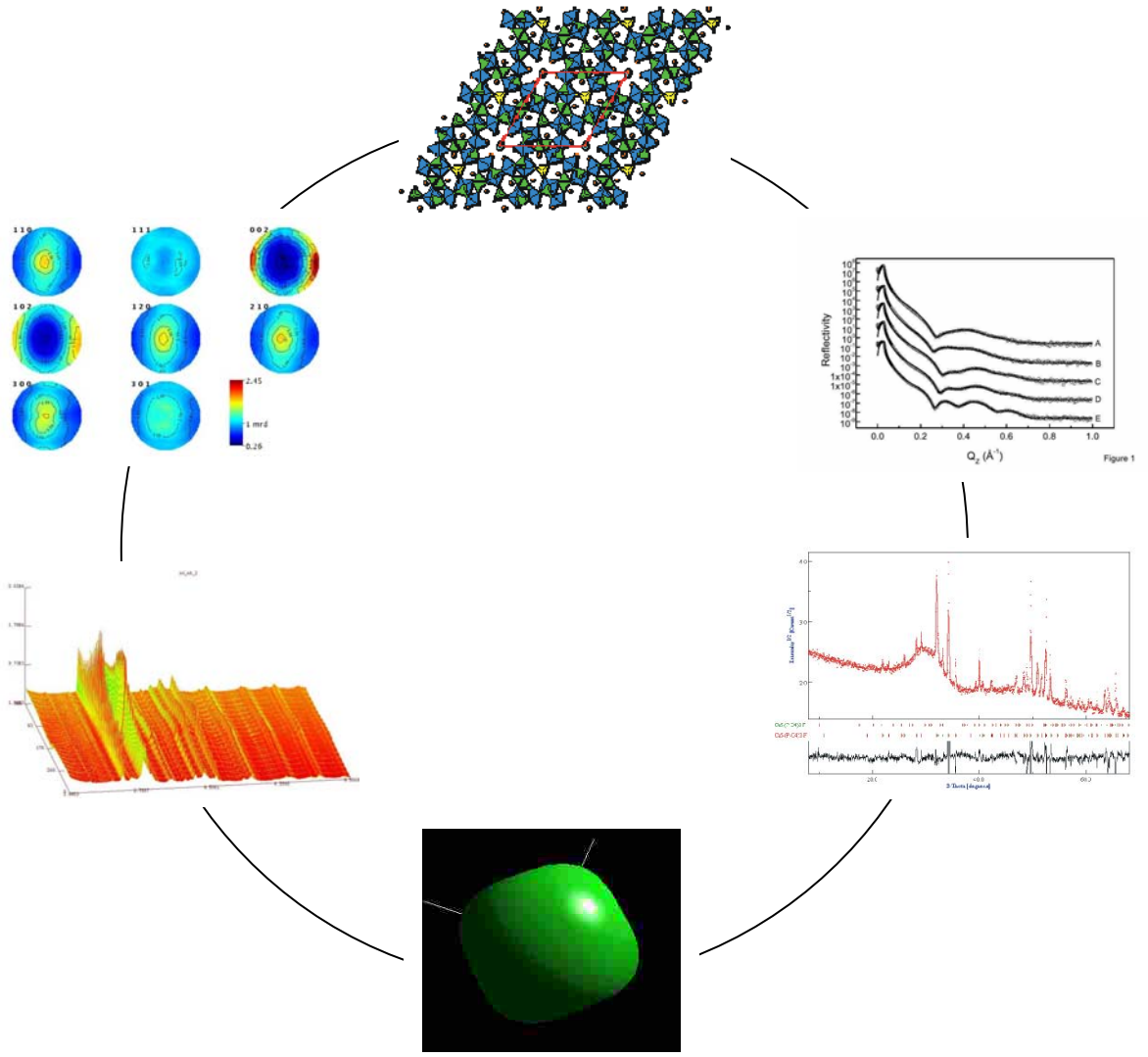
Combined Analysis: structure-texture-microstructure-phase-stresses-reflectivity determination by x-ray and neutron scattering



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http://www.ecole.ensicaen.fr/~chateign/texture/combined.pdf

Some typographical mistakes may have been introduced throughout this document.
Suggestions and corrections are very welcome.

0 Introduction

Solid state chemistry and technology recent developments gave rise to the necessity of intensive structural analysis from single crystal diffraction. However for many solids, single crystal growth is not easy to manage and sometimes impossible. When this is the case, or when structural defects cannot be overcome, the corresponding phases have often been forsaken, due to the inherent difficulties to carry out crystallographic characterisations on polycrystals. But in the last decades powder diffraction techniques progressed significantly, notably due to the Rietveld approach (Rietveld, 1969) and computer science developments. Undoubtedly these developments are of prior importance in the study of solids that do not form large crystals, but also of all materials elaborated by classical solid state reactions, thin deposited structures, natural materials like clays and more recently nanomaterials in which the required properties are intimately linked to the stabilisation of small crystals.

Since the Rietveld method's birth, several ten thousands of structures have been refined and some thousands have been resolved *ab-initio* from the only diffraction data of powder samples. The number of laboratories and industries using this technique, still fairly new when dealing with the incorporation of various formalisms like in the combined approach, does not stop increasing.

However, materials having specific properties are often elaborated from low symmetry phases, which are consequently anisotropic. Property's optimisation is then conditioned by the elaboration processes which have to keep the intrinsic microscopic anisotropy of the constituting crystals at the macroscopic level. These elaboration techniques are complex (alignment under uniaxial pressure, magnetic or electric fields, thermal gradients, flux or substrate growing ... and combinations) and often sample preparation is a hard, time consuming, matter. Naturally, non-destructive characterisations are then required. Unfortunately, when samples are oriented, which was not often the case until recently, most of the characterisation techniques (as the Rietveld analysis of concerns here) require samples grinding. Very often this grinding is not acceptable, for the previously described reasons, but also in the case of rare samples (fossils, comets ...) or simply when grinding modifies the physical behaviour of the samples themselves (thin films, residual stress materials ...). Sometimes grinding is simply not possible, imagine peeling off a 10 nm thick film on a substrate !

In all these cases, the combined analysis becomes essential.

The first part of this document is dedicated to some basic notions concerning diffraction by polycrystals. The various peak profiles used are described and some, most common combined analysis instrumental set-up detailed.

In the second part, powder diffraction data treatment is introduced. In particular, the Rietveld analysis is detailed, including treatment of all the information provided by diffraction diagrams, when texture is not present in the sample or simple to treat.

The third part deals with the automatic phase indexing, necessary step to solve a structure *ab-initio*.

Since its effect prevails on real samples where textures are often stabilised, quantitative texture analysis is detailed in the fourth part.

The fifth part is dedicated to microstructural aspects (isotropic and anisotropic crystal sizes and microdistortions) of the poder diffraction profiles.

In part six, quantitative phase analysis from Rietveld analysis is introduced.

Part seven describes residual stress analysis for isotropic and anisotropic materials.

The eighth part focuses on specular x-ray reflectivity and the various models associated.

Part nine introduces the combined analysis concept, showing all the dilemma that show up when one looks at only one part of the analyses, and case examples are shown as illustration of the methodology.

The 10^{th} part is dedicated to the anisotropic and tensorial macroscopic properties and their simulations to account for the distribution of crystallite orientations in samples.

This book is not intended to provide the reader a complete description of all the approached dealt within it, though quantitative texture analysis is more deeply detailed than others since texture appears to be the largest signal biaser, but a red wire to follow the many concepts introduced through so many years and necessary to understand scattering patterns.

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