Clip session 2007

François Léon

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Magnetic Quantitative Texture Analysis (MQTA) using neutron diffraction from powder and Laue single-crystal data.

Supervisors:

D. Chateigner, Professor at Université de Caen-Basse Normandie, Laboratoire CRISMAT-ENSICAEN UMR CNRS n°6508,

B. Ouladdiaf, Researcher at Institut Laue Langevin-Grenoble.

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➢ *Quantitative texture analysis (QTA).*

Cristalline texture : Knowledge of the different crystallite orientations

Orientation Distribution Function (ODF,f(g)) DV/V = f(g)dg :

g is the cristallite orientation with regards to the sample.

Random orientation → f(g)=1

Pole figures :

Represent the distribution of normals **h**=<hkl>* to the {hkl} planes of the sample, With $I_h(y)$ diffracted intensity.

The fundamental equation of the analysis of texture: $P_h(y) = \frac{1}{2\pi}\int_{hPy} f(g)d\bar{\varphi}$

Quantitative texture analysis

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MAUD software and combined analysis

Rietveld refinement and quantitative texture analysis

Does not take into account only the texture components, but also crystallite anisotropy, thickness, phase ratio, stresses…

Structure refinement by diffraction profile adjustment: Rietveld method (1969).

Minimises the following function : $M = \sum_i \frac{1}{\sigma_i^2}(y_i - y_{ic})^2$

σ_i : Is the variance associated to the observed y_i

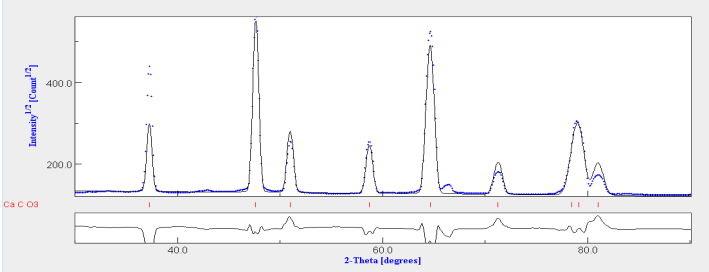
Calculated intensities : $Y_{ci} = Y_{bi} + \sum_{\phi=1}^{N_\phi} S_\phi \sum_{k=K_1}^{k} j_{\phi k} Lp_{\phi k} P_{\phi k} \left|F_{\phi k}\right|^2 \Omega_{i\phi k}$

Crystal structure of the sample is known as a closed model.

Quantitative texture analysis

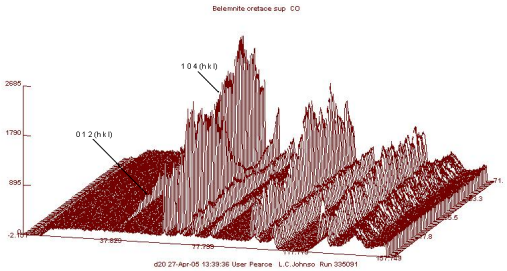
➢ Quantitative texture analysis developpement on D19.

- ➢ ***Results from the D20 instrument.***

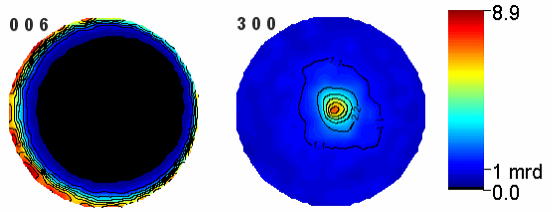


Sum of the 1368 diagrams measured on a belemnite rostrum standard from the Cretaceous (Lambda=2.4Å).

The refinement of the whole dataset using the Rietveld approach in the MAUD software and the E-WIMV algorithm to refine the ODF



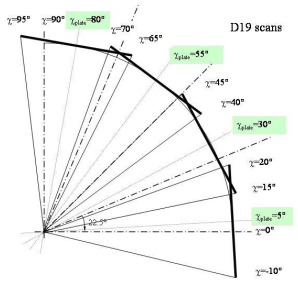
Pseudo-3D Plot



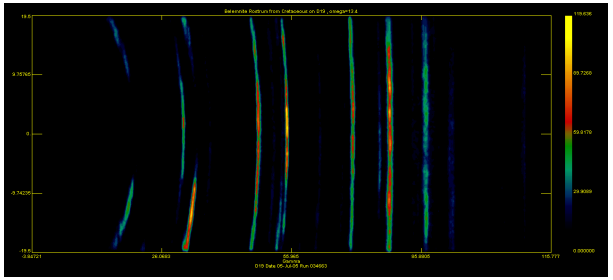
{006} and {300} pole figures.

Quantitative texture analysis

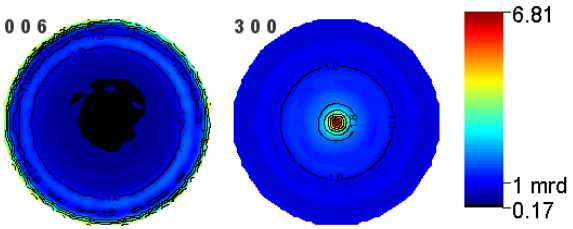
➢ ***Results from the D19 instrument.***



detector position χ



One Debye-Scherrer diagram (0°=χ, φ=0°)



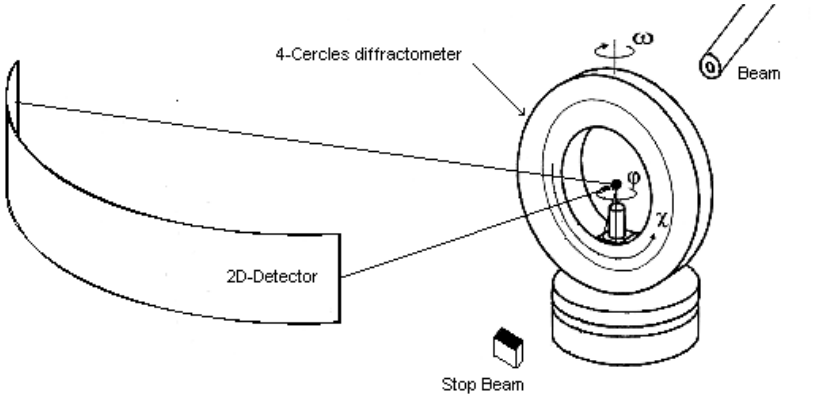
Sum of the diagrams measured on the belemnite rostrum (λ=1.315Å), and corresponding pole figures. Ou est la somme ?

➢ For this acquisition only 4 scans (vs 19 for D20).

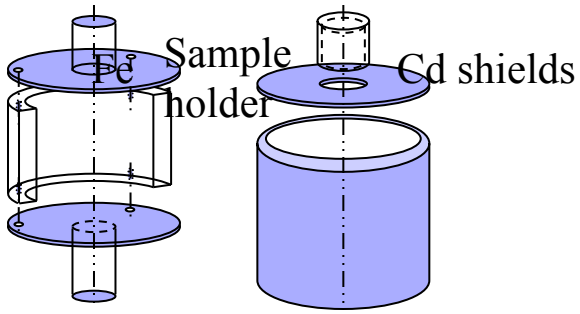
➢This reduces the acquisition time to less than 1h. This study aimed at checking the quality of the approach developed for quantitative texture analysis using two dimensional position sensitive detector (D19).

Magnetic quantitative texture analysis

➢ *Magnetic quantitative texture analysis (MQTA).*

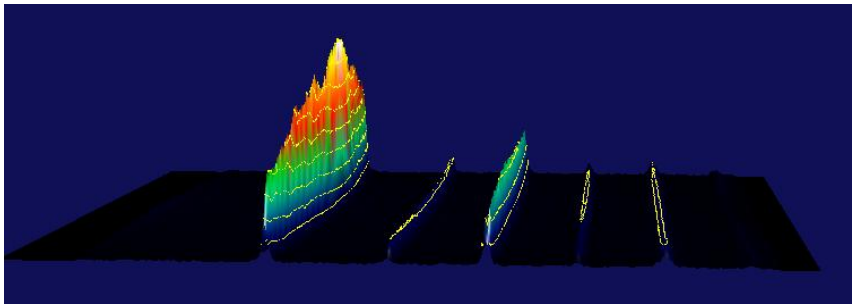


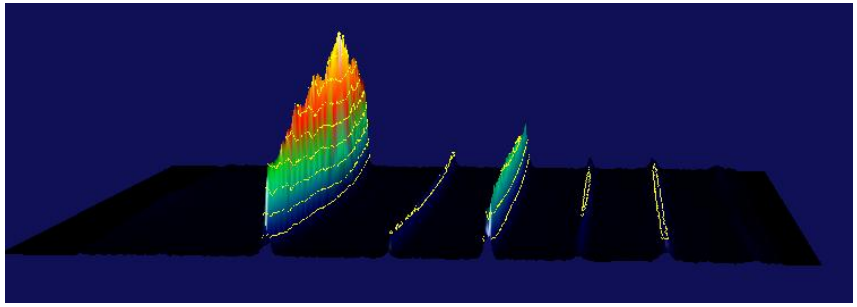
4-Cercles difractometer



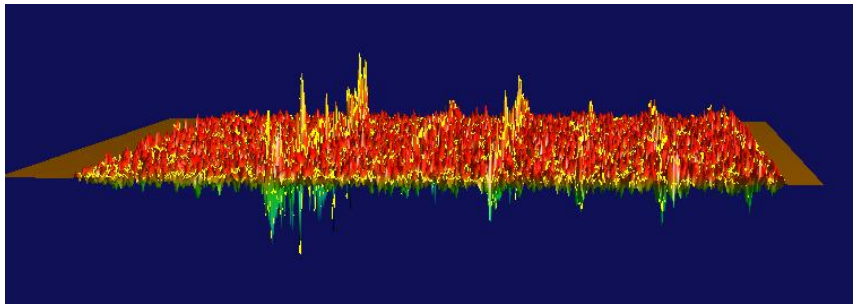
Magnetic sample holder to apply a fixed magnetic field during χ and φ rotations.

Magnetic quantitative texture analysis





Debye-Scherrer diagrams measured for 90°= ϰ et φ= -175° without (left) and with a field of 0.5T (right). Quel échantillon ?!!!



Difference between the two diagrams for 90°= ϰ et φ= -175°

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Aim of this study

Characterisation of magnetic materials in terms of angular dispersion of macroscopic magnetic moments (classically accessed using magnetisation measurements).

Extension of classical measurements which are not able to investigate how the resulting magnetic signals are linked to the crystallites and microstructures since they do not probe crystal lattices.

Interesting issues from

such developments can be outlined:

- - It could inform on how magnetic moments are linked to individual crystallites in the structure, how this link depends on external applied magnetic fields and how the macroscopic magnetisation establishes (e.g. by magnetic moment rotations) under applied fields.
- - Using tensor approaches, similarly as what was developed for other anisotropic properties, the MODF may serve as a predictive tool in the quantitative estimate of macroscopic magnetic properties of oriented samples [1].
- - As a non-destructive technique, the MODF technique would be useful to characterise real samples, using the newly developed formalism in a combined approach [2] for powder and in the orientation imaging [3] for Laue diagrams, for industrials and geologists for instance.

References :
[1]: M. Morales, D. Chateigner, D. Fruchart: *Journal of Magnetism and Magnetic Materials* , **257(2)**, 2003, 258-269.
[2]: M. Morales, D. Chateigner, L. Lutterotti, J. Ricote: *Materials Science Forum*, **408-412**, 2002, 113-118.
[3] H.-R. Wenk, F. Heidelbach, D. Chateigner, F. Zontone: *Journal of Synchrotron Radiation*, **4**, 1997, 95-101.

Acknowledgements

D.Richard (ILL)
S.Rivoirard (CRETA)

Thanks for you attention…