unit cells in the sample. If a crystal structure shows disorder, i.e. if different cells look differently, some of the scattered intensity is lost from the Bragg peaks and distributed throughout reciprocal space as diffuse scattering.

The interpretation of such scattering is far from routine. Sometimes it can be done with qualitative arguments and simple simulations; sometimes it requires computationally demanding modeling including Monte-Carlo (MC) simulations combined with optimization of the parameters of the MC simulation [1,2]. Fortunately this computationally most demanding approach involving global optimization using differential evolution or other population based methods is embarrassingly parallel and therefore well suited for taking advantage of the rapidly growing accessibility of parallel computers [3].

We develop software (ZODS: Zürich – Oak Ridge Disorder Simulations) for analyzing diffuse scattering from disordered single crystals whose average structure is (at least approximately) known. ZODS aims to take advantage of parallel processing in various computational environments ranging from personal computers to supercomputers.

The refinement of the diffuse scattering model is parallelized on two levels. (1) A global optimization method calculates an objective function at many points in parameter space simultaneously. (2) Calculation of the objective function at one point involves simultaneous simulation of multiple disordered crystals with the same set of parameters, merging of the corresponding intensities and calculation of the objective function at that point.

The software is tested for correctness and scalability with experimental data for β-$NaLaF_4$ [4] and artificial test data.

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The disordered and modulated crystal structure of the zeolite SSZ-57

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SSZ-57 has the most complex zeolite structure found to date, with both modulations and significant disorder. High quality X-ray diffraction data could be measured on a *ca*. 2 x 2 x 8 µm microcrystal using a Pilatus 6M pixel detector installed on the beamline X06SA at the Swiss Light Source. The high performance of the experimental setup allowed a full data set (1800 frames, oscillation angle: 0.1° / frame) to be collected in just 15 minutes. The Bragg structure can be described in the three-dimensional space group $P\bar{4}m2$ ($a = b = 20.091$ Å, $c = 110.0$ Å). A better representation of the symmetry, of the sparse density of Bragg reflections and of systematic extinctions in the diffraction pattern, however, was obtained in the four-dimensional super-space group $I4_1/amd(00\gamma)s00s$ ($\gamma = 0.125$), which allowed a refinement with only 648 parameters instead of the 5433 parameters required with the three-dimensional approach. The framework of SSZ-57 is related to that of ZSM-11 (**MEL**, $I\bar{4}m2$, $a = b = 20.12$ Å, $c = 13.44$ Å). The **MEL** units are stacked along **c**, but the sequences are interrupted by 12-rings having their channel direction perpendicular to the *c*-axis. **MEL** units on either side of the 12-rings are rotated with respect to one another by 90° around **c**. Subsequent 12-rings are rotated in the same manner, so there are two mutually perpendicular 12-ring channels per three-dimensional unit cell. The presence of significant disorder did not allow the structure to be understood in detail without considering information from diffuse scattering. In particular, the distribution of the 12-rings, which is of crucial importance to the understanding of the catalytic properties of this zeolite, could not be determined. Monte Carlo modeling of the real structure resulted in an excellent agreement between the experimental and calculated diffuse scattering with the application of just a few rules. When looking along their channel directions, the 12-rings can be stacked directly on top of each other, or, alternatively and with higher probability, they can be shifted to lie above one of the neighboring 10-rings along the positive or negative **c**-directions. Along perpendicular directions in the **a**,**b** planes, the 12-rings form (almost) long-range ordered chains without any off-sets along **c**. The positions of the 12-rings along **c** are uncorrelated within the constraints given by the average structure. Though simple from a conceptual point of view, the complexity of the structure required a Monte Carlo computer model describing more than 10^9 atoms. The handling of such a huge model only became feasible with the application of some simplifications, but these did not seriously hamper the modeling of the experimental observations.

Keywords: zeolites, disorder, modulated structures

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X-ray scattering as a tool for the study of finite size effects in polymers

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The current trends in Polymer Science evolve towards the development of nano-scaled materials. Much effort has been carried out in the last decade to understand the influence of confined media in fundamental phenomena [1]. There is a general agreement that the polymer morphology and nanostructure, which in turn control the physical properties of the material, changes under spatial confinement. The present work contributes to the understanding of finite size effects in polymer materials by means of X-ray scattering methods. Nanolayered polymer systems are employed for this purpose.

Multilayered films with thousands of alternating layers of two immiscible polymers were prepared using a layer multiplying coextrusion process [2]. Films of poly(ethylene terephthalate) (PET) and polycarbonate (PC) with individual layer thicknesses of 65 nm are here investigated. Both materials are initially in the glassy state. Information on the appearance and evolution of PET lamellae (typically several nanometers in one dimension) was obtained by means of isothermal experiments using small-angle X-ray scattering (SAXS) in a synchrotron radiation source. Room temperature wide angle X-ray diffraction studies were also used to provide complementary information of chain orientation.

Real time SAXS studies during the crystallization of nanolayered PET at 150 ºC reveal that lamellae oriented with the basal surfaces parallel to the layer stacking (flat-on lamellae) appear. The distribution of directions normal to the lamellar surfaces broadens as crystallization proceeds. This could be explained as arising from the insertion of new lamellae with slightly inclined surfaces between the first developed crystals. Analysis of the SAXS profiles using the intensity profile method allows determining the long period *L* (periodicity along the