3-1-2018

# Revisiting Polymorphism of Molecular Crystals from the Melt

Alexander Shtukenberg
*New York University*

Qiang Zhu
*University of Nevada, Las Vegas*, qiang.zhu@unlv.edu

Bart Kahr
*New York University*

## MS39-O5

### The argentinean neutron beams laboratory project

Gabriela Aurelio[1], Javier Santisteban[2], Karina Pierpauli[2], Florencia Cantargi[2], Miguel Ángel Vicente[2], Aureliano Tartaglione[2]

1. Centro Atómico Bariloche, San Carlos de Bariloche, Argentina
2. Centro Atómico Bariloche, Comisión Nacional de Energía Atómica, S. C. de Bariloche, Argentina

**email: gaurelio@cab.cnea.gov.ar**

The RA-10 is a 30 MW multi-purpose reactor under construction in Buenos Aires, designed to satisfy national and regional demand for radioisotopes, nuclear materials testing and neutron beams research. The reactor will start operations on 2021, it will have a liquid deuterium cold source and a large guide hall for instruments.

Since 2016 the National Atomic Energy Commission has started a project called "The Argentinean neutron beams laboratory for the RA-10 reactor" (LAHN); aimed at implementing state-of-the-art instruments, developing a user community and the laboratory staff. Two instruments are being designed for the first stage of this laboratory:

(i) a neutron imaging instrument on a cold beam; and (ii) a multi-purpose diffractometer on a thermal beam, optimized for non-destructive studies on large objects.

Both instruments will be placed on the reactor face, in order to exploit very intense, undisturbed, neutron beams. Besides this, an ambitious program has started to popularize neutron techniques in Argentina and create new users. A second phase for the project has been launched, taking into consideration the demands of the local and regional scientific community. Several instruments are being evaluated for this second phase in view of the proposals we have received from laboratories in Europe.

In this talk, the present state of the project will described, providing details of the instruments design and the strategies implemented to develop the Argentinean users community.

**Keywords: large-scale facilities, neutron diffractometer, research reactor**

# MS40 Crystallization for small and large molecules

**Chairs: Prof. Bernhard Spingler, Prof. Terese Bergfors**

## MS40-O1

### Revisiting polymorphism of molecular crystals from the melt

Alexander Shtukenberg[1], Qiang Zhu[2], Bart Kahr[1]

1. Department of Chemistry, New York University, New York, United States of America
2. Department of Physics and Astronomy, High Pressure Science and Engineering Center, University of Nevada Las Vegas, Las Vegas, United States of America

**email: shtukenberg@mail.ru**

Polymorphism is a typical feature of molecular crystals. Since polymorphic modifications exhibit different physical properties, polymorph screening has become an important part of drug formulation process and is required for other applications of molecular crystals. Despite being not as universal as solution screening, melt crystallization typically combines high driving forces for crystallization with low nucleation and growth rates and can provide polymorphs not accessible in a standard solution screening. The screening process itself is simple, fast, and cheap, while determination of the crystal structures is often complicated by the absence of crystals suitable for the single crystal X-ray diffraction analysis. Nevertheless, advances in powder X-ray diffraction and crystal structure prediction algorithms, today, can fill the breach in order to extract structure from polycrystalline samples. Various organic compounds were crystallized from the melt and observed with a polarized light optical microscope. Polymorphs distinguished optically were further analyzed using Raman spectroscopy and X-ray powder diffraction. The crystal structures were typically solved using a combination of X-ray powder diffraction, crystal structure prediction, and Rietveld refinement. We illustrate this approach by discovering and characterizing new polymorphs of several common and well-studied compounds including resorcinol, coumarin, aspirin, and benzamide.

This work was primarily supported by the New York University Materials Research Science and Engineering Center (MRSEC) program of the National Science Foundation under award number DMR-1420073.

**Keywords: polymorphism, molecular crystals, melt crystallization**