s3.m12.p3 **X-ray diffraction study of decagonal Al-Co-Ni as a function of composition.** Sergiy Katrych and Walter Steurer, *Laboratory of Crystallography, Department of Materials, ETH Zurich, CH-Zurich, Switzerland. E-mail: walter.steurer@mat.ethz.ch*

Keywords: Decagonal quasicrystal; X-ray diffraction

The evolution was studied of structural order/disorder phenomena across the wide stability field of the decagonal phase in the system Al-Co-Ni. Full single-crystal X-ray diffraction data sets were collected of 31 samples annealed at 900°C. Based on reciprocal space reconstructions [1, 2] of the imaging-plate-scanner data, the variation in Bragg as well as in diffuse scattering is discussed in detail. The samples were also by powder X-ray diffraction. The all obtained data are in good agreement with the known phase diagram investigations [3-7]. The (quasi)lattice parameters vary smoothly over the stability range of decagonal $Al_{71.5}Co_{28.5-x}Ni_x$ ($8 \leq x \leq 20$). The composition dependence $a(x_{Ni})$ can be described by the linear function $a(x_{Ni}) = 3.8435 - 0.406x_{Ni}$ Å with x_{Ni} the Ni concentration. The smaller parabolic composition dependence $c(x_{Ni})$ follows a polynomial of second order $c(x_{Ni}) = 3.9943 + 1.113x_{Ni} - 3.2773x_{Ni}^2$ Å. The quasi-unit cell volume $V = a^2c\sin(3\pi/5)$ shows a linear dependence dominated by that of a: $V(x_{Ni}) = 57.2016 - 10.753x_{Ni}$ Å^3. A smooth variation is also observed for the diffuse scattering related to the ≈8 Å superstructure. These observations indicate a continuous ordering process at 900°C from the basic Co-rich phase via the type II and type I superstructures to the basic Ni-rich phase.

The substitution of Co by Ni causes complex ordering phenomena of the decagonal phase in the system Al-Co-Ni. At the isothermal section at 900°C five distinct ordering states have been identified, the basic Co-rich and the basic Ni-rich phase which can be indexed on the same reciprocal basis; the Edagawa phase [8], i.e. the superstructure type I (S1+S2) and (S1), a fivefold superstructure in the 5D description; the superstructure type II.

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s3.m12.p4 **Simulation of Disorder Phenomena in Decagonal Quasicrystals.** Miroslav Kobas, Thomas Weber and Walter Steurer, *Laboratory for Crystallography, ETH Zurich, Switzerland. E-mail: miroslav.kobas@mat.ethz.ch*

Keywords: Quasicrystal; Disorder; Simulation

The decagonal quasicrystal with nominal composition $Al_{70}Co_{12}Ni_{18}$, the so-called Edagawa-phase [1], features an extraordinary richness of complex scattering. The view perpendicular to the tenfold axis shows alternating 'Bragg layers' and 'diffuse interlayers'. Bragg layers contain both Bragg reflections and diffuse scattering, while diffuse interlayers contain diffuse scattering only. In the present study, the focus lies on the diffuse scattering inside the Bragg layers. To understand the origin of these diffuse features, simulations of disorder phenomena on different scales and in different dimensions have been performed. In a first approach, the 'cluster' form factors of about 6Å-sized sub-clusters are calculated. The goal of this approach is to identify essential structural building units of the quasicrystal structure. Good agreement with experimental observations are obtained with sub-clusters reported by Saitoh et al. [2]. In a second approach, disorder phenomena of 20-32 Å sized clusters reported in literature [3-6] are simulated. The goal of this approach is to determine local disorder phenomena in the quasicrystal structure. Best agreement with experimental results is achieved with a fivefold orientational disorder of the Abe-cluster [3]. These results are discussed in the framework of electron microscopy studies done by other groups. Especially, links between cluster-models showing *m* symmetry and *5m* symmetry are discussed with regard to plausible disorder phenomena. Furthermore, the influence of some disorder phenomena on the formation of quasicrystalline order is pointed out. In a third approach, disorder related to thermal diffuse scattering (TDS) and phasonic diffuse scattering (PDS) of the Edagawa-phase is calculated [7]. With this technique it is possible to describe complex disorder in three-dimensional space by just a few parameters in five-dimensional space. The goal of this approach is to evaluate the importance of TDS and PDS for the Edagawa-phase. Good agreement with experimental data is achieved and it can be concluded that TDS and PDS constitute the major part of the experimentally observed diffuse scattering inside the Bragg layers. In a next step, the results from these five-dimensional simulations need to be translated into three-dimensional structural information. Combining the results of all approaches will provide insight into the disordered, real structure of the Edagawa-phase. This will be another piece in the puzzle to the comprehension of a real quasicrystal structure.

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