

## Poster Sessions

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 Kantardjiev [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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[1] *Crystals: A handbook for school teachers*, E.A. Wood, 1972. (Spanish, translated by Juan F. Van der Maelen Uria with Carmen Alvarez-Rua Alvarez, Javier Borge, and Santiago Garcia-Granda) [2] K.A. Kantardjiev, C. Lind, J. Ng, B.D. Santarsiero, *J. Appl. Cryst.* **2010**, *43*, 1181. [3] L. Roces, R. Santisteban-Bailón, C. Ruiz-Martínez, S. García-Granda, J. López-Garriga, J.M. García-Ruiz, *Crystallisation in the School*, 1<sup>st</sup> North African Crystallographic Meeting, Casablanca, 2010.

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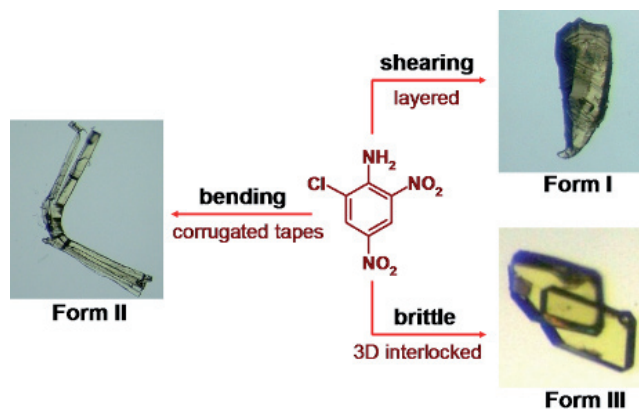
#### Structural basis for the mechanical deformation in organic solids

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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.



[1] C.M. Reddy, S. Basavoju, G.R. Desiraju *Chem. Commun.* **2005**, 2439. [2] C. M. Reddy, R.C. Gundakaram, S. Basavoju, M.T. Kirchner, K.A. Padmanabhan, G.R. Desiraju *Chem. Commun.* **2005**, 3945. [3] C.M. Reddy, G.R. Krishna, S. Ghosh *CrystEngComm* **2010**, *12*, 2296–2314. [4] C.C. Sun *J. Pharm. Sci.* **2009**, *5*, 1671. [5] C.M. Reddy, K.A. Padmanabhan, G.R. Desiraju *Cryst. Growth Des.* **2006**, *6*, 2720.

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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