low temperatures [4].

In the present work, we have prepared Cd_6R single grains by a self-flux method and have measured their physical properties such as electrical, thermal and magnetic properties. We have also performed high-magnetic field measurements up to ~50 Tesla at low temperatures down to 1.3 K.

For most of Cd_6R compounds, the magnetic susceptibility is found to obey the Curie-Weiss law, say, above 50 K, indicating that R atoms at the vertices of the R_{12} icosahedron are well localized in a trivalent state. At low temperatures, heat capacity exhibits peaks attributed to occurrences of long-range magnetic orders. In Cd_6Tb, measurements under high-magnetic field show two clearly meta-magnetic transitions below 10 Tesla. This result suggests that several magnetic states are nearly degenerate at low temperatures. Detail of the physical properties of Cd_6R will be discussed in the presentation.

[1] C. P. Gómez, S. Lidin, *Physical Review B* **2003**, *68* ,024203. [2] R. Tamura, Y. Murao, S. Takeuchi, M. Ichihara, M. Isobe, Y. Ueda, *Japanese Journal of Applied Physics* **2002**, *part 2 41*, L524. [3] R. Tamura, Y. Muro, T. Hiroto, K. Nishimoto, T. Takabatake, *Physical Review B* **2010**, 220201(R). [4] S. Ibuka, K. Iida, T. J. Sato, *Journal of Physics : Condensed Matter* **2011**, *23*, 056001.

Keywords: quasicrystal, magnetism

MS63.P09

Acta Cryst. (2011) A**67,** C625

Synthesis of single-grained $Zn_{88}Sc_{12}$ quasicrystal and its electrical resistivity

Keita Noguchi, Simpei Kawanishi, Kazue Nishimoto,Ryuji Tamura, *Dept. of Mater. Sci. & Tech., Tokyo University of Science, Noda,Chiba 278-8510, (Japan).* E-mail: j8210639@ed.noda.tus.ac.jp

$Zn_{88}Sc_{12}$ icosahedral qusicrystal (iQC) has recently been discovered by Canfield et al.[1] It is a stable binary iQC and is expected to contain no chemical disorder. An interesting feature about the iQC is that two different shapes, i.e., morphologies, of single grains are obtained depending on the initial composition, the reason of which has not been understood[1]. In this study, we have prepared $Zn_{88}Sc_{12}$ single grains and investigated the electrical properties of the $Zn_{88}Sc_{12}$ single grains having two different morphologies.

Single-grained $Zn_{88}Sc_{12}$ quaicrystals were prepared using a self-flux method. Pure elements of Zn(6N) and Sc(3N) with initial compositions of $Zn_{100-X}Sc_X$ with X in the range between 1.5 and 4 were placed in an alumina crucible, sealed inside a quartz tube under argon atmosphere. The elements were melted at 860° C for 3h, and slowly cooled to 490～500 ° C . Then, single grains were separated from the melt using a centrifuge. The obtained grains are found to exhibit two types of growth morphologies as reported[1] depending on the initial composition; PD(Pentagonal Dodecahedron)-shaped grains were obtained for the initial compositions of $Zn_{96}Sc_4$, $Zn_{97}Sc_3$, $Zn_{97.5}Sc_{1.5}$, while RT(Rhombic Triacontahedron)-shaped grains were obtained for the initial compositions of $Zn_{98}Sc_2$ and $Zn_{98.5}Sc_{1.5}$.

Temperature dependences of the electrical resistivity ρ(T) are found to be almost the same for all the grains, exhibiting a negative temperature coefficient, which is a typical behavior of ternary iQCs. We note that the PD-shaped grains exhibit slightly higher values of the resistivity ratio ρ_{16K}/ρ_{290K} than the RT-shaped grains. In the presentation, the results on annealed grains will be also discussed.

[1] P.C. Canfield, et al., *Phys. Rev.* **2010,** *B81*, 20201.

Keywords: quasicrystal

MS63.P10

Acta Cryst. (2011) A**67,** C625

Dislocation mobility in icosahedral quasicrystals

Galina N. Lazareva, Alexander S. Bakai *National Science Center "Kharkov Institute of Physics and Technology"-Kharkov (Ukraine).* E-mail: g_lazareva@kipt.kharkov.ua

A theoretical description of the dislocation motion in quasicrystals is developed. The hydrodynamic approximation is used in deriving the expression for dissipation losses of a moving dislocation. The continuum theory of dislocation mobility [1] and the dynamic equations of elastic and phason fields [2] are combined. Hence the dependence of dislocation mobility on vacancy concentration is found explicitly [3,4]. The numerical analysis of dislocation mobility shows that phason deformations make the major contribution to the drag of free dislocations in icosahedral quasicrysal Al-Pd-Mn. The influence of vacancies on dislocation mobility becomes noticeable only at very large vacancy concentration, $C_v > 10^{-3}$, and at very low dislocation velocity, $v_D < 10^{-8}$ cm/s.

The study of existing experimental data reveals the considerable contribution of mutual pinning of dislocations to their mobility in icosahedral quasicrystal. The expressions obtained for dislocation mobility are valid for temperatures close to the melting temperature since the role of mutual pinning decreases with the increase of temperature. Dislocation drag on pinning centers has a dominant role at lower temperatures.

[1] T.C. Lubensky, S. Ramaswamy, *Phys. Rev. B* **1986**, *33, 11*, 7715. [2] Sh. Kh. Khannanov, *The Physics of Metals and Metallography* **2002**, *93*, *5*, 397. [3] A. S. Bakai, G.N. Lazareva, *Metallophysika i Noveishie Technologii* **2008**, *30*, *12*, 1681-1700 (in Russian). [4] G.N. Lazareva, A.S. Bakai, *J. Phys.: Condens. Matter* **2009**, *21*, 295401.

Keywords: quasicrystal, dislocation, mobility

MS63.P11

Acta Cryst. (2011) A**67,** C625-C626

Structural characterization of thin AlPdRe quisicristalline film formation during annealing process

A. Yu. Seregin,[a,b] I. A. Makhotkin ,[a,c] S .N. Yakunin ,[a,b] D. S. Shaitura,[b] M. B. Tsetlin,[b] E. Yu. Tereschenko,[a] M.V.Kovalchuk,[a,b] [a]*Institute of Crystallography RAS, Moscow.* [b]*Russian Research Centre Kurchatov Institute, Moscow (Rusia).* [c]*FOM Institute for Plasma Physics Rijnhuizen, Nieuwegein, (The Netherlands).* E-mail: seregin.a83@gmail.com

One of the possible ways to form ultrathin $Al_{70}Pd_{20}Re_{10}$ quasicristalline film is the annealing of 3-layer (Al/Pd/Re) structure. Layer-by-layer ion-plasma deposition allows forming thin quasicrystalline film with precisely controlled thickness and homogeneity. Deposition was performed in a vacuum system with a sputtering chamber in the form of a Penning cell by Kr assisted magnetron sputtering from separate pure materials targets. After deposition of a layered structure, the films were coated with a layer of aluminum oxide, which was formed by sputtering of aluminum in a krypton atmosphere with addition of oxygen. The aluminum oxide layer was deposited to prevent selective escape of elements from the film upon vacuum annealing. The concentration range for the films prepared coincided with the known range of quasicrystalline phase formation in bulk samples [1].

We have studied phase evaluation of Al/Pd/Re layered structures in-situ during heat treatment and layer intermixing on intermediate annealing steps ex-situ. In-situ phase evolution study was done with X-ray diffraction and ex-situ layers intermixing analysis was done with

grazing incidence X-ray standing waves technique [2].

Samples under examination were studied stratified Al/Pd/Re structures with layer thicknesses 30/8/3 nm correspondently. Layer thicknesses were controlled by numerical modeling combined with ex-situ calibrations. As a substrate we used super polished sapphire. Order of layers were selected as substrate- Pd-Al-Re to inctear contrast of X-ray standing waves All samples were covered with 10 nm Al_2O_3 layer to prevent oxidation of top layer.

All experiments were done on KMC-2 station BESSY-II synchrotron radiation source. For in-situ phase ID analysis samples were annealed in the high vacuum oven with beryllium dome and tilted for 0.7 degree with respect to the x-ray beam. Diffracted radiation was measured using 2D CCD detector. Samples were heated up to 700 degrees C with the speed 5 degrees per minute then annealed during 1 hour and then cooled down with the speed 10 degrees per minute. Diffraction patterns were detected every 2 seconds. For intermediate layer intermixing study samples were similarly heated and annealed at 250˚C, 300˚C, 350˚C, 450˚C, 550˚C, 650˚C and 700˚C.

We have found that ultrathin quasicrystalline film is formed in 3 steps. At first step at 350˚C forms homogeneous polycrystalline Al_3Pd layer, while Re layer remains separate. Second, between 450 and 680˚C Al_3Pd phase transforms into AlPd phase. At this step Re starts to diffuse into Al-Pd layer. Finally homogeneous Al-Pd-Re intermixed layer forms at 700˚C and with major icosahedra *i*-$Al_{70}Pd_{20}Re_{10}$ quasicristalline phase. First indication of Quasicristalline phase formation was detected at 680˚C.

This work was supported by RFBR grant № 08-02-01393a.

[1] A.D. Bianchi, F. Bommeli, M.A. Chernikov, et al., *Phys. Rev. B*: *Condens. Matter Mater. Phys*.**1997**, *55*, 5730.[2] M.V. Kovalchuk, S.I. Zheludeva, N.N. Novikova et al., *J. Appl. Cryst*. **1997**, *30*, 833-838.

Keywords: quasicrystals, X-ray, in-situ

MS63.P12

Acta Cryst. (2011) A**67,** C626

Multiple diffraction in icosahedral and decagonal quasicrystal

Changzeng Fan, Thomas Weber, Walter Steurer, *Laboratory of Crystallography, ETH Zurich, Zurich (Switzerland).* E-mail: changzeng.fan@mat.ethz.ch.

Multiple diffraction (MD) may be stimulated if more than one set of atomic planes of a crystal are simultaneously in reflection position. When a sample rotates around the diffraction vector of the main reflection and brings another reciprocal lattice point (the so called *simultaneous* or *operative* reflection) onto the surface of the Ewald sphere, the diffracted beam of the primary reflection may also serve as an incident beam for the operative reflection. As a consequence the total amount of intensity will be redistributed among both of them.

Because of the presence of a dense set of Bragg reflections MD is thought to be omnipresent in diffraction experiments with quasicrystal. Accurate measurement of weak Bragg intensities is expected to be heavily affected by MD. To reveal its influence on quasicrystal structure analysis, MD effects in an icosahedral Al-Cu-Fe quasicrystal [1] and in a basic Co-rich decagonal Al-Co-Ni quasicrystal [2] were studied with synchrotron radiation. The high flux available at the beam line SNBL at ESRF, Grenoble allows large-angle ψ-scans within a reasonable time: 10º and 40º ψ-scans (step size 0.01º) were performed for the reflections from *i*-$Al_{64}Cu_{23}Fe_{13}$ and for from *d*- $Al_{72.5}Co_{18.5}Ni_{9}$., respectively. To compensate for small misalignments a 0.5º ω-scan was performed at each ψ−position. From the ω-ψ-scan patterns, several *Umweganregung* peaks could clearly be observed. Figure 1 illustrates the intensity variation of the primary reflection during such wide ψ-scans at one selected peak from *d*-$Al_{72.5}Co_{18.5}Ni_{9}$.

Either the individual MD peak or the MD events in a full data set has been simulated by the kinematical approach. Preliminary results reveal that the amount of weak reflections affected by MD effects during the collection of a full data set is on the same level as those of outliers recognized in a standard data reduction, however, the data quality of the data sets is not seriously biased by the MD effects.

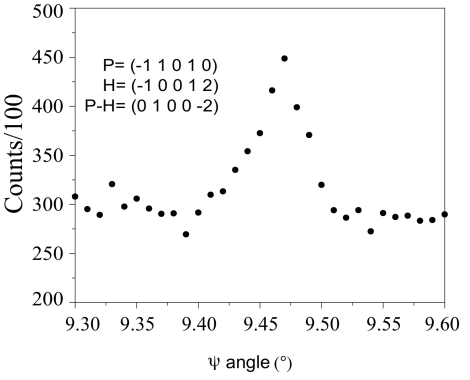

Fig.1 Intensity of a weak reflection $\bar{1}1010$ for *d*-$Al_{72.5}Co_{18.5}Ni_{9}$ as a function of the ψ angle

[1] C.Z. Fan , Th. Weber, S. Deloudi, W. Steurer *Phil. Mag.* **2010,** iFirst, DOI: 10.1080/14786435.2010.512577. [2] A. Strutz, A. Yamamoto, W. Steurer *Physical Review B* **2009**, *80*, 184102-1-9.

Keywords: multiple diffraction, quasicrystals

MS63.P13

Acta Cryst. (2011) A**67,** C626

Localization of current states in one-dimentional aperiodic structures

P.Yu. Korotaev, Yu.Kh. Vekilov, N.E. Kaputkina, *Department of theoretical physics and quantum technologies, Moscow Institute of Steel and Alloys "MISiS", Moscow (Rusia).* E-mail: pvl.korotaev@gmail.com

In periodic one-dimentional atomic structures the current states are impossible. Even the small perturbation leads to localization of electrons [1]. We show that this is not so in some aperiodic structures. For this purose the sequences of quantum dots (QDs) were considered (the QDs can be considered as the artificial atoms, and it is easy to influence on their electronic specta by realistic external fields [2]). As an example the sequence of GaAs and isles of its solid solution $Al_xGa_{1-x}As$ and $In_xGa_{1-x}As$ where x=0.1–1 was considered as sequence of QDs. The energy spectra and transport of electronic excitations in one-dimensional aperiodic sequences of QDs of Thue-Morse and double-periodic type were studied. The influence of the external magnetic field and electric field on energy spectra and transport were studied. For aperiodic sequences of quantum dots the influence of relatively small magnetic and electrical fields is essential (about several Tesla or V/cm), but localization occurs at the finite values of perturbations. The transmission coefficient was determined in quasiclassical approximation taking into account the Coulomb blockade. The resonance tunneling was studied. It takes place when electronic energy levels in neighbor quantum dots are aligned by external fields .

[1] N.F. Mott, W.D. Twose, *Adv. Phys.* **1961**, *10*, 107. [2] P. Yu. Korotaev, N.E. Kaputkina, Yu.E. Lozovik, Yu. Kh. Vekilov, *Journal of Experimental and Theoretical Physics* **2011**, *140(1)*

Keywords: aperiodic sequence, quantum dot, localization