

The structure reveals that the nanobody binds a hydrophobic helix through its CDR1 and CDR3 loops, abolishing a well characterized interaction between the capsid N- and C-terminal domains. Interestingly, the interaction forms a hydrogen bond network with capsid residue N73, which is associated with host antiviral restriction. Structural alignments of this complex with high resolution crystal structures of pentameric and hexameric capsid building blocks suggests that upon binding, the nanobody sterically prevents the incorporation of either pentamers or hexamer to the mature capsid lattice.

Keywords: HIV-1, capsid, assembly

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Modeling diffuse scattering using evolutionary algorithms and super computing

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Materials possessing disorder within their crystalline structure often exhibit unusual and potentially useful properties. An elucidation of the local structure, rather than the average structure, is crucial to understanding the behavior of such materials. Disorder manifests itself as diffuse scattering in a diffraction experiment, but the measurement and interpretation of diffuse scattering is far from routine. It requires high-performance computing for carrying out Monte Carlo and Differential Evolution (DE) modeling techniques, high-flux radiation sources and user-friendly modeling software. With the capabilities at ORNL of high performance computing and the advent of the new \$1.4bn Spallation Neutron Source, we are now exquisitely positioned to quantitatively model the disorder leading to diffuse scattering. An international collaboration was formed between the Universities of Zürich and Bern, the ETH Zürich and the Oak Ridge National Laboratory to develop a new general methodology for modeling diffuse scattering, including the Zürich Oak Ridge Disorder Simulation (ZODS) software, which will be discussed in another contribution.

Our first test case is tris(bicyclo[2.1.1]hexeno)benzene, which exhibits hexagonal symmetry and one-dimensional streaks of diffuse scattering along the hexagonal axis. Layers of coplanar molecules are stacked in a disordered way along the *c*-axis. A four-layer model was initially developed to model the diffuse intensity of fourteen streaks of reciprocal lattice with four probabilistic stacking parameters [1]. These parameters have been optimized with a DE algorithm and parallel computing. Nearly noise free diffraction data were generated using 1280 clones of the best individual after 287 generations of DE refinement. Refinement of the probabilistic parameters against these reference data with a genetic algorithm, a swarm calculation and differential evolution are similarly efficient.

Our second test case is NaLaF₄, a member of a family of rare earth-doped (Er³⁺, Yb³⁺) sodium lanthanide tetra fluorides, which show occupational and displacive disorder reflected in distinct planes (2-D) of diffuse X-ray scattering. These materials are efficient up-conversion phosphors [2-4]. The average crystal structure alone does not allow a complete understanding of the physical properties. Site selective spectroscopic studies could only incompletely ascribe the high efficiency of the light emission to the presence in the crystal structure of multiple optical sites [5]. Specifically, we are reporting on our recently collected neutron data for NaLaF₄. Such data will allow us to better model the positions and site occupancies of the Na and F atoms than is

possible in an X-ray experiment since the relative scattering lengths of Na, La and F for neutrons differ much less than for X-rays. From this data we plan to develop a fully quantitative model; the development and results of this model will be presented.

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Diffuse Scattering from Stacking Faults: Scaling of Pair Correlation Function

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Stacking faults are ubiquitous in several close-packed metals and alloys as also in polytypic compounds like SiC and ZnS where one of the atoms sit approximately on close-packed positions. These faults may result as an accident during growth (so-called growth faults), by plastic deformation (the deformation faults) and during structural phase transition (such as layer displacement faults) involving restacking of the closed-packed layers. The distribution of stacking faults introduced during crystal growth or plastic deformation is random whereas it is non-random for those introduced during restacking transitions. Theory of x-ray diffraction from randomly and non-randomly faulted crystals has been developed several decades ago. In recent years, Monte-Carlo techniques have also been employed to calculate the diffuse scattered intensity. In all these techniques (analytical or Monte Carlo), one first calculates the relevant pair correlation functions P(m), Q(m) and R(m) corresponding to A-A/B-B/C-C, A-B/B-C/ C-A and A-C/C-B/B-A type pairs of layers separated by 'm' intervening layer spacings. The fourier transform of these pair correlation functions yields the scattered intensity distribution along various reciprocal lattice rows. Conversely, the pair correlation function can be directly obtained from inverse fourier transform of the observed scattered intensity [1]. The purpose of this talk is to show a very special property of the pair correlation functions, and that is, their scaling property. It will be shown that the P(m)/Q(m)/R(m) for different values of fault probabilities when plotted against a scaled variable m/ξ (ξ is the correlation length corresponding to the values of P(m), Q(m) and R(m) tending towards 1/3) collapse into a master curve [2-3]. This collapse is also observed in the time domain (t) for the late stages of restacking transitions [4]. The scaling behavior of the pair correlation functions implies a power law dependence of ξ on fault probability or time; the exponent for the latter belongs to a universal class. This scaling property can be conveniently used for calculating the scattered intensity distribution.

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