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Keywords: pharmaceutical crystallography, polymorphs, structural databases

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Different Reasons for Packing with Z'=2: 4-nitroimidazole Derivatives
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The packing of the molecules in crystals is a result of the compromise between different intermolecular interactions, tendency towards close packing, symmetry requirements etc. All these factors, hierarchically organized and influencing one another, determine the unique three-dimensional structure, the molecular crystal.

The compromise between different requirements sometimes requires the presence of more than one molecule in the asymmetric unit. That means that there are molecules in the crystal which are not related by any symmetry operation while still being chemically identical. A study of the connections between this phenomenon and packing conflicts is essential for predicting organic crystal structures. A further goal could be to try to correlate the occurrence of multiple molecules in the asymmetric unit with the presence of certain functional groups in the molecules, space group symmetries etc.

The analysis of the frequency of different Z' values in the crystal structures shows that above-average percentage of the structures with Z'>1 is observed for imidazole derivatives.

The different reasons for packing with Z'=2 will be presented for 4-nitroimidazole derivatives. For example, in two closely-related 1-R-2-methyl-4-nitroimidazoles the creation of bilayers of molecules, the primary building blocks of the crystal structures, is possible because there are two symmetry-independent molecules that have either different conformations or take part in different intermolecular interactions.

Keywords: crystal packing, weak interactions, imidazole derivatives

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Directed Assembly and Covalent Capture of Supramolecular Architectures in the Solid State
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In this presentation, we demonstrate how principles of supramolecular chemistry involving molecules that function as linear templates can be used to direct the formation of finite molecular assemblies with components that react to form covalent bonds. We demonstrate how forces such as hydrogen bonds and coordination bonds can be used to direct the construction of molecules. The targets include linear and bent cyclophanes, as well as molecular ladders. The ability to construct complex molecules in the solid state relies on an ability of the templates to insulate reactants from vexatious structural effects of molecular close packing, effects which have made directing the formation the covalent bonds in organic solids difficult to control. Thus, the templates are able to adapt to changes to size and shape of the reactants and thereby provide a mean to control the size and shape of the resulting products. In that way, the covalent-bonding-forming process provides a means to covalently capture the geometry of reactants within supramolecular architectures with structures largely independent of long-range packing. The molecular targets form in the organized, solvent-free environment of the solid state in 100% yield and gram quantities.

Keywords: supramolecular chemistry, covalent capture, hydrogen bonds

MS46 In-situ Observation of Crystal Growth Processes

Chairpersons: Tadashi Ohachi, Vladimir Kaganer

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Time-Resolved X-ray Topography Study on Growth of 180° Ferroelectric Domains
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Understanding the mechanism of nucleation and growth of 180° ferroelectric domains is an on-going subject of numerous theoretical and experimental investigations. The ferroelectric transition and the domain structure are intimately coupled to dielectric, ferroelectric, piezoelectric, pyroelectric, and nonlinear optical properties in a wide range of materials. In the past, the x-ray topography technique has been applied to investigate the ferroelectric domains in single crystals. However, the lack of sufficient diffraction contrast between the adjacent antiparallel ferroelectric domains made it difficult for investigation of domain dynamics.

Using the coherent x-rays from a third generation synchrotron source, we have greatly enhanced the diffraction contrast from the neighboring antiparallel ferroelectric domains. With this phase-contrast topography technique, we carried out a time-resolved diffraction imaging study of the nucleation and growth of 180° ferroelectric domains in barium titinate single crystals during the polarization switching. The diffraction images were collected with 1-micron spatial resolution and down to 10-ms acquisition time. We have observed drastically different domain growth mechanisms due to the surface treatment at the electrode-sample interfaces, suggesting the nucleation and growth is dominated by the defects at the electrode interface. We present the morphology of 180° domains and describe growth kinetics as a function of temperature and applied potentials.

Keywords: X-ray topography, ferroic domain structure, growth kinetics

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***In-situ* Observation of Surface Kinetics during MBE Growth using Synchrotron X-ray Diffraction**
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The weak interaction of x-rays with matter offers the advantage of not disturbing the system under investigation and in most cases allows us to analyze the results using kinematical scattering theory. Both properties make x-ray diffraction an almost ideal tool to study crystal growth in situ and in real time.

To obtain the necessary sensitivity to study surfaces and interfaces that consist of a very limited number of scatterers, high primary beam intensities usually available at synchrotrons are required. Using a dedicated beamline at BESSY in Berlin, we study the surface kinetics of various III-V materials during deposition and the subsequent recovery under standard molecular-beam epitaxy conditions.

Following the diffraction oscillations during layer-by-layer homoepitaxy on GaAs(001) and the closely related InAs and GaSb surfaces, we can analyze the coverage of the different levels that constitute the growth front. After deposition, the system reduces to a two-level system. This initial, fast recovery is followed by a slower recovery phase in which the two-level structure laterally coarsens until the big terraces of the pre-growth state are recovered.

Despite their similarity in crystal structure, the three materials systems exhibit strong differences in their deposition and recovery kinetics, which are obviously related to the detailed atomistic processes taking place at the reconstructed surface during deposition.

Keywords: molecular-beam epitaxy, coarsening, III-V compounds