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X-RAY AND NEUTRON DIFFUSE SCATTERING OF DECAGONAL QUASICRYSTALS AT TEMPERATURES UP TO 1000°C

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Comparative diffuse neutron (N) and x-ray (x) synchrotron studies of disordered decagonal quasicrystals $Al_{72}Co_{16}Ni_{12}$ were carried out at temperatures up to 1000°C. Various types of diffuse scattering with varying temperature behavior occur. Subsidiary diffuse reflections ('satellites') and streak-like diffuse scattering are tentatively explained by cooperative super- and disordering of the aperiodic order in form of domain structures [1] which exist in 'transient ordering states' [2]. Quite generally, diffuse scattering contributions, including those of phason type, go down in intensity whereas the 'satellites' either gain intensity or vanish at temperatures well above 800°C. Significant differences were found comparing x and n data: so-ray intensities decrease linearly, as expected, whereas neutron intensities show a significant increase for certain reflections above 850°C. This might be related to a Ni/Co-ordering during the formation of (periodic) domains within a quasiperiodic matrix structure. Apparently, disordered Al-Co-Ni phases are governed by a complex domain ordering of twinned lamellar domains with true quasicrystalline order, one-dimensional quasicrystalline and also periodic domains. These ordering phenomena are accompanied by phason straining and fluctuations.

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References

[1] F.Frey, E.Weidner, J.Alloys and Comp. (2002), in the press
[2] E.Weidner, F.Frey, K.Hradil, Phil.Mag. A81(2001)2375

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PHASONS FLUCTUATIONS IN ICOSAHEDRAL PHASES

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Quasicrystals are long range ordered materials without translational symmetry. The long range quasiperiodic order leads to new modes called phason: these collective modes are not propagative and have a diffusive character, unlike phason modes in displacive modulated phases, but similarly to composite structures. Phason fluctuations have been extensively studied in the i-AlPdMn phase: diffuse scattering measurement have shown that most of the diffuse scattering can be interpreted as resulting from long-wavelength phason fluctuations. The temperature dependence of the diffuse scattering is consistent with an interpretation in term of pre-transitional fluctuations. These results will be compared with measurements carried out on i-AlPdRe and i-CdYb phases which have been obtained as single grain recently. These two phases are particularly interesting since the i-AlPdRe is isostructural with the i-AlPdMn and the i-CdYb is a new binary stable phase. We will show that both phases have a significant amount of diffuse scattering due to phason fluctuations, but with a different shape anisotropy.

Keywords: QUASICRYSTAL, PHASON, DIFFUSE SCATTERING

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HOW PERFECT CAN A QUASICRYSTAL BE?

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We determined short range and long range order of the icosahedral Al-Pd-Mn quasicrystalline phase. Furthermore, we showed the high density of vacancies in as-grown samples. These vacancies determine the surface morphology at large scales in a thermodynamic equilibrium.

We studied the perfection of the as-grown icosahedral Al-Pd-Mn phase by the means of X ray Holography and the X ray Standing Wave techniques. Indeed, we analyzed both experiments on the basis of the perfect quasicrystalline structure. The X ray Holography experiment allowed us to reconstruct the 3D local average environment of the Mn atoms without a priori knowledge of the structure. For a fractured as-grown sample we measured a perfect coherency of a periodic standing wave with the quasiperiodic structure. Polishing destroys this coherency for the probed depths. Secondly, we evidenced a condensation of vacancies towards the surface induced by thermal treatments of the sample. During the same thermal treatments we measured by X ray diffraction a small lattice parameter variation in the surface vicinity. This structural modification is not a surface reconstruction as it can be observed in crystalline systems but the relative dilatation of $3x10^{-4}$extends over a surface thickness of few microns. We relate this structure variation to a change in the density of structural vacancies. Our results show that surfaces prepared by sample annealing cannot be analyzed as a cut of the as-grown sample but rather as a cut of a vacancies depleted structure.

Keywords: X RAY HOLOGRAPHY, X RAY STANDING WAVES, QUASICRYSTAL

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STRUCTURAL MODULATION OF Rb_2ZnCl_4 NEAR THE LOCK-IN TRANSITION

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Above 303 K Rb_2ZnCl_4 is isostructural to β-K_2SO_4. At that temperature it undergoes a phase transition towards a one-dimensional incommensurate (IC) phase with superspace group *P(Pmcn)*:ss-1. At 191 K the wave-vector locks into 1/3 c* and a new phase transition takes place towards a commensurate structure of space group $P2_1cn$. The IC structure has already been determined at temperatures far from 191 K where the modulation is constituted by only one harmonic (sinusoidal regime). According to NMR, EPR and dielectric measurements together with certain phenomenological models, the modulation should be strongly anharmonic near 191 K (solution regime). The structural modulation has never been refined near that temperature because of the low intensity and strong overlapping of high-order satellites. Using synchrotron radiation we were able to overcome these experimental difficulties and could measure the intensities of up to fifth-order satellites at 195 K. As it was anticipated in previous analyses[1,2], the refined structure shows that the distortions produced by the different harmonics are essentially the same (up to a global factor) as those of the same symmetry in the lock-in phase. Besides, the phases of the first and fifth harmonics are in agreement with those predicted for a solution regime[3]. Finally, the correlation among the intensities of the first and fifth-order satellites predicted in a previous work[2] has been experimentally confirmed. Making use of this correlation the solution density of the structural modulation has been determined.

References

[1]J. Phys. I France 7 (1997) 371-383
[2]Acta Cryst. (1997) A53, 334-340
[3]J. Phys.:Condens. Matter 7 (1995) 6187-6196

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