

was used for the modelling process, was calculated using a statistical method [1], which allows a purely 3-dimensional, real space optimization of a quasicrystalline structure. Such an approach has already been successfully used for structure refinement of various modifications of the Al-Ni-Co quasicrystal [2], [3], [4]. This is the very first attempt of quantitative structure optimization of Al-Cu-Ir and Al-Cu-Rh quasicrystals based on high resolution, synchrotron diffraction datasets. Up to now the only structure investigation of an Al-Cu-Rh quasicrystal was based on electron microscopy, the structure of the Al-Cu-Ir quasicrystal has not been studied before and the Al-Cu-Co structure was refined only based on a rather limited, in-house diffraction dataset. The current refinement gives much more details about the structure.

All three decagonal phases show  $\sim 4$  Å periodicity (two atomic layers per period). Their space group is centrosymmetric  $P10_3/mmc$ . While the Al-Cu-Co phase shows a significant amount of diffuse scattering in the interlayers of the diffraction pattern, the Al-Cu-Ir and Al-Cu-Rh phases exhibit no diffuse scattering. This fact is well-reflected in the structure of Al-Cu-Ir and Al-Cu-Rh phases, *i.e.* they are well-ordered, the Cu/Ir and Cu/Rh positions can clearly be distinguished and the only disorder present is the partial occupation of several Al positions. All decagonal quasicrystals are ternary alloys based on Al and two transition metals. This is the very first structure refinement of a decagonal phase distinguishing the positions of two different transition metal atoms. The initial model for all phases was the same and based on the rhombic Penrose tiling. The initial decoration of the rhombuses was derived based on a structure solution obtained from charge flipping. The refined structure gives reasonable  $R$  values, and the chemical composition agrees well with the EDX measurements.

[1] B. Kozakowski, J. Wolny, *Acta Cryst.* **2010**, *A66* 489-498. [2] J. Wolny, B. Kozakowski, P. Kuczera, H. Takakura, *Z. Kristallogr.* **2008**, *223*, 847-850. [3] P. Kuczera, B. Kozakowski, J. Wolny, W. Steurer, *J. Phys.: Conf. Ser.* **2010**, *226*, 012001. [4] P. Kuczera, J. Wolny, F. Fleischer, W. Steurer, *Phil. Mag.* **2011**, in print.

**Keywords:** decagonal quasicrystal, structure refinement.

## MS.63.5

*Acta Cryst.* (2011) **A67**, C145

### Variable-Range-Hopping Conductivity in Quasicrystals

Yu. Kh. Vekilov, M. A. Chernikov, *Department of Theoretical Physics and Quantum Technologies, National University of Science and Technology "MISIS", Moscow, (Russia)*. E-mail: yuri.vekilov@gmail.com

Among icosahedral phases, including single crystals of icosahedral Al-Pd-Re, the variable-range-hopping (VRH) regime is only revealed in polygrain samples of icosahedral Al-Pd-Re with the resistivity ratio  $R = \rho(4.2 \text{ K})/\rho(300 \text{ K}) \geq 13$ . Experiments show that this regime relates to the presence of defects, voids and inclusions of secondary phases [1, 2]. Here we analyze the low temperature electronic transport in polygrain samples of icosahedral Al-Pd-Re using an analogy with granular electronic conductors. Our preliminary results are given in Ref. 3.

The density of electronic states at the Fermi energy  $N(E_F)$  in icosahedral quasicrystals is nonzero. We therefore consider a model in which metallic quasicrystalline particles of a size ranging from few nanometers to hundreds of nanometers are embedded into an insulating matrix. The electronic levels are discrete due to electron confinement within a single "grain". The mean level spacing  $\delta$  is inversely proportional to the volume  $V$  of the grain  $\delta = 1/[N(E_F)V]$ . For icosahedral Al-Pd-Re  $\delta$  is an order of magnitude higher than for a typical metal.

Two main factors are responsible for the electronic transport in icosahedral Al-Pd-Re. The first is the dimensionless intergranular conductance  $g$ . Samples with  $g \geq 1$  exhibit metallic properties. Samples with  $g \leq 1$  show an insulating behavior. Depending on the structural state of the material and the temperature, both factors may be important. The notion of granular system means  $g \leq g_0$ , where  $g_0$  is the dimensionless intragranular conductance. The homogeneously disordered case corresponds to  $g \approx g_0$ . The second factor is the electrostatic (Coulomb) energy  $E_s \gg \delta$ , which accounts for the change in the energy of a grain when an electron is added or removed. It plays an important role in the insulating regime when electrons are localized in the grains. At low coupling  $g \ll 1$  an electron has to overcome an electrostatic barrier into a neighboring granule. Depending on the structural state and temperature the both factors may be important for the specific behavior of the electrical conductivity. The character of electrostatic disorder defines either the Efros-Shklovskii or the Mott type of the VRH regime primarily with elastic co-tunneling at  $T \leq (\delta \cdot E_s)^{1/2}$ . For icosahedral Al-Pd-Re this temperature is less than 10 K. For strong intergranular coupling, the metallic regime with a power-law temperature variation of the electrical conductivity  $\sigma$  takes place. At low temperatures the temperature-dependent part of  $\sigma$  is dominated by quantum-interference corrections.

The metallurgical reason for the specific behavior of polygrain icosahedral Al-Pd-Re most likely relates to the fact that the icosahedral phase is the primary crystallization phase only for alloys with rhenium content lower than 5 at.%. For icosahedral phase with 8.5 at.% rhenium the primary crystallization phase is  $\text{Al}_3\text{Re}$  that crystallizes in the shape of needles leading to porous ingots with numerous voids.

[1] I.R. Fisher, X.P. Xie, I. Tudosa, C.W. Gao, C. Song, P.C. Canfield, A. Kracher, K. Dennis, D. Abanoz, M.J. Kramer, *Philos. Mag. Lett.*, **2002**, *82*, 1089. [2] J. Dolinšek, P.J. McGuinness, M. Klanjšek, I. Smiljanić, A. Smontara, E.S. Zijlstra, S.K. Bose, I.R. Fisher, M.J. Kramer, P.C. Canfield, *Phys. Rev. B*, **2006**, *74*, 134201. [3] Yu. Kh. Vekilov, M.A. Chernikov, *EPL* **2009**, *87*, 17010.

**Keywords:** electronic, icosahedral, quasicrystal

## MS.64.1

*Acta Cryst.* (2011) **A67**, C145-C146

### Structural basis for the sequential assembly of photosynthetic multienzyme complex

Hiro Yoshi Matsumura,<sup>a</sup> Akihiro Kai,<sup>a</sup> Takayuki Maeda,<sup>a</sup> Masahiro Tamoi,<sup>b</sup> Mika Hirose,<sup>a</sup> Natsuko Kizu,<sup>a</sup> Akira Wadano,<sup>c</sup> Tsuyoshi Inoue,<sup>a</sup> Shigeru Shigeoka,<sup>b</sup> <sup>a</sup>*Graduate School of Engineering, Osaka University, Osaka (Japan)*. <sup>b</sup>*Faculty of Agriculture, Kinki University, Nara (Japan)*. <sup>c</sup>*Hagoromo International University, Osaka (Japan)*. E-mail: matsumura@chem.eng.osaka-u.ac.jp

Protein-protein interactions are likely to be generally important in coordinated regulation of metabolic pathways. In photosynthetic  $\text{CO}_2$  assimilation pathway (the Calvin cycle), such regulation is partially achieved by an intrinsically disordered protein, CP12, which acts as a linker in the sequential assembly of Calvin cycle enzymes glyceraldehyde-3-phosphate dehydrogenase (GAPDH) and phosphoribulokinase (PRK). Both enzymes activities are inhibited when embedded within the GAPDH/CP12/PRK complex. The reversible association/dissociation of the complex are mediated by light/dark transitions, which are responsible for the changes in redox potential and the concentrations of metabolites such as NAD(H) and NADP(H). However, the molecular mechanisms for the sequential multiprotein assembly still remain elusive.

Here we report the crystal structures of GAPDH-CP12 complex and PRK from *Synechococcus elongatus* (Fig. 1). The structure of GAPDH-CP12 complex represents that the C-terminal region of CP12