

## Microsymposium

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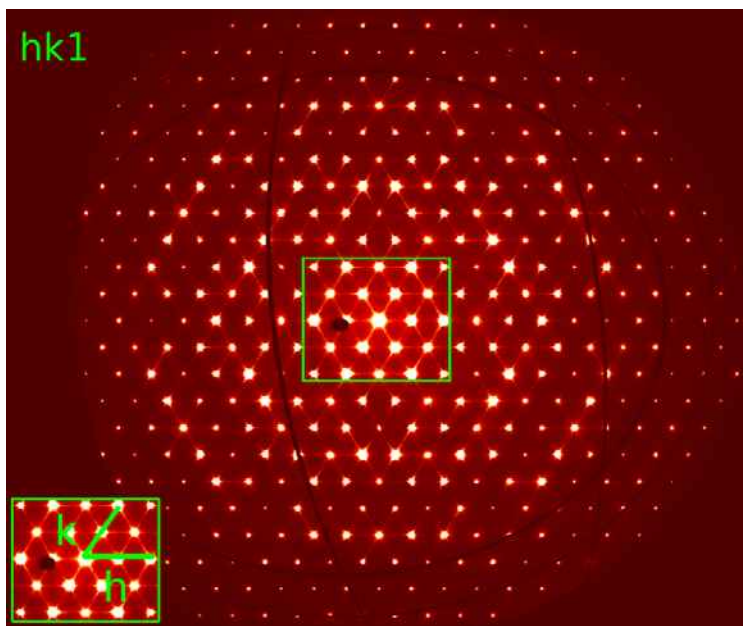
### Modelling diffuse scattering of the disordered crystal structure of $\text{Na}_2\text{SiF}_6$

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Many crystalline materials are not perfectly ordered, but are disordered to a smaller or larger extent. The properties of such materials are often related to the nature of the disorder. In diffraction experiments, disorder is observable as diffuse scattering. In routine X-ray structure determinations, only Bragg reflections are considered, leading to average crystal structure models. Methods to derive the average structure from the Bragg reflections are very well established, whereas diffuse scattering is rarely accounted for and mostly ignored. Our attempts at modelling the disordered structure of crystalline sodium fluorosilicate will be presented. Although the average crystal structure is known [1], there is some uncertainty about the true space group [2].  $\text{Na}_2\text{SiF}_6$  assumes a crystalline morphology that resembles that of ice and is therefore known as an ice-analog material [3]. In the average crystal structure (in space group P321), the asymmetric unit contains two ordered sodium cations (both sitting on a two-fold axis) and two disordered  $\text{SiF}_6^{2-}$  anions (one sitting on a 3-fold axis and the other on a 32 site). Each anion can occupy two alternative sites in the unit cell, related by a non-crystallographic mirror plane at  $z = \frac{1}{4}$ . The occupation is mutually exclusive for both anions. Diffuse scattering can be observed as planes perpendicular to  $l$  in the  $hkl$  and  $nkl$  precession images where these diffuse planes can be found at integer  $l$ . For  $l$  odd, the diffuse scattering is more intense. Also there are diffuse clouds of intensity around certain Bragg peaks. In the  $hkn$  planes, diffuse streaks are visible parallel to  $a^*$ ,  $b^*$ , and  $a^* - b^*$ , while some Bragg peaks have diffuse clouds of intensity around them. The pattern of streaks and clouds evolves when going to higher order planes. In the figure below, the  $hk1$  precession image is illustrated. The observed diffuse scattering features will be interpreted in terms of structural models obtained by Monte Carlo simulations.

[1] A. Zalkin, J. D. Forrester, D. H. Templeton, *Acta Cryst.*, 1964, 17, 1408, [2] G. F. Schäfer, *Zeitschrift für Kristallography*, 1986, 175, 269-276, [3] H. Jeong, Y. Huh, *Cryst. Materials Letters*, 2010, 64, 1816-1818



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