On the other hand, neutron diffraction experiments have been performed in the La- and Y-doped $TbRhIn_5$ intermetallics in the AFM ordered phase (at the dilution limit of 40% of doping) at the Echidna (HRPD) instrument of the OPAL reactor, Australia. Our results show that there are no change in the magnetic moments orientation when compared to the non-doped compound (along tetragonal c-axis), the propagation vector remains the same and the size of the Tb moment is approximately the expected for a single Tb^{3+} ion.

We will discuss the details of magnetic structures determination as a function of CEF effects and how they are responsible in determining the magnetic moment directions for different *R* ions from this series as well as in determining the T_N evolution along the series and the behavior of magnetic susceptibility and specific heat.

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Structural biology and SAXS beamlines at the photon factory

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The Photon Factory (PF) is currently operating five structural biology beamlines, BL-1A, BL-5A, BL-17A, NW12A, NE3A, and two SAXS beamlines, BL-10C and BL-15A. Whereas all the structural biology beamlines use insertion device sources, the SAXS beamlines are conventional bending magnet sources.

BL-5A, NW12A and NE3A are high-throuput beamlines and we facilitate automation of the beamline operation with developments of sample exchange robots PAM, automated sample centering system and unified beamline control software [1,2]. Recently we started fully-automated data collection operation and it has been well used by the pharmaceutical companies.

BL-1A and BL-17A are small focus beamlines, dedicated to the micro crystal structure determination. In addition, softer xrays, 4 keV (BL-1A) and 6 keV (BL-17A), are available for low energy SAD structure analysis. We are now developing the helium chamber system to reduce the background.

BL-10C and BL-15A are two of the oldest beamlines at the PF and we have started upgrades of the SAXS beamlines [3]. We installed a 2-dimentional detector, RIGAKU R-AXIS 7 at BL-10C for the experiments of liquid samples. At BL-15A, we installed a flat panel detector, Hamamatsu C9728DK-10 for WAXS exeriments. We have a plan to construct a new insertion device SAXS beamline at BL-15A. We will move the current BL-15A to BL-6A this summer and will develop a new BL-15A beamline for SAXS experiments using small focus and softer energy x-rays.

We will present current status of the beamline upgrades and our future plans.

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Magnetic dynamical structures of possible spin-peierls system TiOBr

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Newly proposed spin-Peierls system Ti*OX* (*X*: Cl, Br) has been revealed showing exotic structural and magnetic properties such as a successive phase transition, one-dimensional (1D) nature associated with orbital ordering of Ti ions and super-lattice structure being related to the Peierls instability [1-5]. It is pointed out that resulting only from an arrangement of Ti d_{xy} orbital, the formation of 1D spin chains and the spin-Peierls transition will be realized. Recently, it has been demonstrated that TiOBr also exhibits two successive phase transitions similar to TiOCl at T_{c1}=27K and T_{c2}=47K. Here we carried out inelastic neutron experiments in order to find the evidence of spin-Peierls transition. The inelastic spectrum with a large amount of poly crystalline sample of TiOBr shows the localized signal in the vicinity of the magnetic zone center Q=0.9Å^{-1}. Observed spin gap like signal lies at energy of ΔE~10meV. The gap energy in TiOBr is expected much higher from measured thermodynamic properties and by analogy with TiOCl. Constant Q cuts of the observed $S(Q,E)$ map show some Q-dependent structure in its intensity indicating the signal is sample oriented. The Q structure quite reveals the intensity is well explained by the powder averaged dynamical structure.

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Making crystallography appealing to secondary school students

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Science has been established as a critical part of the secondary school curricula. Sadly, Crystallography is often left out of the teaching curricula for students at secondary school. Educators usually assume that teaching crystallography requires advanced science knowledge and that X-ray instruments are insecure, inaccessible, unsafe or difficult to use.

Several approaches have been made to deal with this issue. One classical teaching pamphlet is that produced by Elizabeth A. Wood, 1972 [1] which was translated to most of the most popular languages. More recently this subject has been discussed in several papers by Kantardjieff [2]. Concerning Spain, some successful attempts have been developed to make crystallography and crystallization close to students. One of these is the so call Crystallization in the School [3]. This crystal growing competition has been organized since 2008 involving several high schools within the region of Andalusia (Spain), Puerto Rico, Asturias and, during the present academic year, it has been extended throughout the whole of Spain.

Within the Spanish initiative for excellence (CEI), the Summer Scientific Campus offered by the University of Oviedo -CEI has the aim of promoting the scientific vocations amongst near-future graduate students who are immersed during 14 days on different profiles of experimental sciences, technologies and innovation within a unique environment of cultural exchange, with the experimental science activity, through their integration into research projects carried out in the university facilities.

We have developed a proper scenario to incorporate Crystallography into the Summer Scientific Campus, presenting the X Ray Diffraction topics in a substantive way and trying to attract the enthusiasm of youngest into Crystallography, using the Forensic Science as an appropriate setup to understand the techniques and authentic processes used within a Crime Scene. Our 'X-Ray diffraction in the Forensic Science Workshop' introduces and develops the skills, understanding and knowledge of X Ray diffraction methods and their application to forensic science.

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Structural basis for the mechanical deformation in organic solids

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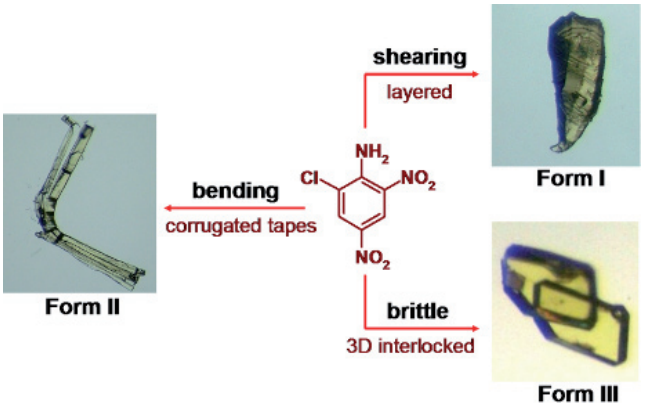
Understanding structure-mechanical property correlations is a key element in material science and engineering that underlies the successful design of materials [1], [2], [3], [4]. Based on mechanical behaviour, molecular crystals may be classified into three categories: (1) shearing, (2) bending and (3) brittle [5]. Crystals with parallel layered structure having strong intralayer and weak interlayer interactions show shearing on application of a mechanical stress. Bending occurs when the strength of intermolecular interactions in orthogonal directions are significantly different. Isotropic crystals with comparable intermolecular interactions in the three orthogonal directions display brittle nature. The experimental characterization of the defects or molecular packing at the deformed region is challenging as the organic materials are generally very sensitive to the microscopy beams.

In our ongoing study, the mechanism of crystal deformation is being investigated by probing the deformed region using a combination of techniques like, single crystal X-ray structure determination, micro Raman, HRTEM and optical microscopy. The preliminary results on bending type crystals suggest that the ordering of molecules at the deformed region is not completely random as in amorphous materials, but the deformed region turns into the polycrystalline domains with slightly altered molecular packing. It was also observed that the severe bending in the crystals leads to the formation of grain boundaries within which the molecules adopt somewhat distinct (high energy) packing.



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Highly symmetric complex intermetallics

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A growing number of structurally highly complex intermetallic phases is being discovered and described with the emergence of new crystallographic methods. We are still not able to understand, why unit cells containing hundreds or even thousands of atoms are being formed by simple, binary and ternary metallic compounds. To approach this important question we are working on a systematization of complex intermetallics, starting with the highest-symmetric lattice, *i.e.* the cubic face-centered structures.

There is a bigger group of phases with approximately 400 atoms per unit cell - 43 reported structures -, which crystallizes in only two different space groups and can be roughly assigned to a common aristotype structure. The few structures with even bigger unit cells - 11 phases with around 1000 atoms per unit cell, not mentioning the even bigger Al-Cu-Ta compounds [1] ,[2] - show a slightly broader structural variety but can also largely be traced back to some common geometrical characteristics. We try to understand all of these structures in terms of the cluster approach, describing them as packings or coverings of highly symmetric building blocks. In addition, features of the average structure and findings from first-principle studies are