Outline

1. **Summary of the simplified method (double-Voigt approximation) for analyzing microstructure of materials**
2. **Isotropic cases**
3. **Anisotropic cases**

Live presentation: (Cont. isotropic) Complete creation of an IRF file using the case of spinel MgAl$_2$O$_4$
Live presentation: (Anisotropic) Examples of anisotropic cases

Summary: IRF for microstructure analysis

1. **Collect a diffraction pattern with a well crystalized sample free of defects (Al_2O_3, Garnet, LaB_6, $Na_2Ca_3Al_2F_{14}$, etc.) for each used conditions of the diffractometer**
2. **Refine the collected patterns to obtain either the Gaussian and Lorentzian components of each peak (Peak fitting, Res=4, 8) or the instrumental U_{ins}, V_{ins}, W_{ins}, X_{ins}, Y_{ins} (Le Bail fits or Rietveld, Res=1)**
3. **Use EdPCR to copy the refined parameters in the dialog: Template > Instrumental Resolution File. Save the IRF file.**
4. **Refine a diffraction pattern of a normal sample using the IRF file putting, for starting the refinement, all the UVWXY parameters equal to zero. Select a microstructural model and refine it.**

Observed, instrumental and intrinsic profiles

$$h(x) = g(x) \otimes f(x)$$

GAUSSIAN   *U, V, W, I_G*   *LORENTZIAN*   *X, Y*

The parameters *U, V, W, I_G, X, Y* appearing in the PCR file make reference to the observed profile $h(x)$ **if no IRF file is used** (*U_h, V_h, W_h, I_{hG}, X_h, Y_h*).

The same parameters refer to the intrinsic profile $f(x)$ **if an IRF file is used** (*U_f, I_{fG}, X_f, Y_f*). Normally *V_f=0, W_f=0*

The IRF file stores the characteristics (*U_g, V_g, W_g, X_g, Y_g*) of the instrumental profile $g(x)$

Simplified methods for treating the intrinsic profile as implemented in FullProf

Parameters controlling the Full-Width at half maximum (isotropic case)

Isotropic Gaussian Strain

Isotropic Gaussian Size

$$H_{hG}^2 = (U_g + U_f)\tan^2\theta + V_g\tan\theta + W_g + \frac{I_{fG}}{\cos^2\theta}$$

Isotropic Lorentzian Strain

Isotropic Lorentzian Size

$$H_{hL} = (X_g + X_f)\tan\theta + \frac{Y_g + Y_f}{\cos\theta}$$

Simplified methods for treating the intrinsic profile as implemented in FullProf

Parameters controlling the Full-Width at half maximum (anisotropic case)

Isotropic Strain   Anisotropic Strain   Isotropic Size   Instrumental

$$H_{hG}^2 = (U_f + (1 - \xi_f)^2 D_{fST}^2(\boldsymbol{\alpha}_D)) \tan^2 \theta + \frac{I_{fG}}{\cos^2 \theta} + H_{gG}^2$$

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Isotropic Strain   Anisotropic Strain   Isotropic Size   Anisotropic Size   Instrumental

$$H_{hL} = (X_f + \xi_f D_{fST}(\boldsymbol{\alpha}_D)) \tan \theta + \frac{[Y_f + F_f(\boldsymbol{\alpha}_S)]}{\cos \theta} + H_{gL}$$

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Anisotropic strains

Position of peaks determined by:

$$\{\alpha_i\}=\{A,B,C,D,E,F\}$$

$$M_{hkl} = \frac{1}{d_{hkl}^2} = M\left(\alpha_i; hkl\right)$$

$$\frac{1}{d_{hkl}^2} = Ah^2 + Bk^2 + Cl^2 + Dkl + Ehl + Fhk$$

The mean and the variance of the function M_{hkl} are given by :

Average cell parameters

$$\langle M_{hkl} \rangle = M\left(\langle \alpha_i \rangle; hkl\right)$$

Spread of peaks (variance) :

$$\boxed{D_{fST}^2\left(\boldsymbol{\alpha}_D\right) \sim} \; \sigma^2\left(M_{hkl}\right) = \sum_{i,j} C_{ij} \frac{\partial M}{\partial \alpha_i} \frac{\partial M}{\partial \alpha_j}$$

$$\sigma^2\left(M_{hkl}\right) = \sum_{\substack{HKL \\ \{H+K+L=4\}}} S_{HKL} h^H k^K l^L$$

$$\boxed{\boldsymbol{\alpha}_D}$$

Anisotropic strain parameters

Anisotropic size

$$H_{sizeL} = k\beta_{size} = \frac{[Y_f + F_f(\boldsymbol{\alpha}_S)]}{\cos\theta} = \frac{k\lambda}{D_{\mathbf{h}}\cos\theta}$$

Integral breadth (β) and FWHM (H) are related by the constant k

Ellipsoidal shapes of crystallites .

$$\frac{\lambda}{D_{\mathbf{h}}} = Y_f + F_f(\boldsymbol{\alpha}_S) = \mathrm{k}_s\, d_{\mathbf{h}}^2(\alpha_1 h^2 + \alpha_2 k^2 + \alpha_3 l^2 + 2\alpha_4 hk + 2\alpha_5 hl + 2\alpha_6 kl)$$

Arbitrary shapes of crystallites can be simulated using spherical harmonics.

$$\frac{\lambda}{D_{\mathbf{h}}} = Y_f + F_f(\boldsymbol{\alpha}_S) = \sum_{lmp} a_{lmp} P_{lm}\left(\cos\Theta_{\mathbf{h}}\right) \begin{Bmatrix} \cos m\Phi_{\mathbf{h}} \\ \sin m\Phi_{\mathbf{h}} \end{Bmatrix} ; \quad p = +/-$$

Volume averaged shape of crystallites is obtained from the refined parameters

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