TEMPERATURE DEPENDENCE OF THE 8A SUPERSTRUCTURE IN DECAGONAL Al-Co-Ni PHASES

F. Frey[1] E. Weidner[1] K. Hradil[2] M. de Boissieu[3] A. Letoublon[5] G. McIntyre[4]
[1]Institut F.Kristallographie, LMU Geoscience Dept. Theresienstr.41 MUENCHEN 80333 GERMANY [2]Institut fuer Mineralogie, JM University, Wuerzburg, Germany [3]LTPCM, ENSEEG, St.Martin d'Heres, France [4]ILL, Grenoble, France [5]Lab. de Crist., CNRS, Grenoble, France

Diffraction patterns of decagonal Al-Co-Ni phases show diffuse layers perpendicular to the unique ('periodic') axis. These layers are basically due to a one-dimensional 8 Å superstructure [1]. Purely elastic neutron measurements of a $Al_{72}Co_{16}Ni_{12}$ sample revealed that short-range order (sro) maxima within these layers exhibit a different temperature dependence as compared to a homogeneous diffuse background intensity of the layers [2]. The weak diffuse maxima loose intensity, but remain observable up to 980°C, which is close to the melting point. The diffuse layers are no more detectable above 950°C. The temperature evolution of both phenomena is analyzed in terms of critical power laws. The critical exponents can be interpreted within the following ordering scenario: at very high temperatures the structure has a 4 Å period along the periodic axis. During cooling there is an onset of displacive and/or migrational short-range ordering within the aperiodic layers. This gives rise to the diffuse maxima with 8 Å period. Below 905°C an additional one-dimensional ordering ensues with a freezing of thermal motions along the unique direction. Long-range correlated displacements within columns cause the diffuse layers in the diffraction pattern. Computer simulations of different models are compared to the experimental data.

Refereces
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MONTE CARLO STUDY OF 'ATOMIC SIZE EFFECT' SCATTERING IN DECAGONAL AlCoNi

M. Honal T.R. Welberry
Australian National University Research School of Chemistry Science Road CANBERRA ACT 0200 AUSTRALIA

In addition to sharp Bragg peaks that correspond to correlation lengths of several micrometers many stable quasicrystals show diffuse scattering effects that indicate significant deviations from a perfectly quasiperiodic structure. A feature that became apparent in recent high quality diffraction patterns (cf. Fig. 4 in [1]) is one reminiscent of the so-called 'atomic size effect' scattering common in crystalline alloys. The term originates from static displacements in disordered alloys which are caused by differences in atomic radii. The primary effect on the diffraction pattern is a transfer of intensity from regions on one (e.g. low-angle) side of a line joining prominent Bragg peaks to regions on the other (e.g. high-angle) side, leading to a sharp step in the diffuse background. Using structural information froAFS [2] and Monte Carlo (MC) techniques to study the size effect [3] different model systems have been developed for decagonal AlCoNi. Although experimental diffraction patterns could not be reproduced by simply introducing size effects due to different local structures around Ni and Co, as speculated in [1], our MC studies clearly show that this effect can contribute to the overall appearance of diffuse scattering in different decagonal AlCoNi samples.

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STRUCTURE AND PHASE TRANSITION OF *P*-CHLOROBENZAMIDE DESCRIBED IN THE SUPERSPACE FORMALISM

A. Schoenleber[1] P. Pattison[1,2] G. Chapuis[1]
[1]University of Lausanne Institute of Crystallography BSP - Dorigny LAUSANNE CH-1015 SWITZERLAND [2]Swiss Norwegian Beamline, SNBL/ESRF, PO Box 220, F-38043 Grenoble, France

The superspace formalism cannot only be used to describe incommensurately modulated but also commensurately modulated structures. This particular type of structures is commonly referred to in the literature as superstructure. This approach is illustrated with the structure of p-chlorobenzamide. The molecule of p-chlorobenzamide, C_7H_6ClNO, consists of a benzene ring and an amide group that together form two planar sub-units. The dihedral angle between the two planes formed by the sub-units is about 25°. The room temperature phase can be described as: 1) A three-dimensional supercell structure with three molecules in the asymmetric unit, space group *P*-1. The three molecules show different dihedral angles (19.95(9)°, 33.65(8)° and 29.45(8)°, respectively). 2) A (3+1)-dimensional, commensurate modulated structure with only one molecule in the asymmetric unit, superspace group P-1($\alpha\beta\gamma$) and modulation vector q = (0.333, 0, 0). The variation of the dihedral angle is described by a positional and a temperature parameter modulation of the individual atoms (dihedral angle of the basic structure: 27.79(5)°). Both models reproduce the observations of the X-ray diffraction measurements equally well. The diffraction pattern is characterized by a clear difference in intensity between main and satellite reflections. A reversible phase transition occurs at T = 317 K. The high-temperature (HT) phase contains one molecule in the asymmetric unit, space group *P*-1. The molecular structure of the HT-phase resembles the non-modulated basic structure at room temperature. The physical mechanism of the phase transition can therefore be understood as a loss of modulation at high temperature.

HIGH-TEMPERATURE SYNCHROTRON MEASUREMENTS OF DECAGONAL Al-Co-Ni QUASICRYSTAL POWDERS

C. Soltmann[1] C. Beeli[1] C. Baehtz[2] R. Lück[3]
[1]ETH Zürich Laboratorium Für Festkörperphysik Hpf ZüRICH 8093 SWITZERLAND [2]DESY, HASYLAB, Notkestrasse 85, D-22603 Hamburg [3]MPI für Metallforschung, Seestrasse 75, D-70174 Stuttgart

The goal of our investigations was to correlate structural information with expansion data which is based on dilatometric measurements of Al-Co-Ni quasicrystals by Lück et al. [1]. In addition, indications of high-temperature phase transitions, i.e. the transitions type I $\leftrightarrow$ S1 and S1$\leftrightarrow$ β Ni found by Lück et al. [1], should be revised. For this reason, precise high-temperature synchrotron diffraction measurements were carried out using a new fixed image plate detector system at HASYLAB (Hamburg, F.R.G.).
Al-Co-Ni quasicrystal powders of the composition $Al_{71.5}Co_{13.5}Ni_{15}$ - $Al_{71}Co_{11.5}Ni_{17.5}$, synthesised by arc-melting and subsequent tempering, were sealed in silica glass capillaries under argon atmosphere. The measuring temperature was calibrated accurately with the thermal expansion of sodium chloride [2]. Diffraction patterns were taken in the temperature range 300 K - 1150 K at 0.071 nm. 13 Bragg reflections were selected and fitted in order to determine the quasicrystalline a and c lattice parameters. Based on the lattice parameter data, the thermal expansion of the quasicrystals was calculated. In addition, the temperature ranges of the indicated phase transitions could be characterized accurately. Our high-temperature diffraction measurements enabled to state quantitatively the high-temperature changes of the Al-Co-Ni quasicrystalline lattice.

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