Ph.D. Course in Materials Science and Nanotechnology

University of Milano-Bicocca, Department of Materials Science, via Cozzi 55, 20125 Milano

February 15, 2019 – 10.30 a.m.

Seminar room - Department of Materials Science U5

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New Experimental Techniques for Exploring Crystallization Pathways and Structural Properties of Solids

The lecture will highlight three experimental strategies that we are currently developing for exploring crystallization pathways and structural properties of solids: (i) in-situ solid-state NMR techniques for understanding the time-evolution of crystallization processes, (ii) exploiting the phenomenon of X-ray birefringence for spatially resolved mapping of molecular orientational distributions in materials, and (iii) structure determination of organic materials directly from powder X-ray diffraction (XRD) data.

Our in-situ solid-state NMR techniques for studying crystallization pathways exploit the ability of NMR to selectively detect the solid phase in heterogeneous solid/liquid systems of the type that exist during crystallization from solution, and this strategy has been applied to establish the sequence of solid phases formed during crystallization processes, including the discovery of new transient polymorphs. Our most recent development is an in-situ NMR strategy (called "CLASSIC" NMR) that yields simultaneous information on the time-evolution of both the solid phase and the liquid phase during crystallization.

We recently reported an experimental method that allows spatially resolved measurements of X-ray birefringence to be carried out in "imaging mode", representing the X-ray analogue of the polarizing optical microscope. The lecture will describe applications of the X-ray Birefringence Imaging technique: (a) to study changes in molecular orientational ordering associated with solid-state phase transitions, (b) to determine the size and spatial distribution of domain structures, and (c) to establish the degree of molecular orientational ordering in anisotropic materials, including liquid crystal phases.

Finally, although single-crystal XRD is a very powerful technique for determining structures of crystalline materials, the requirement for a single crystal limits the scope of this technique. For materials that cannot be prepared as suitable single crystals, structure determination must be tackled instead using powder XRD data. However, structure determination from powder XRD data is significantly more challenging than from single-crystal XRD data, particularly for organic materials.

For several years, we have been focusing on the development of new methodology (particularly the direct-space strategy for structure solution) to enable crystal structures of organic materials to be determined directly from powder XRD data. The lecture will describe the current state-of-the-art and future prospects in this field.

PhD students and all interested in the seminar are kindly invited to participate.

The PhD Coordinator
Prof. Marco Bernasconi