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Transient ordering states in decagonal Al–Co–Ni at temperatures up to 1000 °C

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Abstract

Disordered decagonal quasicrystals with the nominal compositions $Al_{72}Ni_{12}Co_{16}$ and $Al_{72.5}Ni_{11}Co_{16.5}$ were investigated by comparative diffuse neutron (N) and X-ray (X) synchrotron studies, respectively, at temperatures up to 1000 °C. High resolution X-ray measurements reveal peak splitting consistent with a domain structure of 2D qp and 1D qp lamellae. At higher temperatures the strain fluctuations decrease, giving rise to larger areas of the 2D qp and 1D qp domains. In summary, this disordered Al–Co–Ni phase is governed by complex transient ordering states, i.e. twinned lamellar domains of true 2D qc sequences, 1D and periodic domains accompanied by phason straining and phason fluctuations.

Keywords: Transient ordering states; Decagonal Al–Co–Ni; Temperature

1. Introduction

X-ray and neutron diffraction investigations were carried out to contrast a dis- or superorder behaviour in decagonal Al–Co–Ni of the transition metal atoms. The almost isoelectronic Ni and Co atoms differ significantly in their neutron scattering power. The use of an analyser in the neutron experiments allows to separate diffuse scattering contributions of inelastic origin. Different types of diffuse scattering have been reported for decagonal quasicrystals, caused by structural disorder such as phason and phonon type fluctuations [4], chemical disorder, straining and strain fluctuations, intergrowth of domains, e.g. twin domains, 1D quasicrystals, approximant phases, and superordering. In some of the decagonal phases there is an additional superorder along the unique periodic axis, which gives rise to a particular 1D-columnar cluster ordering. (This was also investigated in high-temperature experiments; cf. Frey et al., this conference.). The type and amount of disorder depends on the sample composition, prior history and the temperature. A summary is given in Ref. [1].

2. Experimental

High temperature synchrotron studies were performed with samples $Al_{72.5}Co_{16.5}Ni_{11}$ (Z), and $Al_{72}Co_{16}Ni_{12}$ (T), high temperature neutron work with sample (T). The codes refer to the origin of the samples, cf. [1]. The highest temperature achieved was between 950 and 1000 °C, close to the melting point, which is around 1060 °C (varying with the composition of the sample). At the synchrotron facility HASYLAB-DESY the four-circle diffractometer D3 ($\lambda = 0.7$ Å) was used. The neutron diffraction experiments were carried out at the instrument D10 of the ILL. The cylindrical sample (T) had a height of 15 mm and a diameter of 7 mm, with a mosaic of roughly 1°. At the D10 experiment ($\lambda = 2.36$ Å, in combination with a $\lambda/2$ filter) an analyser was used, set to zero-energy transfer to get rid of possible diffuse scattering of inelastic origin (within the resolution limits of the analyser).

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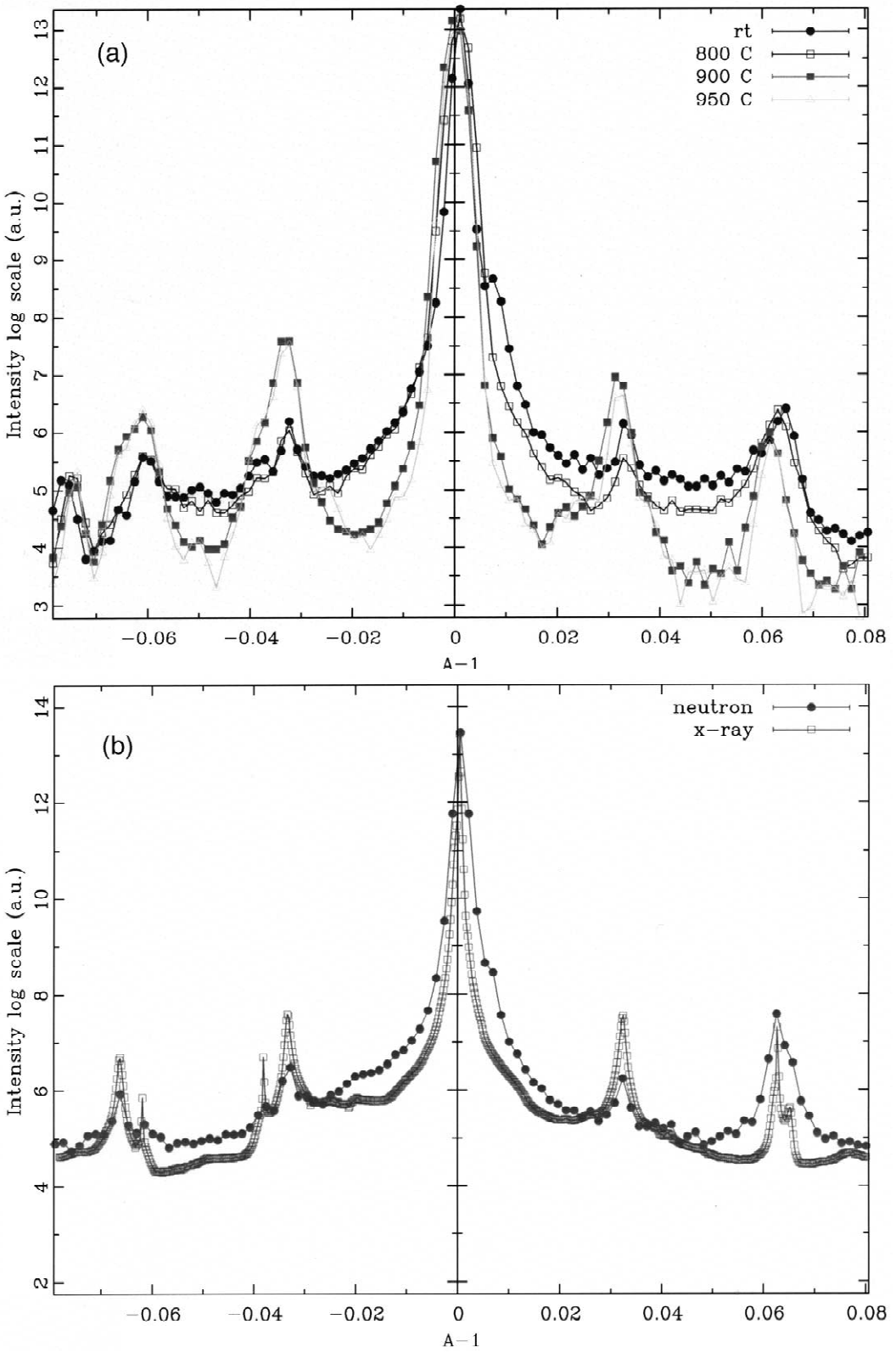

Fig. 1. $100\bar{1}0$ reflection, neutron measurement, sample (T) (a): temperature evolution (b): comparison to X-ray measurement.

3. Results and discussion

Around the Bragg reflections (sample T, Z) with high intensity, extended diffuse scattering can be observed (Fig. 1a). The profile analysis of reflections with different $Q_\perp$ components reveal a systematic dependence of the ratio of integral intensities $I_{\text{diff}}/I_{\text{Bragg}}$ which increases with increasing $Q_\perp$ value. The diffuse part has lost most intensity at temperatures above 800 °C and is hardly detectable at 980 °C (Fig. 1a). Owing to the $Q_\perp$ dependence we conclude that the major diffuse part is due to (frozen-in) phason fluctuations which vanish correspondingly at high temperatures. This type of scattering was also observed for the X-ray experiment (Fig. 1b) but there is no comparable difference between the low and high temperature measurements. The contrast between the neutron and X-ray results is difficult to interpret, since in the X-ray case no analyser was used, so TDS might be obscuring the effect. This is, however, not very likely as the Bragg intensity itself stays almost unchanged when heating to 950 °C. A possible explanation might be a 'transition' from a low T domain structure, which is governed by a Co–Ni concentration fluctuation (and accompanied by planar defects), to a more homogenous, with repect to the Ni–Co distribution, high T structure. The difference could also be due to the unequal sample sizes. The large neutron sample may be affected by various 'microstructural' disorder phenomena, which are absent in the very small specimens used for synchrotron studies. In particular, surface-related disorder might be more important in X-ray diffraction.

In addition to the diffuse scattering around the Bragg reflections, subsidiary reflections have been reported, which have been explained as satellites, arising from a 2-fold superstructure [3] or from domains with 1D qp ordering [2,5]. Around the strong Bragg reflections, a pattern of diffuse maxima seems to correspond to satellites with a $1/8\ a_i^*$ satellite vector. High resolution experiments revealed, however, that these satellites consist of weak Bragg reflections and four additional weak diffuse maxima, the strongest of which is close to the reported 1/8th satellite position. This type of pattern is easily explained by assuming a loss of quasiperiodicity in one direction, corresponding to a certain value of linear phason strain. We followed the temperature behaviour of the additional reflections as shown in Fig. 1. The diffuse maxima measured show a strong increase above 800 °C for the neutron experiment. In the X-ray case the intensity behaviour is much more complicated. At first glance, the two samples seem to give contrary results. For the Z sample, the 'satellite' reflections vanish at ≈900 °C, only to appear again at 950 °C with much higher intensity (see Fig. 2a and b). This type of reflection (belonging to domains with a 1D quasiperiodic structure) also occurs in the shape of the 'diffuse pentagons', a reflection group made up of five weak diffuse reflections. These maxima are not visible above 750 °C. In the case of the T sample, the intensity of the strong subsidiary reflections generally decreases, an example is shown in Fig. 3. It has to be noted, however, that the so-called 'satellite' reflections were not measured during this experiment. A tentative_explanation may be that the reflections around the 10010 reflection do lose their intensity, as in the case for the T sample investigated by X-rays, and are 'replaced' by reflections of the 4/6 approximant (some positions overlap, see Fig. 2), which may be a more stable phase at high temperatures than the 1D qc. We assume that this effect would only be observed for high intensity approximant reflections.

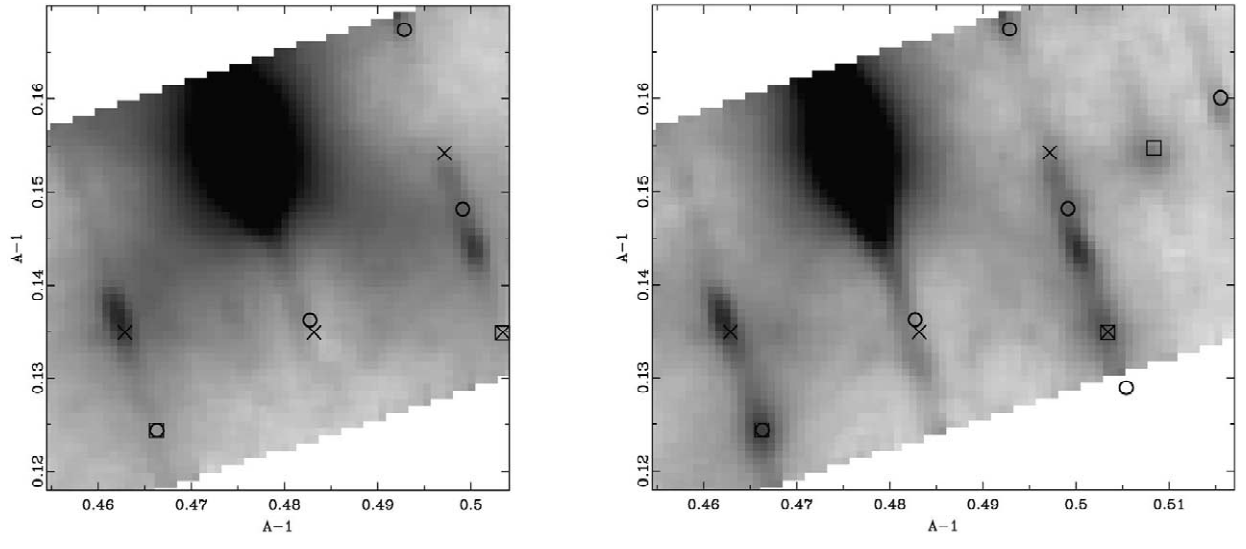

Fig. 2. $100\bar{1}0$ reflection, sample Z, X-ray measurement, left: 900 °C, right: 950 °C, squares denote positions of 1D qc ('satellites'), circles and crosses two orientations of the 4/6 approximant.

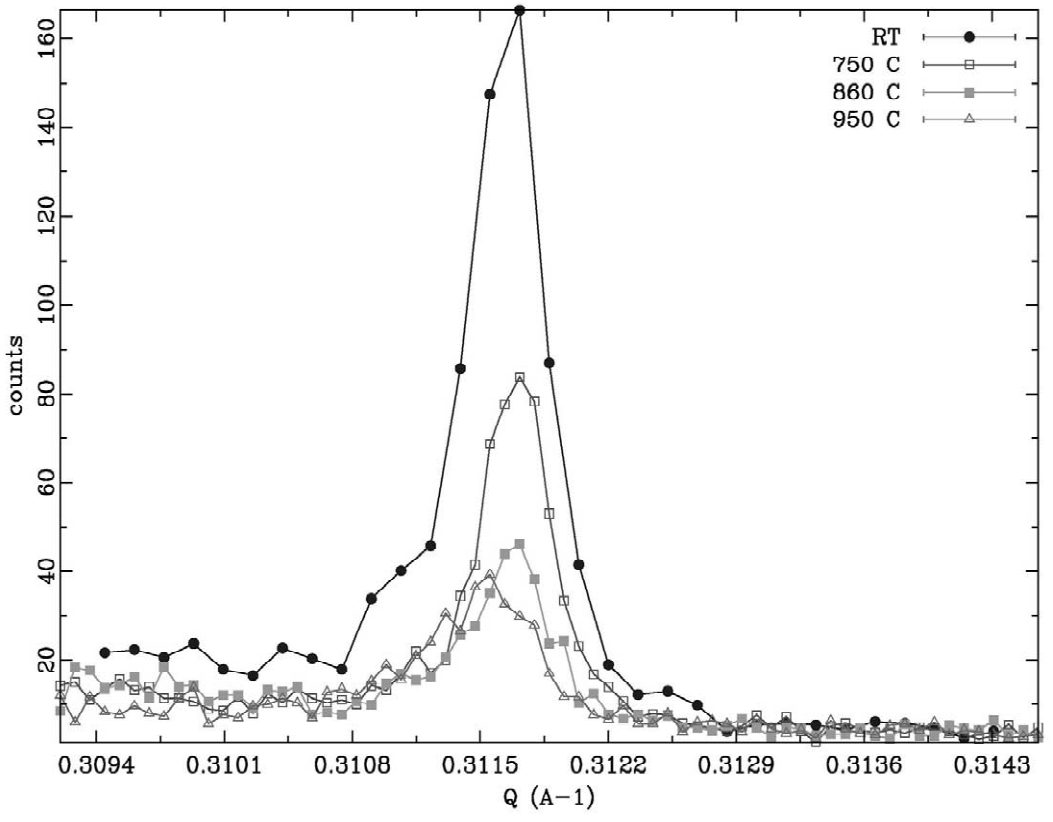

Fig. 3. DESY/D3, sample T, subsidiary reflection close to $10\bar{2}10$.

4. Conclusions

A tentative scenario is proposed: At low temperatures the samples probably consist of coherently intergrown domains of (disordered) 1D and 2D quasicrystalline domains. At higher temperatures part of this disorder, i.e. chemical concentration fluctuations, decrease. At temperatures above 900 °C, approximant phases form, and increase their volume. The mechanism of this transition could be either due to a growth of preformed nuclei of the approximant, facilitated by the decreasing structural disorder or, additionally/alternatively via phase transitions of the 1D qc domains to approximant domains. It is unclear, however, which energy or entropy term governs such a transformation into one of the microstructural states as long as the (elastic or phason) energy of such a microstructure is largely unknown.

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