MS10.04.02 OBSERVING AND UNDERSTANDING ARCS OF DIFFUSE SCATTERING FROM QUASICRYSTALS.

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Localized arcs of diffuse scattering are caused by particular short-range correlations between bonded icosahedral clusters. They were observed in AlMn, the first quasicrystal discovered, after annealing. They were observed in the TiMnSi quasicrystal on the day of its discovery; in that material they appear with high contrast and their shapes and locations in reciprocal space were mapped in detail. Electron diffraction in the TEM, on selected planes in reciprocal space, produces two-dimensional images from which the full three-dimensional structure of the arcs can be inferred. X-ray diffraction has also been useful in observing the arcs, especially in materials in which their contrast is not as great as in TiMnSi. TEM investigations demonstrated that the disorder producing the arcs in TiMnSi is topological rather than chemical. Simulations of the scattering of waves from icosahedral glass models and from random canonical-cell tiling models contain arcs very similar to those observed. They can be traced to the contribution of nearest-neighbor icosahedral clusters to the pair correlation function. Improving the quality of the glasses (as assessed by the widths of the simulated diffraction peaks) with constraints that force a uniform, high density of clusters increases the contrast of the arcs in the simulations. In the best glasses weak diffraction peaks can be resolved within the arcs, like those sometimes seen in the measurements. Too-tight constraints produce a crystal structure, the 1/1 1.3 -nm cubic approximant (a bcc cell with icosahedral clusters at the corner and body center sites). Local correlations in the glass like those in the 1/1 crystal phase are strongly suggested as the source of the arcs. Modeling of these quasicrystals as canonical-cell tilings has led to the same conclusion; indeed, a highly constrained glass is structurally identical to a random canonical-cell tiling. This role of local correlations has been confirmed in a pleasingly direct way in a simulation of the diffraction from polycrystalline 1/1 structure, in which only grain orientations for which the icosahedral clusters in the bcc phase could connect coherently across grain boundaries were allowed. With grain sizes of 1.3 nm, excellent agreement with the data was obtained.

MS10.04.03 METHODS FOR AB INITIO STRUCTURE SOLUTION OF DECAGONAL QUASICRYSTALS

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N-dimensional Patterson methods have been combined with the maximum entropy method for ab initio phase determination of decagonal structures [1].

To unravel the n-dimensional Patterson function the symmetry minimum function has been extended to the embedding dimensions. Given the n-dimensional space group this Patterson superposition method allows the positions of the hyperatoms to be located and a first crude structure model to be derived.

To retrieve the shape and chemical composition of the acceptance domain of each hyperatom, this procedure is combined with the maximum entropy method. This method is exclusively constrained by the positions of the hyperatoms in the n-dimensional unit cell and result of the symmetry minimum function in physical space. These constraints enforce quasiperiodicity and correct atomic distances can be easily implemented.

Applying the maximum entropy method in perpendicular space allows a detailed idealised decagonal structure model to be derived, as only solutions within the planes of the acceptance domains are possible. The physical space approach, however, provides the capability to determine more complex non-periodic structures as well as to introduce deviations from the ideal quasiperiodic structures.

The combined algorithm has been tested on decagonal $Al_{70}Co_{15}Ni_{15}$, where the existing structure model could be improved. The structure models of decagonal $Al_{71}Fe_5Ni_{24}$, $Al_{70.5}Mn_{16.5}Pd_{13}$ (using multiple anomalous dispersion data) and $Al_{80}Os_{10}Pd_{10}$ will be presented.

[1]   Haibach, T, Steurer, W.: Five-dimensional Symmetry Minimum Function and Maximum Entropy Method for ab initio Solution of Decagonal Structures. Acta Crystallogr. A (1995) in press.

MS10.04.04 DYNAMICAL X-RAY DIFFRACTION IN ICOSAHEDRAL Al-Pd-Mn QUASICRYSTAL.

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Large size crystals of $Al_{70}Pd_{21.5}$ $Mn_{8.5}$ were grown by the Bridgman method. Berg-Barrett topographs of a thick specimen showed three large grains approximately equal in size. Regions extending several mm² in size could be identified, over which the diffracted intensity was uniform, an indication of crystal perfection. The integrated intensity of several reflections was measured on an absolute basis with $\lambda = 1.54$ Å and the structure factor was extracted from the experimental value of the integrated intensity by making use of dynamical theory. Such procedure is justified by the fact that the rocking curves were extremely sharp ($\simeq 30$ arcseconds) and that anomalous transmission has been observed in similar samples (S.W. Kycia et al., Phys. Rev. B48, 3544 (1993)). While good agreement is found between theory and experiment for the strong reflections, large discrepancies are observed for the weak reflections, which are more sensitive to the details of the atomic surfaces in 6D space.
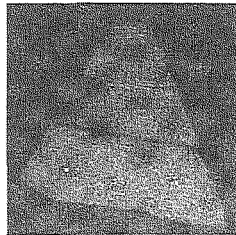
Berg-Barrett topographic photo. Symmetric Bragg geometry; $\lambda = 1.54$ Å. Reflection excited: (0 2 4 0 $\bar{2}$ 4) on a two-fold axis, normal to the specimen surface. The dark circle is due to surface stain. The white lines are regions of strain.

MS10.04.05 THE INCOMMENSURATELY MODULATED PHASES OF HEXAMINE DERIVATIVES.

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Hexamine suberate, azelate and sebacate form layer structures with alternating sheets of hexamine and alkanedioic acid linked by H-bonds between N and O atoms. The acid molecules are totally extended with 6, 7 and 8 carbon atoms and an acid group at each end. They form a two-dimensional array with their axis inclined by 30° with respect to the layer normal.

At room temperature, hexamine suberate and sebacate (even number of carbons) are strongly modulated, as witnessed by satellite reflections up to the fourth, respectively sixth order. The modulations are very stable between 120 and 300K. Hexamine azelate (odd number of carbons) is commensurate. However, strong diffuse scattering observed on precession photographs reveals some disorder in the structure.

The two incommensurate compounds have been refined using the superspace group formalism. Displacive atomic modulations including up to eight harmonics lead to satisfactory models. The analysis of the refinements indicates that in a layer, the zig-zag