Poster Presentation

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Studying structure disorder in DL-Norvaline by single crystal diffuse scattering

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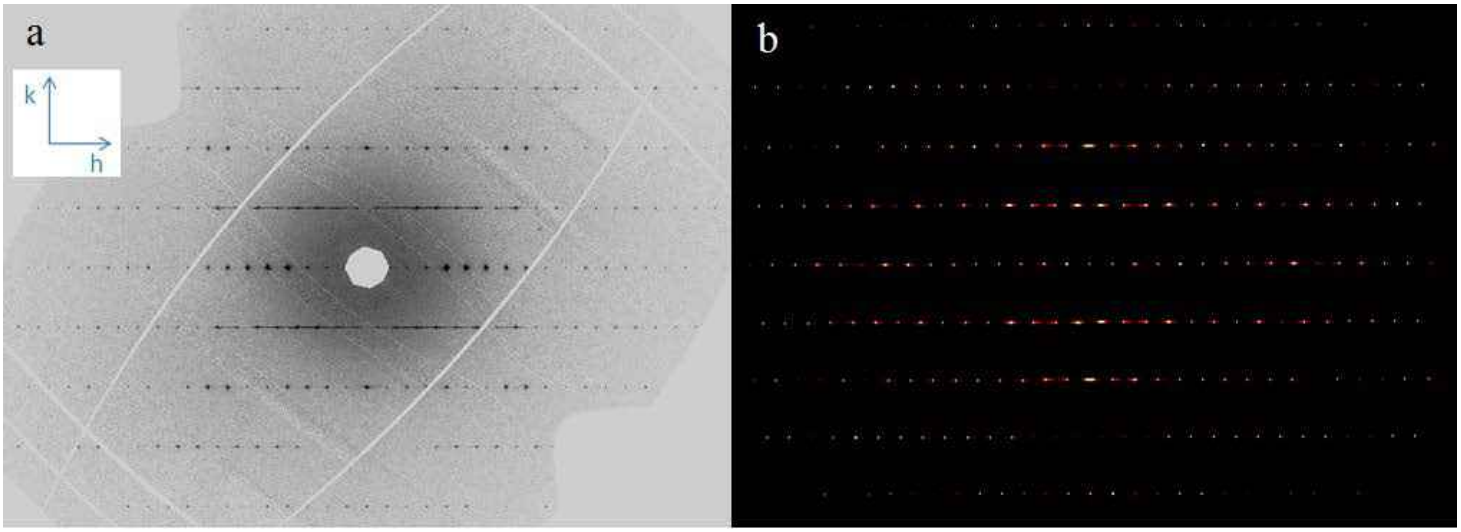
Diffraction methods are the most important methods to study the three-dimensional arrangement of matter at the atomic level. Real materials are often not perfectly ordered and the resulting diffraction pattern may contain a weak continuous or structured background known as diffuse scattering, in addition to sharp Bragg peaks. Our motivation is to analyse diffuse scattering in order to learn about the Short Range Order (SRO) of disordered crystals and improve the tools to model disorder phenomena. We are now investigating the SRO in DL-Norvaline which crystallizes in three known temperature-dependent phases. At least two of them (beta-phase space group C2/c above -70°C, alpha-phase P21/c around -90°C) show disordered average structures in which the alkyl side chain adopts several conformations [1]. The scattering data were collected using synchrotron radiation and a noise-free Pilatus pixel detector at the ESRF BM01A station. The diffraction pattern of the β-phase shows diffuse streaks parallel to a reciprocal lattice axis and diffuse clouds around low angle reflections [2] (Fig. 1). These features result from static and dynamic disorder. The diffuse streaks indicate disorder amongst stacks of layers of molecules, while the diffuse clouds arise from thermal motion. The modelling of the disorder involves the use of the Monte Carlo and differential evolution algorithms embedded in ZODS [3]. Our progress with model development will be presented.

[1] *C.H. Görbitz, J. Phys. Chem. B 2011, 115, 2447,* ***[2]*** *Agilent Technologies (2012). CrysAlisPro, Agilent Technologies, Yarnton, Oxfordshire, England,* ***[3]*** *ZODS: Zurich-Oak Ridge Disorder Simulation software, ETH/UZH, under development*



Keywords: structure disorder, diffuse scattering, static and dynamic disorder