



Transferència de coneixement: CURSOS DE FORMACIÓ EN DIFRAC.EVA i TOPAS

Experiència des de 2001 impartint més de 60 cursos intensius per empreses, centres de recerca i universitats (modalitat on-line o presencial) en els temes següents:

- Introducció a la difracció de raigs-X de pols
- Preparació de mostres per difracció de raigs-X de pols
- Interpretació de difractograms amb Diffrac.EVA
- Bases de dades disponibles
- El mètode de Rietveld
- TOPAS. Introducció
- TOPAS. Anàlisi quantitatiu (mode GUI)
- TOPAS. Anàlisi quantitatiu avançat (mode LAUNCH)
- TOPAS. Mode LAUNCH
- TOPAS. Anàlisi quantitatiu automatitzat (mode LAUNCH)
- TOPAS. Anàlisi de la microestructura (mode GUI)
- TOPAS. Anàlisi de la microestructura avançat (mode LAUNCH)



Característiques dels cursos:

- Pressupostos a mida sense compromís
- Notes del curs en PDF i exemples treballs
- Suport bibliogràfic
- Contingut personalitzat a les necessitats del client
- Exemples de casos reals
- Treball intensiu amb difractogrames del client
- Suport científic després del curs

1. TOPAS. Introduction
 1.10 Sample preparation and analysis

We fill the cavity of the sample holder homogeneously.

We lightly press the sample so that it is evenly distributed. It is necessary to hold the sample holder to the glass.

We remove the compression accessory.

We remove the adapter from the sample holder.

Geometrical description of the diffractometer

7. TOPAS. Basic quantitative analysis
 7.2 Introduction of structures

Mullite structure:
 $Al_2[Al_2Si_2Si_2O_{10}]_{n-1}$
 $0.25 \leq x \leq 0.4$

It is a solid solution where the end members have the composition:
 $2Al_2O_3 \cdot SiO_2$ Mullite 2:1 or primary
 $3Al_2O_3 \cdot 2SiO_2$ Mullite 3:2 or secondary

Chains of AlO_6 octahedra parallel to the c axis joined by tetrahedra (Si, Al)O₄.

8. Quantification of diffractograms
 8.3 Proposed problems

7. TOPAS. Basic quantitative analysis
 7.5 Microabsorption effect and corrections

Effect of microabsorption
 In a two-phase system, the intensity ratio between two phases I_1/I_2 depends on the size of the particles in each phase and the difference between their absorption coefficients ($\mu_1 - \mu_2$).

$\mu_1 > \mu_2$ decrease I_1/I_2
 $\mu_1 < \mu_2$ increase I_1/I_2

1. TOPAS. Introduction
 1.4 Working with hkl_phases

Diffraction profile fitting:

Input data files → Emission profile → Background → Add hkl phase → G.E.S. a.b.c.a.r.y → Environmental Parameters? → YES → Select Peak Type (P, G, D, P, S) → Enter standard parameters and fit → Run (F6) → Zero error → U.V.W.X

PROPERTY window of each diffractogram. It is located under the diffractogram and the area under the curve. It is used on the relationship between these two areas.

Original diffractogram
 Diffractogram with X-offset: 0.1°
 Diffractogram with Displacement: -0.485 mm

Crystal Data:
 Molecular weight: 334.8
 Volume (Å³): 197.45
 Dn: 5.83
 Dm: 5.63
 I/Beer: 6.10

Chemical Formula: $(Ti_{0.4}Ni_{0.6})(Sb_{1.2}Ti_{0.8})O_6$

Mo 0.70932 Å
Cr 4.2897 Å



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The collage includes several key components:

- 2. Powder X-ray diffractometer** and **2.3 Sampleholder**: Diagrams showing the effect of sample parafocality on Bragg-Brentano geometry for different 2θ angles. It illustrates the focalization circle and the illuminated area being tangential.
- 8. Quantification of diffractograms with posed problems**: A summary of steps to follow, including a table for phase identification and a list of parameters like d_{hkl} and d_{hkl}^{obs} .
- 1. X-ray diffraction fundamentals** and **1.4 The diffraction phenomena**: Text explaining that depending on the symmetry of the crystal structure, some reflections (hkl) that are not systematically absent (extincts) in certain structures can have some reflections to almost zero intensity. It also mentions that these extinctions or diffraction conditions are tabulated in the International Tables of Crystallography.
- 2. TOPAS. Diffraction profile analysis** and **2.1 Basic concepts**: Graphically explains what is measured by X-ray diffraction and how it does not correspond to a simple model. It includes a diagram of secondary particles or grains and a scanning electron microscopy image of a crystal.
- 2. TOPAS. Diffraction profile analysis** and **2.4 Anisotropic broadening**: Shows a whole powder pattern fitting for a sample of nanocrystalline bricks. It lists steps: 1. File / Close All, 2. File / Load Files / MRI32085.RAW or MCI011070.raw / Add hkl phase, 3. MRI32085.RAW or P-3m, 4. Space Group / P-3m, 5. a (Å) / 3.14, b (Å) / 4.78 Refinings. It also shows parameters for d_{hkl} and d_{hkl}^{obs} .
- 7. TOPAS. Basic quantitative analysis** and **7.8 Quantification of clays**: Shows the initial cell parameters and the TOPAS program allowing stacking defects to be modeled using the LAUNCH programming mode. It includes a list of parameters for the structure resolution.
- Diffractogram interpretation with DIFFRAC.EVA (1)** and **Working with patterns**: Shows a diffractogram with peaks labeled (111) $Cu_{K\alpha 1} + K_{\alpha 2}$, (200) $Cu_{K\alpha 1} + K_{\alpha 2}$, (400) $Cu_{K\alpha 1} + K_{\alpha 2}$, and (400) $W_{L\alpha 1}$. It notes that in this case all reflections are generated for a cubic cell with $a = 5.4308\text{\AA}$, regardless of the extinctions.
- 2. TOPAS. Diffraction profile analysis** and **2.5 Proposed examples**: Shows a Williamson-Hall plot for CeO_2 with a slope of zero, indicating no microstrain. It also shows a plot for $\alpha-Fe$ with a slope, indicating microstrain induced.