

MS28-O5**Magnetic structure determination of EuPtIn₄ through resonant X-ray magnetic scattering**

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Zintl phases are ionic intermetallic compounds characterized by a polyanionic network with covalent bonds. These compounds are studied because of their structural variability and their electronic and physical properties [1,2]. An interesting case is the compound EuPtIn₄, which presents a phase transition from a paramagnetic to an antiferromagnetic structure below a Néel temperature of 13 K and for which a spin-flop transition was observed under a high magnetic field applied along the *ac*-plane at low temperature. Due to the strong neutron absorption of Eu, the resonant X-ray magnetic scattering (RXMS) technique was employed to investigate the magnetic structure in EuPtIn₄, taking advantage of the significant enhancement of the magnetic signal obtained at the L₂ edge of Eu. The RXMS experiments were performed at beamline P09 of PETRA III, employing different experimental possibilities, including a double phase retarder for full polarization analysis and a vertical 14 T cryomagnet [3]. The measurements confirm the phase transition at the mentioned Néel temperature and reveal an incommensurate antiferromagnetic structure with a propagation vector $\mathbf{k} = (\frac{1}{2}, \frac{1}{2}, \gamma)$, where γ is the incommensurate component with a value of 0.4258. The intensities of a set of reflections with indices $(\frac{1}{2}, n + \frac{1}{2}, \gamma)$ have been measured in the $\sigma\pi'$ channel (with n being an integer between 6 and 14) to infer the magnetic structure in the ground state while full linear polarization analysis was used to study the changes under high magnetic fields. Hereby, we will report on the magnetic structure of EuPtIn₄ as solved using the equations for RXMS and the density matrix formalism and on its corresponding magnetic superspace group.

References:

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Keywords: magnetic structure, resonant X-ray scattering, superspace formalism

MS29 Mathematical crystallography: special aspects of symmetry and other topics

Chairs: Prof. Berthold Stöger, Prof. Bernd Souvignier

MS29-O1**Z-modules in crystallography: structures and defects**

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Z-modules¹ are natural extensions of lattices. They have been introduced in crystallography by A. Janner and T. Janssen [1] in reciprocal space as the convenient tool to index the diffraction diagrams of incommensurate phases using a set of N integers ($N > d$, d being the dimension of the physical space). This generated the idea of extending crystallography to N -dimensional spaces, defining thus super-periodic crystals (incommensurate phases, composite crystals and quasicrystals).

Our present goal is to discuss the consequences of the presence of Z-modules of rank N in direct space in the crystallographic description of certain structures, revealing thus hidden symmetries when embedded in a N -dimensional superspace: *what kind of new defects could possibly be generated when the atoms of the crystal are located on a long range ordered subset of the nodes of a Z-module?* [2,3]

After recalling the basic definitions and properties of Z-modules, we exemplify the embedding process from d - to N -dimensional spaces, using the specific case of the NiZr orthorhombic *Cmcm* structure that is fully defined on a single Z-module generated by the vertices of the regular pentagon. We will then explain the symmetry breaking in the process of backwards projection from N - to d -dimensional spaces that generates the defects leaving the module invariant but not the crystal. In NiZr, there are essentially two such basic defects: a quinary twin and a translation boundary (plus its corresponding dislocation).

Observations by HREM and HAADF electron microscopy show the perfect agreement at the atomic level between theoretical models and experiments. This justifies the physical pertinence of introducing Z-modules in the crystallography of those kind of alloys that have local hidden non crystallographic symmetries.

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1 A Z -module of rank N in R^d with $N > d$ is the set S of points of R^d that are linear combinations with integer coefficients of N vectors arithmetically independent:

- a Z -module of rank N in R^d is the (irrational) projection of a lattice ZN in R^N ;
- a Z -module of rank N in R^d forms an enumerable dense set of points in R^d or in a non-empty subspace of R^d ;
- if $d = N$ the Z -module is trivially a lattice ZN .

Keywords: Z -modules, twins, dislocations

MS29-O2

The theory of twisted X-rays and their diffraction patterns

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Most molecular structures that are known today have been found by X-ray crystallography. However, a main drawback of the method is the need to crystallize the structures under consideration. As proteins often do not form crystals, but aggregate in other highly symmetric assemblies, like rods or sheets, we proposed to design electromagnetic radiation that reflects the symmetry of the structures in the same way as plane waves do for crystals [1,2].

In the special case of helical structures, like carbon nanotubes or helical viruses, this approach yields a class of radiations that we call twisted X-rays [1,2], and that are closely related to X-ray beams carrying orbital angular momentum [3].

In this talk, the theory of twisted X-rays and their diffraction patterns will be presented. Furthermore, it will be shown that structure analysis using twisted X-ray diffraction has the potential to solve molecular structures that are recently inaccessible.

Keywords: twisted X-rays, orbital angular momentum