Does the March-Dollase underdetermined texture model influence structural determination ?

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Single crystal

Mean atomic positions

z_{Al}: 0.35222 (4) Å

$x_{O:}$ 0.3063 (2) Å

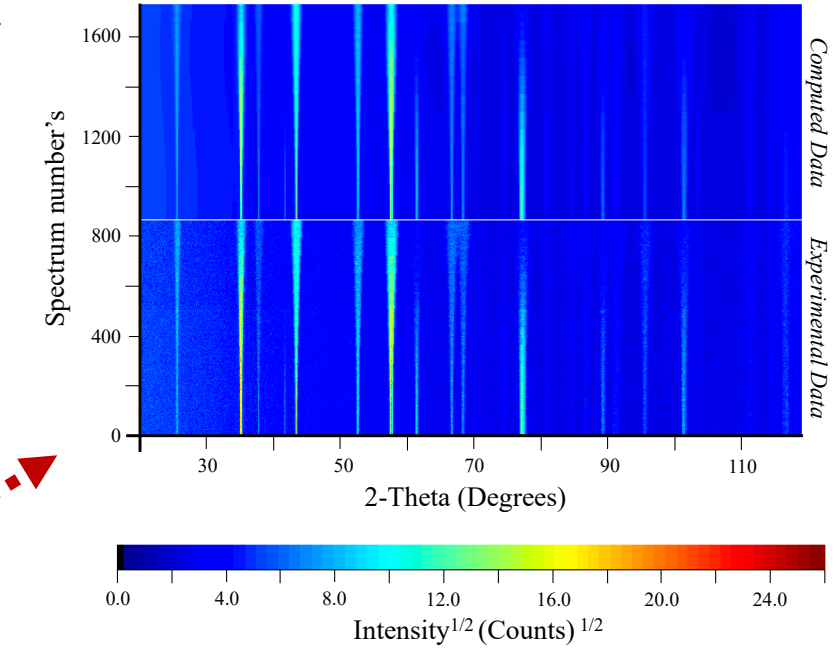

Fig 1 : *864 X-ray diffraction patterns for the α-Al_2O_3 sample acquired with a 4-circles diffractometer in as many sample orientations. Represented as 2D plots, bottom figure is for all observed diagrams and top diagrams for ODF-corrected Rietveld fits.*

	Bruker D8 Advance *2 circles diffractometer*		**ThermoFisher-Inel CPS-120** *4 circles diffractometer*	
	Atomic positions (Å)	*Reliability factors*	*Atomic positions (Å)*	*Reliability factors*
March-Dollase 2 components $\ell 00$ (99%) $-$ $\hbar 00$ (1%)	z_{Al}: 0.35232 (2) x_O: 0.3094 (2)	$\sqrt{GoF}$: 4.9 R_{wp} (%): 16.4 R_b (%): 13.3 R_{exp} (%): 3.3	z_{Al}: 0.35210 (1) x_O: 0.31464 (7)	$\sqrt{GoF}$: 1.4 R_{wp} (%): 33.9 R_b (%): 26.5 R_{exp} (%): 24.0
E-WIMV ODF : 3.75°	-		**z_{Al}: 0.352225 (7)** **x_O: 0.30633 (5)**	**$\sqrt{GoF}$: 1.2** **R_{wp} (%): 29.1** **R_b (%): 22.2** **R_{exp} (%): 24.0**

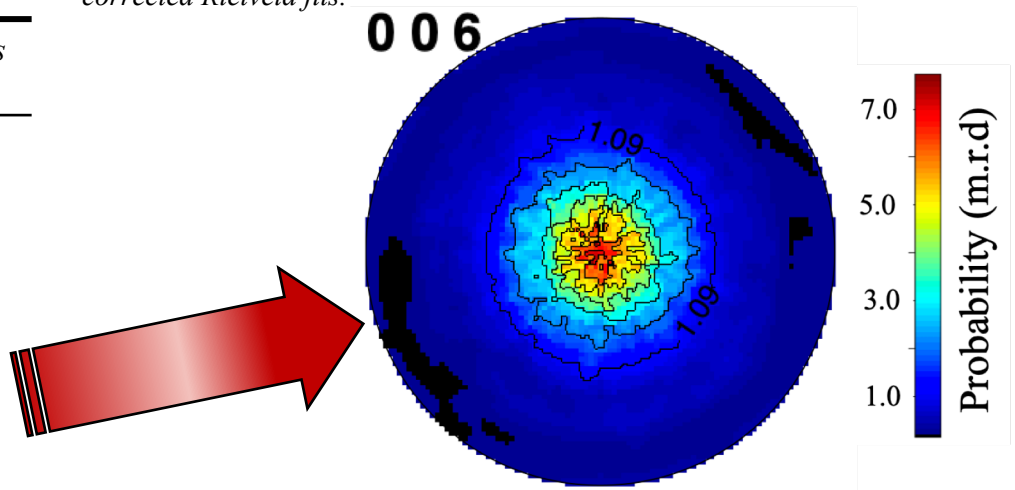

Fig 2 : *Normalized pole obtained after ODF refinement using E-WIMV.*