwheel tilings with singular centre and rotational symmetry without ‘forbidden’ vertices will be characterized. Possible colour symmetries of these tilings will be discussed.

[1] R. Lück, Proc. Aperiodic'09 (accepted).
[2] D. Frettlöh, E. Harris,
http://tilings.math.uni-bielefeld.de/substitution_rules/pinwheel

P03-02

TILINGS WITH GLOBAL ROTATIONAL SYMMETRY BASED ON PENROSE RHOMBI

Reinhard Lück[1]

[1] *Weilstetter Weg 16, D-70567 Stuttgart, Germany*

Penrose rhombi are well known from the Penrose pattern, the thick ones are formed by 72° and the thin ones by 36°. The Penrose patterns allow only an almost global tenfold pattern with a decagon at the centre which is usually termed cartwheel pattern. However, Penrose rhombi form tilings with global tenfold symmetry; necessarily the central star is represented by ten thin rhombi. Several tilings of this kind have been listed previously [1]. A study of some acceptance domains was performed by Scheffer [2]. Unfortunately, a pattern grown by substitution with the linear scaling factor of τ^3 (τ is the Golden Mean) described by Warrington [3] was not taken into account. All these tilings are characterized by a shift in internal space of $\gamma = 1/2$. The tilings will be compared considering the patterns, the acceptance domains, substitution rules and other properties. Colouring of these patterns is possible without essential differences.

[1] R. Lück, Phil. Mag. 88 (2008) 2049-2058.
[2] M. Scheffer, Ph. D. thesis, Stuttgart University, 1998.
[3] D.H. Warrington, Quasicrystalline Materials, Eds. Ch. Janot, J.M. Dubois, World Scientific, Singapore, 1988, pp. 243-254.

SEMI-PERFECT COLORINGS OF HYPERBOLIC TILINGS

Glenn R. Laigo, Beaunonie R. Gozo, Jr. and Ma. Louise Antonette N. De Las Peñas

Mathematics Department, Ateneo de Manila University, Quezon City, Philippines

The discovery of quasicrystals generated interest in the study of colorings exhibiting non-periodic color symmetries such as 5-, 8- and 12-fold rotations. While these symmetries are abundant among tilings in the hyperbolic plane, colored hyperbolic tilings are still not widely studied. One of the problems being dealt with in previous works is deriving a systematic approach in arriving at colored symmetrical hyperbolic patterns.

In [1], a framework has been established to obtain perfect colorings of hyperbolic semi-regular tilings. By a perfectly colored hyperbolic tiling, we mean that all the elements of the symmetry group *G* of the uncolored tiling permute the colors of the tiling. In this paper, we extend the method to construct semi-perfect colorings of hyperbolic tilings. A coloring of a hyperbolic tiling is semi-perfect if the group *H* of symmetries that induce a permutation of the colors in the colored tiling is a subgroup of *G* of index 2.

We illustrate the method by enumerating the semi-perfect colorings of the semi-regular 8·5·8·5 tiling on the hyperbolic plane using up to ten colors. This tiling is interesting since it exhibits 5- and 8-fold symmetries not seen in Euclidean periodic patterns.

[1] De Las Peñas, M.L.A.N.; Felix, R.P.; Laigo, G.R.: Colorings of hyperbolic plane crystallographic patterns. Z. Kristallogr. **221/10** (2006) 665-672.

P03-04

Presented as S09-01

P03-05

CANCELED

P03-06

DIFFRACTION OF LIMIT PERIODIC POINT SETS

Michael Baake[1] and Uwe Grimm[2]

[1] *Fakultät für Mathematik, Universität Bielefeld, Postfach 100131, 33501 Bielefeld, Germany*
[2] *Department of Mathematics and Statistics, The Open University, Walton Hall, Milton Keynes MK7 6AA, UK*

The kinematic diffraction measure of a point set is the Fourier transform of its natural autocorrelation, provided the latter exists. In general, the diffraction measure may contain pure point, singular continuous and absolutely continuous components with respect to Lebesgue measure. Lattice periodic and quasiperiodic measures are examples of structures with a pure point diffraction measure, supported on a finitely generated module of points.

Limit periodic point sets are aperiodic structures with pure point diffraction which are characterised by a countably, but not finitely generated Fourier module. Examples are cut and project sets with p-adic internal space. We illustrate this by presenting explicit results for the diffraction measures of two examples with 2-adic internal space. The first, well-known example is the period doubling chain in one dimension, based on the period doubling substitution rule. The second example is a planar point set derived from the chair tiling in the plane, which can be described as a fixed point of a block substitution rule.

APERIODIC STRUCTURES, ORDER AND DISORDER

S.I. Ben-Abraham[1] and A. Quandt[2]

[1] *Department of Physics, Ben-Gurion University, IL-84105 Beer-Sheba, Israel*
[2] *Department of Physics, Ernst-Moritz-Arndt Universität, D-17487 Greifswald, Germany*

The motivation of this research is twofold: (1) Artificial aperiodic structures, such as quasiregular heterostructures, have been the subject of intensive research activities. Considerable progress has been achieved in recent years, where some of the most promising physical realizations of structures are photonic or phononic meta-materials. It turns out that the fabrication of such structures is mostly governed by algorithms based on substitution sequences. (2) The commonplace notions of "order" and "disorder" are heavily context-dependent and rather subjective. Even though in most cases their meaning might be more or less clear, they are, in fact, not defined at all.

In order to gain more insight into these fundamental issues, we undertook a study of double-sided substitution sequences and their multidimensional generalizations. Here we present double-sided versions of the Fibonacci (F), Prouhet-Thue-Morse (PTM), paperfolding (PF), period doubling (PD) and Golay-Rudin-Shapiro (GRS) sequences, as well as their two-dimensional counterparts (except for F whose two-dimensional representatives are the well known Penrose tilings). The main topic of our analysis is their degrees of order vs. disorder. A rough measure is the topological entropy, but better insight might be provided by the symbolic complexity. While in the 1D case these concepts for F, PTM, PF, PD and GRS are well known, virtually nothing is known about their 2D counterparts. Therefore we try to quantify the rectangle complexity of PTM, but we also mention some aspects of the corresponding lattice-animals (polyominoes) complexity. Finally we want to suggest a definition for the entropy of multidimensional structures. It leads us to conjecture that the entropy of 2D PTM is ln2 (at least in the present version). And irrespective of future refinements, $\ln 2$ may certainly be considered to be a safe upper entropy bound.

P03-08

APPLICATION OF THE AVERAGE UNIT CELL CONCEPT TO THE 3D APERIODIC AMMAN TILING

P. Kuczera, R. Strzałka, J. Wolny

Faculty of Physics and Applied Computer Science, AGH – University of Science and Technology, Krakow, Poland

Amman tiling is a 3D generalization of the Penrose tiling. It consists of two kinds of structure units: prolate and oblate equilateral rhombohedra. All faces of the structure units are identical rhombuses. The ratio of the face diagonals is equal to τ, and the acute angle amounts to atan(2) = 63.44^{o}. The volume ratio of the unit tiles as well as the ratio of their frequencies in the Amman tiling is also equal to τ. Amman tiling reveals an icosahedral symmetry, thus it can be used as a quasilattice for building a model of an icosahedral quasicrystal.

One can generate the set of points of the Amman tiling by projecting a 6D hypercubic lattice via 3D window – the so called atomic surface. In case of the Amman tiling the atomic surface has the shape of a rhombic triacontahedron.

We present a derivation of the structure factor of the Amman tiling on the basis of the average unit cell concept [2], which allows a structure factor calculation in 3D physical space only. This method is similar to the one used for a successful structure refinement of the decagonal basic Ni-rich Al-Ni-Co phase [3,4].

Any point of the Amman tiling can be written in the so called reference lattice: $r_i = p_i \cdot \alpha_i + u_i$, $\alpha_i = 2\pi/k_i$, where: $i = x,y,z$, p_i is an integer, α_i is a reference lattice constant for a given direction and u_i is a position in the reference lattice. The reference lattice constant is related to a scattering vector k_i, which is observed in the diffraction pattern. The position distribution of Amman tiling points $P(u_x,u_y,u_z)$ is called an average unit cell. Because of the aperiodicity of the Amman tiling the distribution $P(u_x,u_y,u_z)$ should be related to another one $P(v_x,v_y,v_z)$, whose lattice constants are elongated by τ. A 6D distribution $P(u_x,u_y,u_z,v_x,v_y,v_z)$ is only nonzero along lines: $v_i = -\tau^2 u_i$, This is a characteristic feature of quasicrystalline lattices. One can show that there is a linear relation between the shape of the distribution $P(u_x,u_y,u_z,v_x,v_y,v_z)$ and the shape of the atomic surface. A structure factor for any scattering vector can be calculated as a Fourier transform of this distribution. It is important to notice, that because of the characteristic relation between v_i and u_i, the Fourier transform actually reduces to a 3D integral.

[1] Levine D., Steinhardt P. J. *Phys. Rev.* B **34** (1986) 596-616.
[2] Wolny J. *Phil. Mag.* **77** (1998) 395-412.
[3] Wolny J., Kozakowski B., Kuczera P., Takakura H. *Z. Kristallogr.* **223** (2008) 847-850.
[4] Kuczera P., Kozakowski B., Wolny J., Steurer W. *JPCS* (2010)- in print.

P03-09

A LONG-RANGE ORDER FOR GROWING PERFECT QUASI-CRYSTALLINE FORMATIONS

R. Al Ajlouni[1]

[1] *Department of Architecture, Texas Tech Univ., Lubbock, TX 79409-2091, USA*

Since their discovery, the unique structural signature of quasicrystals has posed a perplexing puzzle. While significant progress has been made in determining their physical properties, a deeper understanding of the structure of quasicrystals at an atomic scale remains an open question. To date, no available structural model has been successful in describing the long-range transitional and rotational order of quasicrystalline formations. Available structural models depend heavily on local rules, and hence they cannot explain the global quasiperiodic order.

In this paper, I present a global multi-level hierarchical framework that is able to describe the long-range transitional and orientational order of the global empire pertaining to Perfect Penrose Tiling (PPT) models of quasicrystal growth. In this order, the global empire is constructed of infinite levels of hierarchical clusters. Any cluster level, in this hierarchy, is composed of four smaller building clusters; two highly symmetrical clusters and their two fragments. Cluster configurations and the geometric arrangements of the multi-level clusters are determined entirely by a geometric progression of framework of nested decagrams. I further demonstrate the use of this framework to construct the global empires of two types of PPTs to produce an infinite and defect-free covering of the two-dimensional plane (fig.1). The proposed model suggests that the position of atoms, locally and globally, is defined by one global framework, and not tiled based on local rules (matching or overlapping, etc). In this way, quasicrystal formations can grow rapidly ad infinitum without the need for any defects or mismatches.

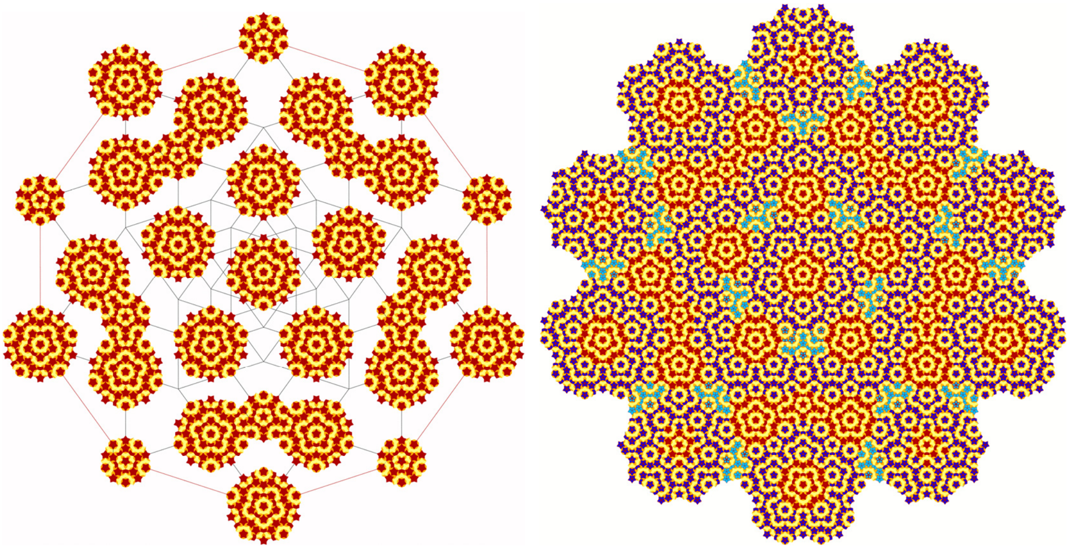

Fig. 1.Constructing the empire of on type of Perfect Penrose Tile.