From molecular dynamics simulations to diffuse scattering maps

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Modern materials often exhibit a considerable portion of structural disorder, playing a key role in their functionalities. In order to characterise local atomic arrangements and short-range correlations one has to study the shape of Bragg lines and the distribution of diffuse scattering below and between them.

To extract information from experimental data one has to compare model-based intensities with the observed ones. The progress in computing techniques in last decades permits to produce realistic models of crystalline lattices by a variety of approaches ranging from ab initio DFT methods via molecular dynamics (MD) to phase-field models based on the Landau formalism. Alternatively, one may retrieve the displacement pattern without making assumptions on its origin by reverse Monte-Carlo (RMC) modelling

With this progress in place the bottleneck has shifted from producing supercell models to generating the corresponding diffuse scattering distributions in reciprocal space. The principal issue being the fact that scattering amplitudes from a distorted lattice cannot be summed up using fast Fourier transform algorithms (FFT) because of the displacement phase factor exp(-iQR) being Q-dependent. As a consequence, many efforts in recent years have been restricted to simple models on small supercells [1,2] or to more involved pair distribution function (PDF) analysis [3-5], where the summation problem is reduced to a single dimension.

To address this issue, we will present the results of a new approach [6], based on recent developments of the non-uniform fast Fourier transform algorithm [7], implemented in the MP_tools program suite [8]. Diffracted intensities from model supercells containing millions of atoms as well as dynamic scattering functions $S(Q,\omega)$ based on time sequences of thousands of frames can be addressed in an interactive manner.

Many motivating discussions with my colleagues Marek Pasciak, Petr Ondrejkovic and Jirka Hlinka from the Institute of Physics (AS CR) are kindly acknowledged.

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