



JOURNAL OF
APPLIED
CRYSTALLOGRAPHY

Volume 50 (2017)

Supporting information for article:

A Bayesian approach to modeling diffraction profiles and application to ferroelectric materials

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The error used for least squares statistical approach is based on the variance equations as seen in Equation S1:

$$\text{Error} = 2 \frac{\left\{ I_{00h}^2 I_{h00}^2 \left((I_{h00} - \text{LCI}_{h00})^2 I_{00h}^2 + (I_{00h} - \text{LCI}_{00h})^2 I_{h00}^2 \right) \right\}^{1/2}}{(2I'_{00h} I_{h00} + I'_{h00} I_{00h})^2} \quad (\text{S1})$$

where LCI_{00h} and LCI_{h00} are the lower confidence interval (one standard deviation from the mean value) of the $(00h)$ reflection and the $(h00)$ reflection, respectively.

Table S.1 Extracted parameter values using least squares minimization for PZT thin film at 0 V.

I_{002}	x_{002}	m_{002}	F_{002}	I_{200}	x_{200}	m_{200}	F_{200}
12.77	3.28	1.0	0.059	119.02	3.38	0.041	0.081

Table S.2 Minimum and maximum of a uniform prior distributions for PZT thin film.

	I_{002}	x_{002}	m_{002}	F_{002}	I_{200}	x_{200}	m_{200}	F_{200}
Min	0.1	3.25	0	0.005	0.1	3.36	0	0.005
Max	100	3.32	1.0	0.5	500	3.40	1.0	0.5

Table S.3 Minimum and maximum of a uniform prior distributions for the PZT bulk material.

	I_{001}	x_{001}	F_{001}	I_{100}	x_{100}	F_{100}
Min	1.0	1.61	0.005	0.01	1.65	0.005
Max	100	1.65	0.5	1000	1.7	0.5

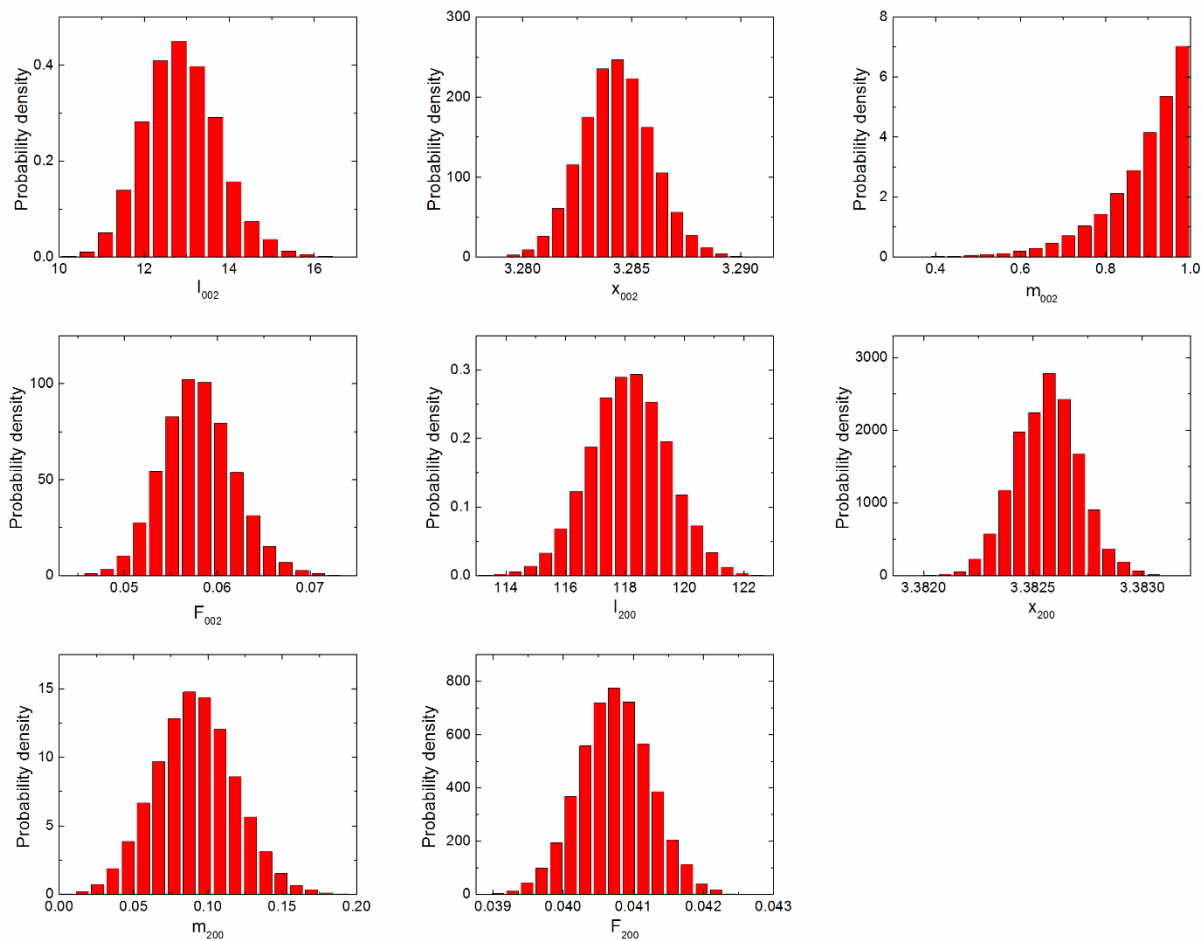


Figure S1. Representative posterior distributions of parameters for thin film PZT at 0 V.

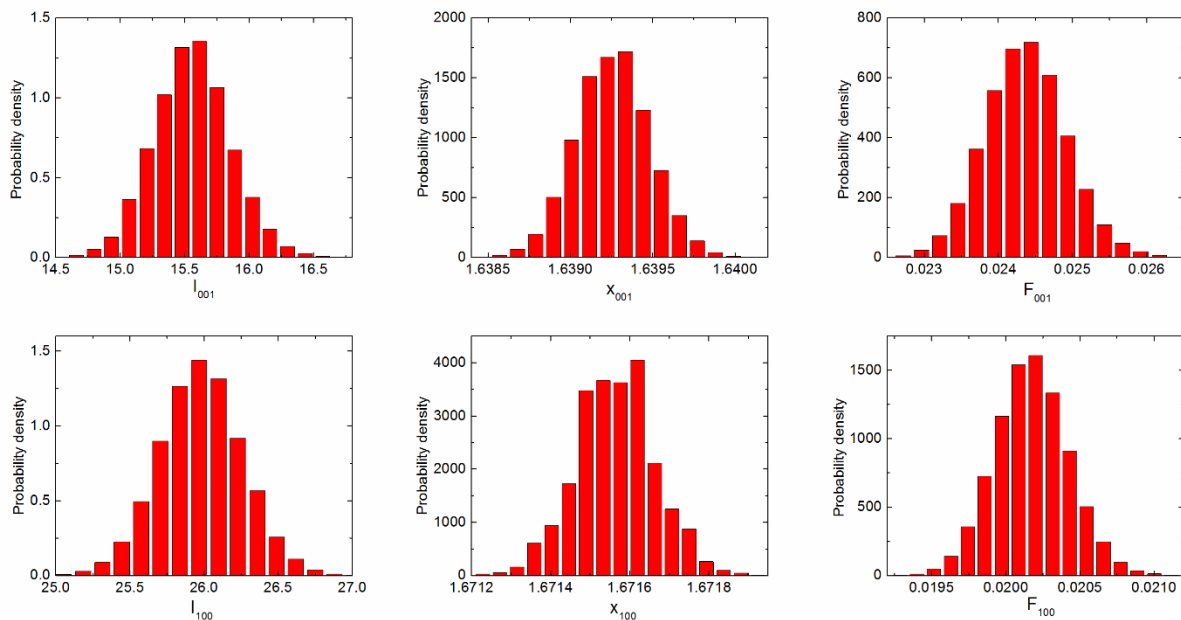


Figure S2. Representative posterior distributions of parameters for bulk K350 at 0 V.

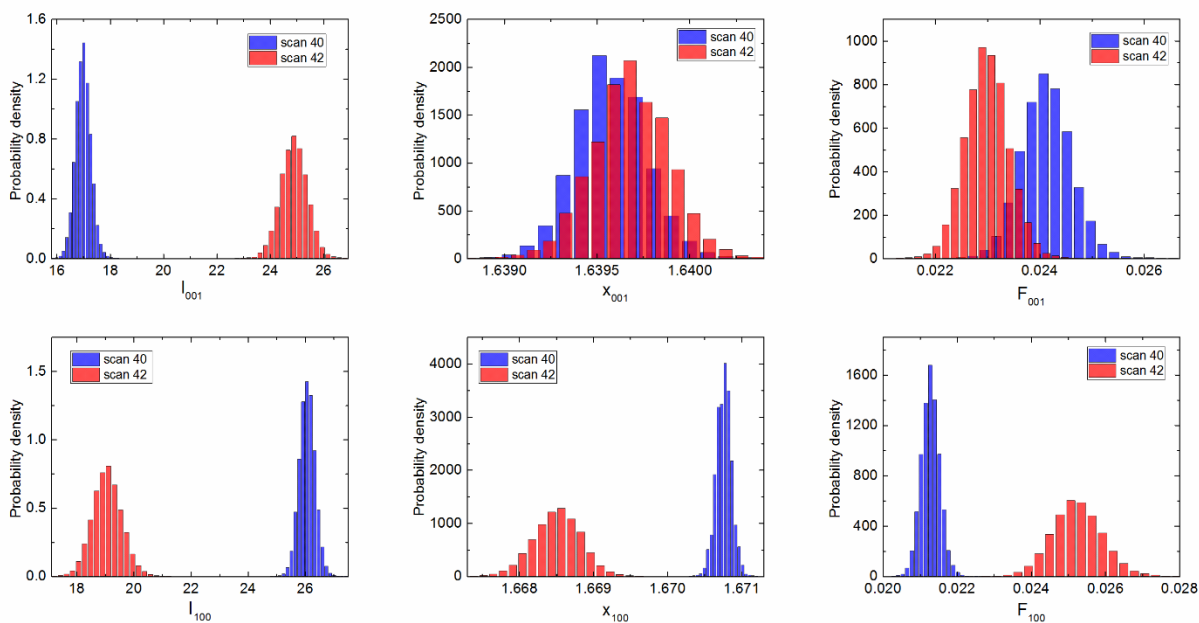


Figure S3. Posterior parameter distribution comparisons between broad and narrow domain reorientation distribution sets in PZT bulk material.