

Collège de France
Chimie du Solide et de l'Énergie

SÉMINAIRE

Jeudi 11 décembre 2014, 10h30

Salle 2

*(entrée principale visiteurs à droite dans la cour d'entrée)
Collège de France*

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Understanding defective materials using powder diffraction (FullProf). The case of layered materials (FAULTS).

The analysis of the microstructure using “macroscopic” diffraction (x-rays or neutrons) consists on the determination of a series of parameters characterizing the crystallite size (coherent domains), the microstrain due to the presence of a variety of defects (dislocations, interstitials, vacancies, disorder), probabilities of stacking faults or micro-twinning, etc. Except for the latter case an extension of the Rietveld method, taking into account the instrumental resolution, is enough for a large kind of materials. The programs of the FullProf suite allow the full treatment of diffraction data in those cases. For the case of layered materials with a strong concentration of extended defects (stacking faults) simulation techniques have been applied by using mainly the DiFFAX program. We have created a new program (FAULTS), using the DiFFAX kernel, that allows a Rietveld-type of refinement in which the probabilities and shifts of the different kind of stacking faults are refinable parameters. In the present seminar I will present a general overview of what can be done in microstructural analysis using the programs of the FullProf Suite and an introduction to the new FAULTS program that will be shortly distributed within the FullProf Suite.