

Institut de Minéralogie et de Physique des Milieux Condensés
Unité Mixte de Recherche 7590
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SÉMINAIRE

Vendredi 13 décembre, 10h30

*Salle de conférence, 4ème étage, Tour 22-23
IMPMC, Université P. et M. Curie, 4, Place Jussieu, 75005 Paris*

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RECENT DEVELOPMENTS OF FULLPROF FOR CRYSTAL STRUCTURE AND MICROSTRUCTURAL ANALYSIS

The FullProf Suite is one of the program suites most used in the world for the analysis of powder diffraction data. The programs of the suite allow the full treatment of diffraction data in complex cases: multiphase analysis using databases, microstructural parameters developed for treating micro-strain and size effects, symmetry modes for the analysis of structural distortions, incommensurate magnetic structures, powder and single crystal data, simultaneous refinement of multiple datasets, structure determination using simulated annealing, etc. In the present seminar I will present a general overview of what can be done using the programs of the FullProf Suite through a series of examples ranging from structure determination and refinement using symmetry modes to quantitative phase analysis through user-built databases.