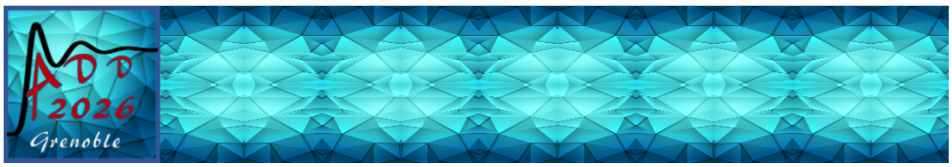

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DISCUS, Simulation and refinement of disordered crystal structures

Content

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DISCUS is a program that can simulate crystal structures and can calculate the corresponding diffraction pattern[1]. Its scope includes the possibility to simulate perfect crystal structures, as well as disordered structures. The program includes several toolboxes to introduce defects into the crystal structure. The strength of the program is the nearly unlimited flexibility that it offers to the user. One can use the program to simulate individual atoms, molecules, small clusters, finite-sized nanoparticles or crystals that are essentially infinite in size. Into each of these structures many different defects can be introduced via a set of tools integrated into the program.that still as an average periodic crystal structure, or a complex core/shell nanoparticles as well as a glass like structure without periodicity.

The tools to create disorder include basic options like the manipulation of individual atoms and extended tools to manipulate the crystal at large. These tools include short range order concepts to distribute different atom species or to distribute displacement correlations throughout the crystal. Empirical potential functions allow to introduce local distortions to the structure. Another tool builds stacking faults. These can be created as growth faults or use a short range order mechanism to build faults with more complex layer sequences. A new companion program allows the use of abstract generators to create essentially any stacking fault sequence. DISCUS uses an abstract domain concept to incorporate defects into a host structure. These defects might be anything from an individual atom, a small cluster, a guest crystal with regular or irregular internal host-guest surface or a set of molecules on top of a surface. The domains themselves may be subject to a short-range order distribution. Finally, modulated structures can be simulated with the use of displacement or density waves. To build finite crystals, options exist to create crystals limited by a suitable surface.

DISCUS calculates single crystal diffraction pattern of as well as powder diffraction pattern, the pair distribution function (PDF), and the 3D-PDF. The DISCUS program suite [2] includes two generic optimizer sections to refine disordered crystal structures with respect to experimental data. The DISCUS suite is available for Linux, Mac and Windows. The programm includes an MPICH option to allow fast parallel refinement on multiple core architectures or supercomputer frames. A set of interactive teaching pages is available to introduce disorder diffraction concepts [3].

[1] R.B. Neder, T. Proffen, *Diffuse Scattering and Defect Structure Simulation*, Oxford (2008).

[2] DISCUS is available on https://github.com/tproffen/DiffuseCode.

[3] DISCUS Teaching pages available on https://www.icsp.nat.fau.eu/neder-group/ (Under revision).

[4] K. Page, T.C. Hood, Th. Proffen, R.B. Neder, *J. Appl. Cryst.* **44**, 327 (2011).

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