o.m10.o1 **Diffuse scattering in quasicrystals.** M. de Boissieu, A. Létoublon, M. Boudard, *LTPCM, UMR CNRS 5614 , ENSEEG BP 75 38402 St Martin d'Hères Cedex (France).*
Keywords: diffuse scattering.

Quasicrystals are materials presenting a new kind of long-range order: their diffraction pattern present sharp Bragg reflections with a symmetry which is incompatible with translation invariance. They can be obtained as large single grains in several systems and their quality is such that they show X-ray dynamical diffraction effect.

Although they present extremely sharp Bragg reflections, most of diffraction patterns of quasicrystals contain a significant amount of diffuse scattering: this is in particular true for the icosahedral AlPdMn phase, and the decagonal AlNiCo phase.

The origin of this diffuse scattering and its microscopical interpretation is one of the key issue in the understanding of the long-range quasiperiodic order propagation.

We will review results obtained in the i_AlPdMn phase. In this system, the diffuse scattering has been shown to be the result of long-wavelength phasons fluctuations[1-3]. At the atomic level, phasons fluctuations will result in a series of atomic rearrangements. Each rearrangement consists of an atomic 'jump' (on a length of the order 1 Å) between two atomic sites having almost the same local environment. Longwavelength phasons fluctuations are thus collective diffuse modes, which are frozen at room temperature.

A temperature study of the diffuse scattering gave a counterintuitive result: the diffuse scattering intensity decreases when the temperature is raised. This was interpreted as being the result of pretransitional fluctuations, and was confirmed by phase transitions observed for samples having a slightly different chemical composition.

Finally, absolute scale measurement of the diffuse scattering intensity showed that the amount of diffuse scattering is almost the same for all studied samples, and can be considered as an intrinsic property of i-AlPdMn phases. Similar results have been obtained for decagonal quasicrystals, which indicates that most likely these phases are only stable at high temperature.

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o.m10.o2 **Diffuse Scattering Studies at Beamline F1, HASYLAB/DESY: Recent Developments and Applications**. C. Paulmann, U. Bismayer, *Mineralogisch-Petrographisches Institut, Universität Hamburg, Grindelallee 48, D-20146 Hamburg, Germany*.
Keywords: diffuse scattering, synchrotron, CCD.

The availability of a commercial CCD-detector-system recommends the beamline F1 (Kappa-diffractometer) for studies of weak diffraction phenomena and time-resolved studies. Several disordered compounds were studied showing different characteristics of additional defect-induced scattering. The studies include REE-doped germanates with an intense broad and structured distribution of diffuse scattering, Al-excess NiAl-spinell with weak diffuse scattering due to cation-defect reordering as well as recrystallization studies of metamict minerals (allanite, titanite)[1]. The latter compounds show very broad and weak Bragg-reflections due to severe structural damage caused by alpha-recoil collision cascades. On annealing, a time- and temperature-dependent sharpening and intensity increase indicates progressive recrystallization effects.

The studies lead to the development and GUI-implementation of a range of advanced data processing routines to cover problems beyond the capabilities of the standard software system of the CCD-detector.

Apart from the beamline-specific accomodation of the diffraction geometry, a more flexible processing of large data sets arising from diffuse scattering studies is provided for a 3D-mapping of diffuse scattering (e.g. calculations of initial backgrounds across arbitrary scan ranges, background corrections for sample-external scattering, enhanced numerical data-processing of extended data-sets, interfaces to standard applications).

To avoid the blooming effect of strong Bragg-reflections due to long exposure times in diffuse scattering studies several identical data collections with shorter times and a later addition are more favourable. This implies an exact scaling of the different data sets against the varying primary beam intensities. In consequence, different off-line scaling strategies were implemented and successfully tested including a) external monitor data b) scaling against the storage ring current, c) scaling against a range of standard frames, d) computing frame internal scale factors from definite frame-areas.

Studies of diffuse scattering demand an exact correction of detector-intrinsic distortions caused by the fibre-optic taper between phosphor and CCD-chip. Internal look-up tables with an resolution of four pixels are calculated using bicubic spline algorithms to give an accurate correction. An interface to external appli-cations for processing large data sets was implemented.

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