## MS28-03 | A Disordered Superspace Approach to Understand Highly Structured Diffuse Scattering

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Single crystal diffuse scattering is generally interpreted using correlation parameters, that describe probabilities for certain configurations on a local scale. If the diffuse maxima are at a general position in reciprocal space many parameters are needed to simulate a short range ordered structure in direct space, which reproduces the observed diffuse maxima.

In the field of incommensurate crystallography a (3+d)-dimensional approach is taken to describe satellite reflections in reciprocal space, that cannot be indexed with integer (h,k,l) . A 3-dimensional aperiodic crystal structure is periodic in (3+d)-dimensional superspace and the atomic positions and/or occupancies of the 3D structure are described by modulation functions.

A perfectly periodic superspace gives rise to sharp satellite reflections. In order to describe broadend satellite reflections we introduce disorder into superspace. By introducing phase domains in the superspace structure we can generate structures that give rise to diffuse maxmia at any position in reciprocal space with an arbitrary width [1]. The disordered superspace approach also allows for a straight forward simulation of a disordered structure using only few parameters.

The compound ThAsSe shows highly structured diffuse planes at **G**±0.14<110>*±Ɛ<110>*±η[001]* with Ɛ and η essentially continuous [2]. The observed extinction conditions and the sharp diffuse rods can be interpreted directly using the disordered superspace approach. The diffuse planes in reciprocal are reproduced from a computational model crystal that was build using the disordered superspace approach.

[1] Schmidt, E.M. and Neder, R.B. submitted.
[2] Withers, R.L. et al. Solid State Chemistry, 177 (2004) 701-708.