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Size and orientation of PNRs characterized by PDF analysis and a statistical model in $Bi(Mg_{1/2}Ti_{1/2})O_3$-$PbTiO_3$ ferroelectric re-entrant relaxor

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Supplementary Information

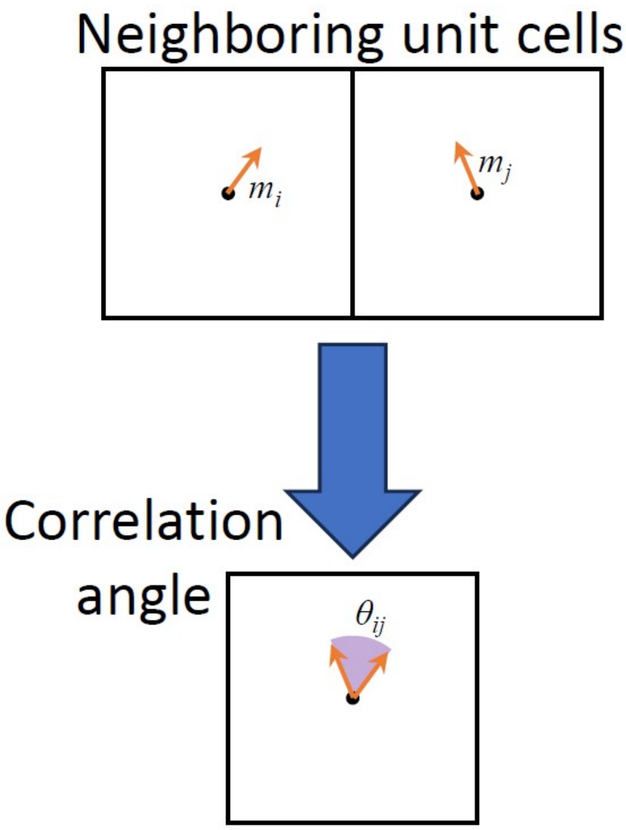

Figure S1: Illustration of the calculation of angular correlations for nearest neighbors in two dimensions. m_i and m_j correspond to the displacement vectors describing atom-atom pair i and j. θ_{ij} is the angle formed between the directions of the two displacement vectors.

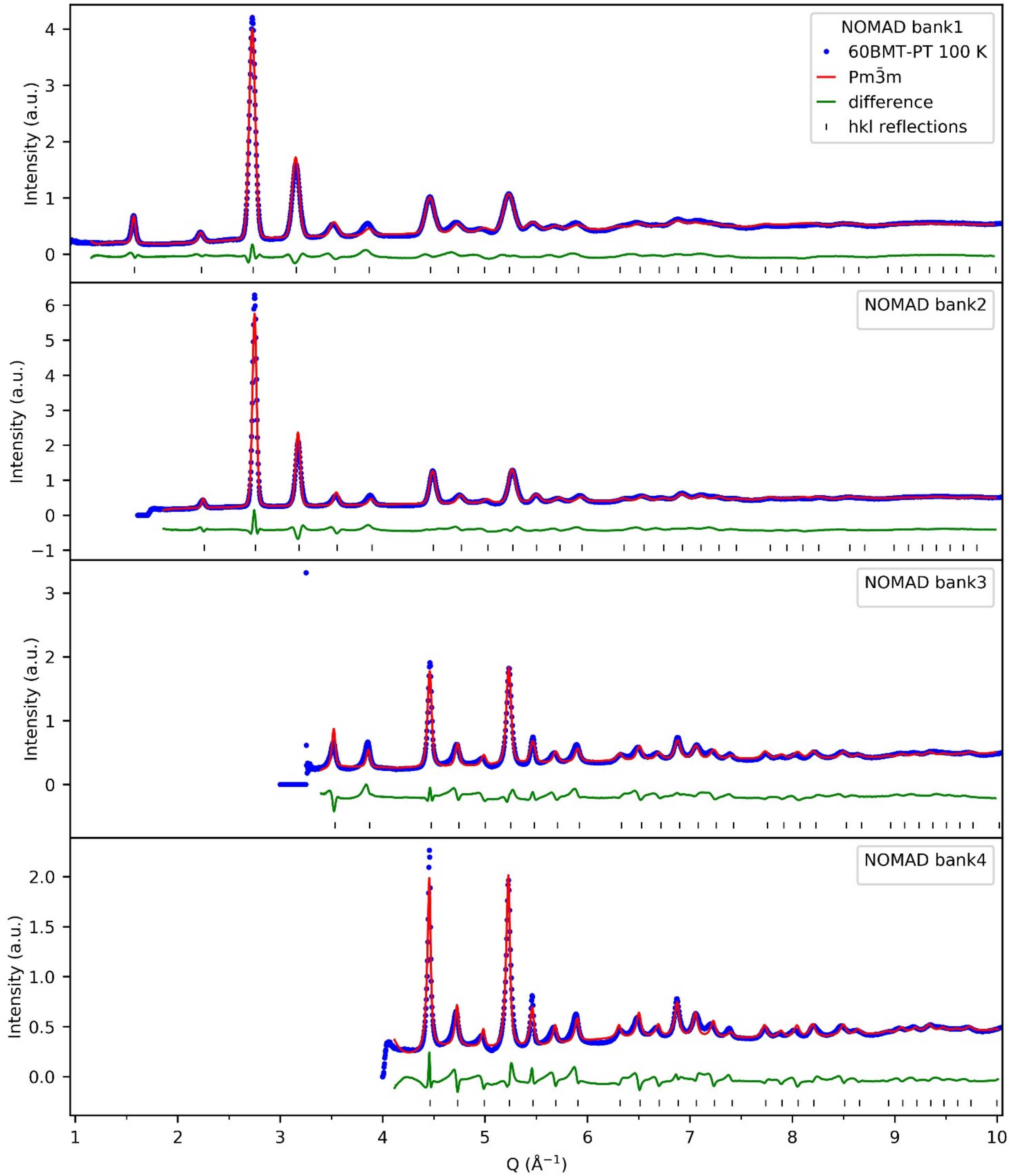

Figure S2 Neutron powder diffraction Rietveld refinement fit of 60BMT-PT at 100 K with a *Pm*-3*m* cubic unit cell.

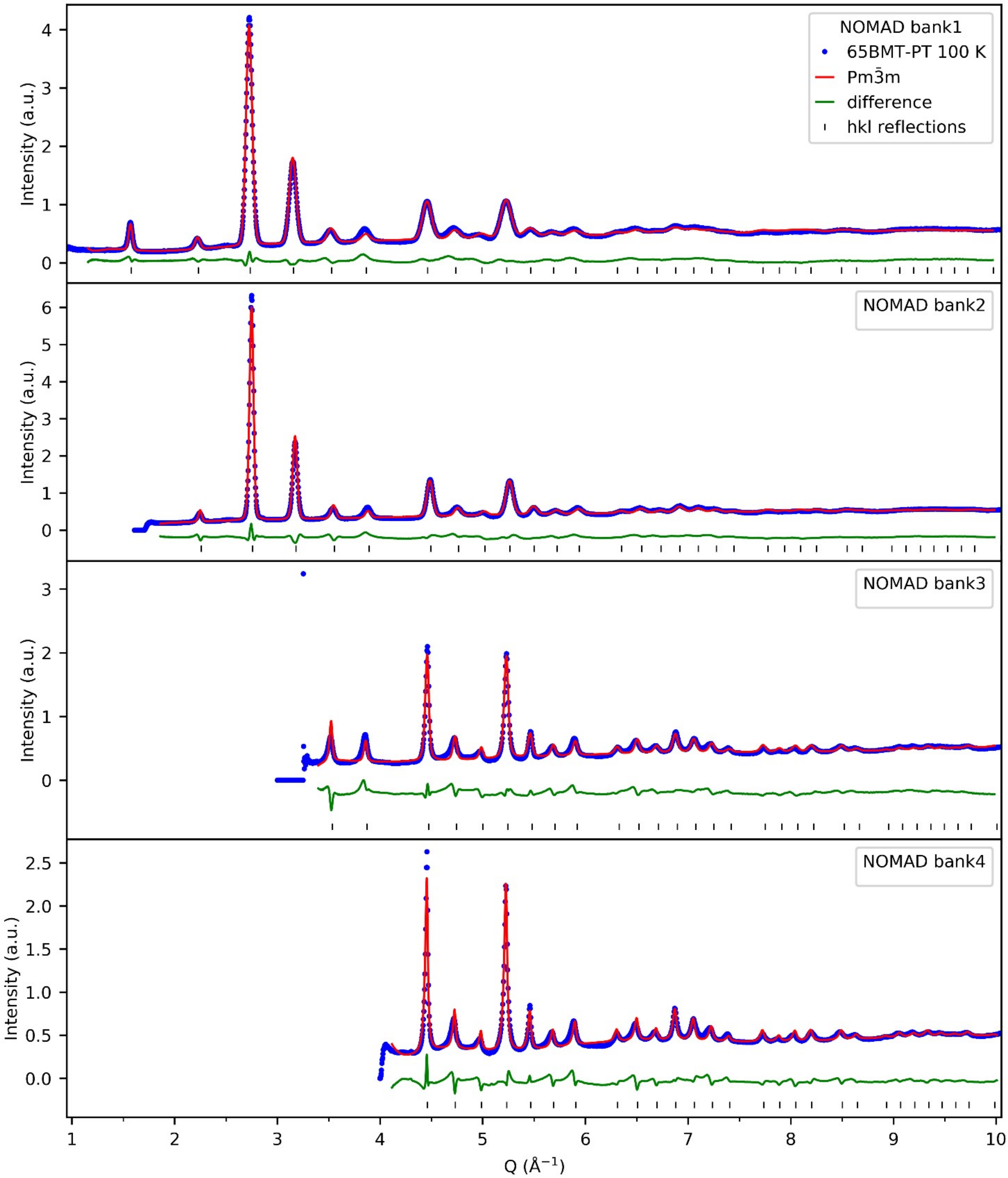

Figure S3 Neutron powder diffraction Rietveld refinement fit of 65BMT-PT at 100 K with a *Pm*-3*m* cubic unit cell.

Table S1 Rietveld refinement results for 60BMT-PT and 65BMT-PT using different models

Sample	Space group	Cell parameter		R value		
		a, *b* and *c* (Å)	*α*, *β* and *γ* (°)	R_p	R_{wp}	R_e
65BMT-PT	*Pm*-3*m*	3.9896	90	17.2	16.7	0.145
	*P*4*mm*	3.9759, 4.0293	90	10.3	11.5	0.126
	*R*3*m*	5.6436, 6.9093	90, 90, 120	16.7	18.4	0.147
	Pm-3*m*+ *R*3*m*	3.9836 5.6582, 6.9281	90 90, 90, 120	6.87	6.39	0.141
	Pm-3*m*+ *P*4*mm*	3.9734 3.9745, 4.0362	90 90	8.12	9.42	0.134
60BMT-PT	*Pm*-3*m*	3.9873	90	9.97	9.26	0.155
	*P*4*mm*	3.9700, 4.0391	90	9.21	10.6	0.133
	*R*3*m*	5.6398, 6.9071	90, 90, 120	16.9	17.0	0.156
	Pm-3*m*+ *R*3*m*	3.9873 5.6517, 6.9276	90 90, 90, 120	13.5	12.1	0.156
	Pm-3*m*+ *P*4*mm*	3.9999 3.9681, 4.0383	90 90	6.92	7.45	0.136

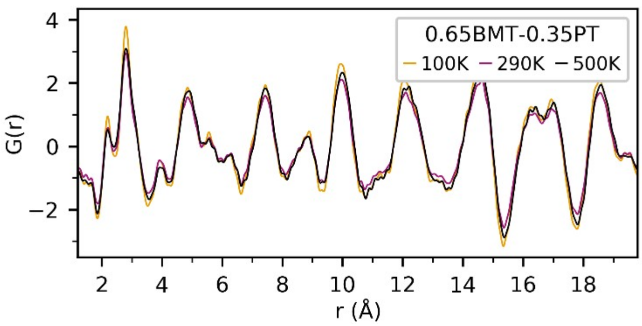

Figure S4 Neutron pair distribution function of 65BMT-PT.

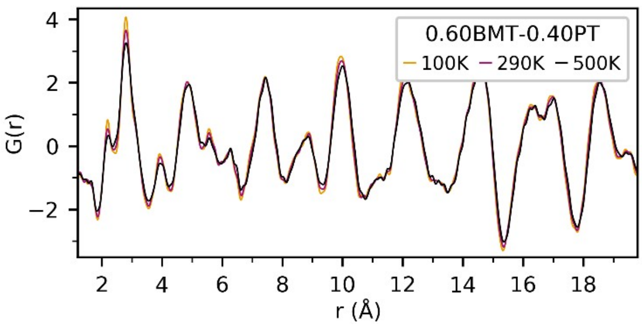

Figure S5 Neutron pair distribution function of 60BMT-PT.

Stereographic projections

For a directional perspective, stereographic projections were produced from the directional atomic displacements. The displacement vectors were determined, and their angles relative to the [001] and [100] cubic directions were calculated and binned into "windows" on the stereograph of an equal solid angle. The brightness of the perceptually uniform color scale indicates the relative number of directional displacements in each angular "window".

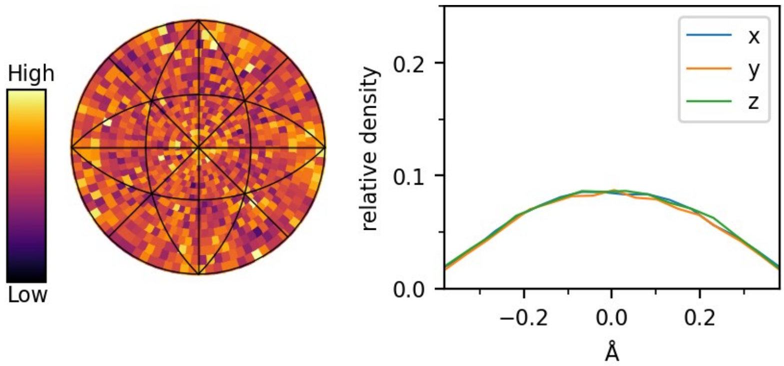

Figure S6 The directional displacement of Bi plotted on a stereographic projection (left). Histograms of the *x*,*y* and *z* displacements (right).

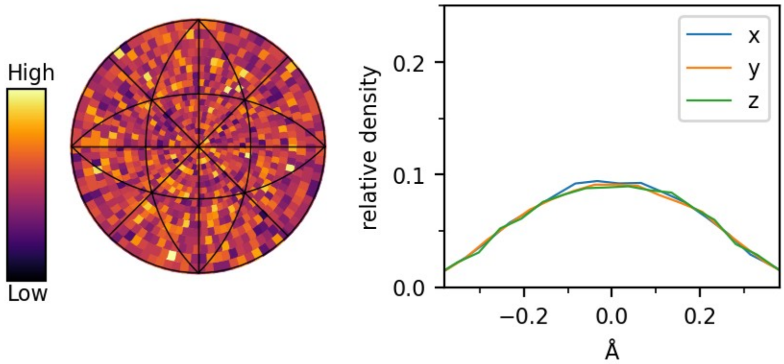

Figure S7 The directional displacement of Pb plotted on a stereographic projection (left). Histograms of the *x*,*y* and *z* displacements (right).

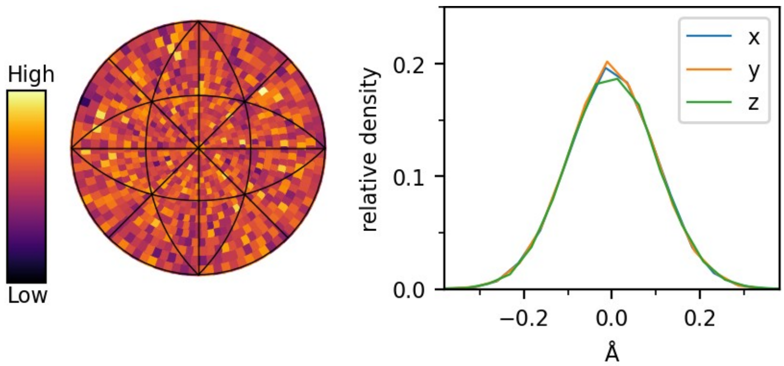

Figure S8 The directional displacement of Ti plotted on a stereographic projection (left). Histograms of the *x*,*y* and *z* displacements (right).

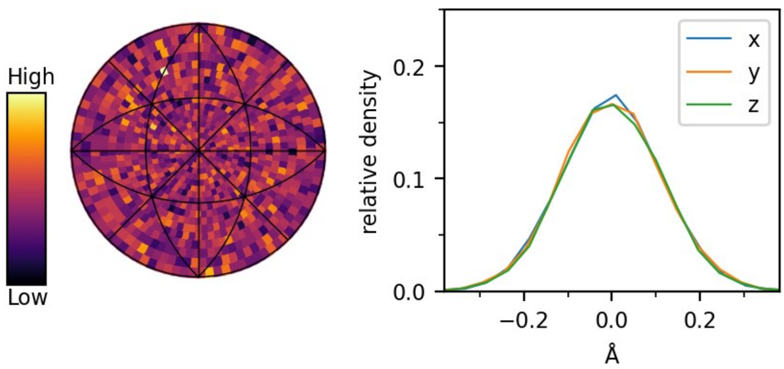

Figure S9 The directional displacement of Mg plotted on a stereographic projection (left). Histograms of the *x*,*y* and *z* displacements (right).