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Diffuse scattering as a probe of local structure

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The strong sharp Bragg reflections that occur in diffraction patterns of all real crystals are used by conventional X-ray crystallography to deduce the average repetitive arrangements of atoms or molecules. Diffuse scattering, on the other hand, contains information about the deviations from the average (i.e., different types of disorder) and gives structural information on a scale that goes beyond that of the average unit cell and extends over a range of 0.1nm-100nm. In many important materials, it is this extended range of structural information that is crucial in determining the unique or novel properties of the material, rather than the average unit cell structure. We review the development of our diffuse scattering methodology using a variety of examples taken from different fields to illustrate the kind of information that can be obtained by current day methods - information that is simply not available from the Bragg experiment. Amongst these will be the zeolite mordenite, the organic pentachloronitrobenzene, which is one of a series of chloronitrobenzene compounds whose anomalous dielectric properties are thought to be related to their disorder, the relaxor ferroelectric PZN and finally examples of organic molecular crystals that exhibit polymorphism - a topic of crucial interest to the pharmaceutical industry. We gratefully acknowledge the support of the Australian Research Council, the Australian Synchrotron Research Program, the Access to Major Research Facilities Program and the Australian Partnership for Advanced Computing.

Keywords: diffuse scattering, Monte Carlo simulation, local structure

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Magnetic short-range order in Pt-rich Pt-Mn alloys

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The magnetism of $Pt_{(1-c)}Mn_c$ between c=0.12 to 0.16 is very unique. The magnetic diffraction pattern shows drastic change with a little difference of atomic arrangement and Mn concentration, while magnetic susceptibility shows a spin-glass like behavior throughout the concentration region. The atomic ordered phase in this Mn concentration range is also unique: it possesses two kinds of atomic ordered structures, Cu_3Au-type as a high temperature phase and ABC_6-type as a low temperature phase. The latter structure has the largest unit cell in the fcc based ordered structures and is only found in Pt-rich Pt-Mn , Pt-rich Pt-Cu and ternary $CuMnPt_6$ alloys. In the neutron diffraction pattern of the alloy with c=0.125, diffuse scattering appears at 1/2,0,0 with fourfold incommensurate peaks. The fourfold peaks also appear at equivalent points in the ABC_6-type structure. The origin of the incommensurate peaks is considered to be a distant interaction through a spin density wave in the conduction-electron gas caused by a Fermi-nesting effect. In the alloy with c=0.144, the incommensurate peaks disappear completely and a new set of magnetic superlattice reflections appears at 1/2 1/4,0, 1/2,0,1/4 and their equivalent points in the ABC_6-type structure. These magnetic peaks indicate that the alloy forms long-rang order of type-II anti-ferromagnetic structure. The origin of the magnetic long-range order is considered to be an antiferromagnetic interaction between the near-neighbor localized spins. These characteristic magnetic scattering disappear completely when the alloys become disordered state. The results indicate a strong coupling between the magnetic and atomic structures and a crossover of dominant magnetic interaction in this Mn concentration region.

Keywords: magnetic ordering, neutron diffuse scattering, spin glasses

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Phason diffuse scattering in the icosahedral quasicrystalline phases Zn-X-Sc, X = Co, Ag, Mg

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According to the hydrodynamic theory of quasicrystalline materials, the long range quasiperiodic order yields in quasicrystals new long-wavelength modes, the phason modes, in addition to the acoustic phonons. Phason excitations are diffusive and associated with internal atomic rearrangements the dynamics of which is expected to lead to a distinctive diffuse scattering signal around Bragg peaks in reciprocal space. Up to now, experimental demonstration for the existence of phason diffuse scattering was given in the enlightening single case of the Al-Pd-Mn Mackay-type icosahedral (i-) phase from which the phason elastic constants were extracted and the thermal activation unvealed. In the present communication, we report on X-ray synchrotron investigations of the diffuse scattering in the i-Zn-X-Sc (X = Mg, Ag, Co) phases and the Zn-Sc 1/1 periodic approximant bringing evidence for the presence of long-wavelength phasons in this new class of icosahedral quasicrystalline phases and ruling it out in the
1/1 approximant structure.

Keywords: diffuse X-ray scattering, quasicrystals, phase transitions and structure

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3D-PDF analysis of single crystal diffuse scattering on the example of disordered quasicrystals

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The three-dimensional pair distribution function (3D-PDF) method