

Single Crystal Diffuse Scattering

Reinhard B. Neder

Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Diffuse scattering has been observed for almost as long as any single crystal diffraction, see [1] for a recent review on the subject. Further reviews are found for example in [2-7] and references therein. Diffuse scattering is observed for all classes of crystalline materials, metal alloys, simple inorganic materials, quasicrystals, molecular structures including protein crystals.

The intensity of the Bragg reflections describes the crystal structure very well with one important limitation. To the Bragg reflections all unit cells look alike. The Bragg reflections thus contain information on the average structure only. Any difference between the unit cells manifests itself in additional, usually weak diffuse scattering between the Bragg reflections. The diffuse scattering may be an almost featureless background or show a pattern of intricate complexity and may consist of streaks, layers, broad peaks or even curved distributions. The origin of the structural deviations may be due to dynamic effects such as the thermal movement of atoms or due to static effects. The first effect is commonly termed thermal diffuse scattering, while the second effect is referred to as disorder diffuse scattering.

The static deviations from the average structure can have many different reasons and may be present at different dimensions within the crystal. The deviations may be something as simple as a distribution of two or more atom types at a single site within the unit cell. Very often these local replacements cause a slight static shift of the surrounding atoms and these may be described as small clusters of slightly different structure. In a molecular structure the simplest defects might be a molecule in a slightly different conformation. From these simple defects one can consider a continuous and gradual change to larger objects such as domains with slightly different order or actual disolutions of a guest phase in the host crystal. Other defect types may disrupt the strict periodicity of the crystal on a larger scale such as stacking faults. Commonly the periodicity is maintained within the layers but the layer sequence deviates from a strictly periodic sequence.

Somewhat independent of the actual defect type, we need to consider the distribution of the defects throughout the host structure. Many times the defects are not randomly distributed and the correlations between neighboring defects introduce structure into the diffuse scattering.

In this lecture an overview of defect types, the arrangement of defects and the corresponding diffuse scattering is given. The lecture will describes current measurement, analysis and modelling techniques.

- [1] T.R. Welberry, T. Weber, *Crystallography Reviews* **22**, (2015).
- [2] B.T.M. Willis, H. Jagodzinski, F. Frey, J.M. Cowley, J. Gjonnes, P.S. Pershan in *Int. Tables for Crystallography Vol B*, U. Shmueli (Ed.), IUCR (1993), 383.
- [3] W. Schweika, *Disordered Alloys*, Springer (1998)
- [4] V.M. Nield, D.A. Keen, *Diffuse Neutron Scattering from Crystalline Materials*, Oxford University Press (2001).
- [5] T.R. Welberry, *Diffuse X-Ray Scattering and Models of Disorder*, Oxford University Press (2004)
- [6] R.B. Neder, T. Proffen, *Diffuse Scattering and Defect Structure Simulation*, Oxford University Press (2008)
- [7] T.R. Welberry, D.J. Goossens., *IUCr J.* **1**, (2014), 550

