Abstract ID : **138**

Monday 17 Oct, 14:00

PDFgui – a small box modelling platform for nanoscale structure analysis

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PDFgui is a user-friendly graphical interface built on the PDFfit2 small box modeling engine to fit neutron and X-ray PDF data and extract nanoscale structure information. The easy to use PDFgui environment organizes fits and simplifies many data analysis tasks, such as configuring and carrying out sequential refinements and plotting multiple fits. PDFfit2 is a program as well as a library for real-space refinement of crystal structures. It is capable of fitting a theoretical three-dimensional (3D) structure to atomic pair distribution function data and is ideal for nanoscale investigations. The fit system accounts for lattice constants, atomic positions and anisotropic atomic displacement parameters, correlated atomic motion, and experimental factors that may affect the data. The atomic positions and thermal coefficients can be constrained to follow the symmetry requirements of an arbitrary space group. PDFfit2 and PDFgui are freely available [1]. In this talk, the PDFgui concept and layout as well as essential capabilities will be presented. To exemplify the small box analysis as applied to bulk systems featuring nanoscale heterogeneities, a brief illustration of a recent hidden local symmetry breaking detection in a high performance thermoelectric system will be shown [2]. PDFgui functionality and typical use cases, such as co-refinement of multiple datasets, phase analysis, sequential refinements of variable length scales, temperature & composition, will be demonstrated during the followup hands-on tutorial. .

[1] "PDFfit2 and PDFgui: computer programs for studying nanostructure in crystals", C L Farrow et al., J. Phys.: Condens. Matter **19** 335219 (2007)

"Hidden local symmetry breaking in silver diamondoid compounds is the root cause of ultralow thermal conductivity", H. Xie et al., Adv. Mater. **34** 2202255 (2022)

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