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Supporting information for article:

New capabilities for enhancement of *RMCProfile* – instrumental profiles with arbitrary peak shapes for structural refinements using the reverse Monte Carlo method

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Supplementary Information

New capabilities for enhancement of RMCProfile – instrumental profiles with arbitrary peak shapes for structural refinements using the Reverse Monte Carlo Method

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Fig. S1: Experimental (open symbols) and calculated (red line) diffraction patterns for $SrTiO_3$. The experimental pattern was measured on NOMAD and the calculated signal corresponds to the model refined in TOPAS.

Fig. S2: Diffraction profiles for $SrTiO_3$ calculated using TOPAS (open symbols) and RMCProfile (red line). The difference trace is shown in blue.

Fig. S3: Portions of the $D(r)$ for the models refined using the Polaris (red) and NOMAD (blue) data, respectively, which correspond to Fig. 7b in the main text. The uncertainty band (±2 standard deviations) associated with the statistical noise in the NOMAD data is indicated using cyan color. The standard deviation for the $D(r)$ is 0.0005. The uncertainty band for the Polaris $D(r)$ is even narrower. As can be seen, in many regions, the red trace falls outside of the uncertainty band.

Table S1. Average fractional atomic coordinates for $SrTiO_3$ referenced to a cubic unit cell with lattice parameter a=3.905 Å. (upper – Polaris, lower - NOMAD). The uncertainties reflect single standard deviations obtained from three independently refined configurations.

	x	*y*	*z*
Sr-1	-0.0005(7)	0.0002(7)	-0.0009(7)
	0.0000(1)	0.0000(2)	-0.0001(1)
Ti-2	0.5001(2)	0.4999(2)	0.5001(3)
	0.4999(1)	0.4999(1)	0.5000(1)
O-3	-0.0002(4)	0.5000(7)	0.5001(6)
	0.0000(1)	0.5000(3)	0.5001(2)
O-4	0.5003(7)	-0.0004(7)	0.5009(2)
	0.4999(2)	-0.0001(1)	0.5000(2)
O-5	0.5005(3)	0.5002(7)	-0.0004(2)
	0.5000(2)	0.5001(2)	-0.0000(2)

Procedure for generating Bragg-peak profiles in TOPAS4RMC

The program starts with generating a list of peak positions for all possible sets of *hkl*s. Since we are interested only in a profile shape, a single entry is used to represent a group of peaks having inequivalent *hkls* but identical (within a certain tolerance) positions. The script then cycles through the generated list, sequentially setting the intensity of a given peak to unity while zeroing all other peaks. At each step, Topas is called to run a zero-step Pawley calculation, outputting a tabulated profile for the selected peak. In these calculations, the scale factor is set equal to 1 to satisfy the normalization conditions. The background signal is extracted by setting the intensities of all *hkl* peaks to zero and running a zero-step Pawley calculation. The tabulated peak-profile

and background functions are supplied to RMCProfile as external input files. RMCProfile combines this information with actual peak intensities, which are calculated from atomic positions in the refined configuration, to generate a calculated Bragg pattern. The workflow for this procedure is summarized in Fig. 2 of the main text.

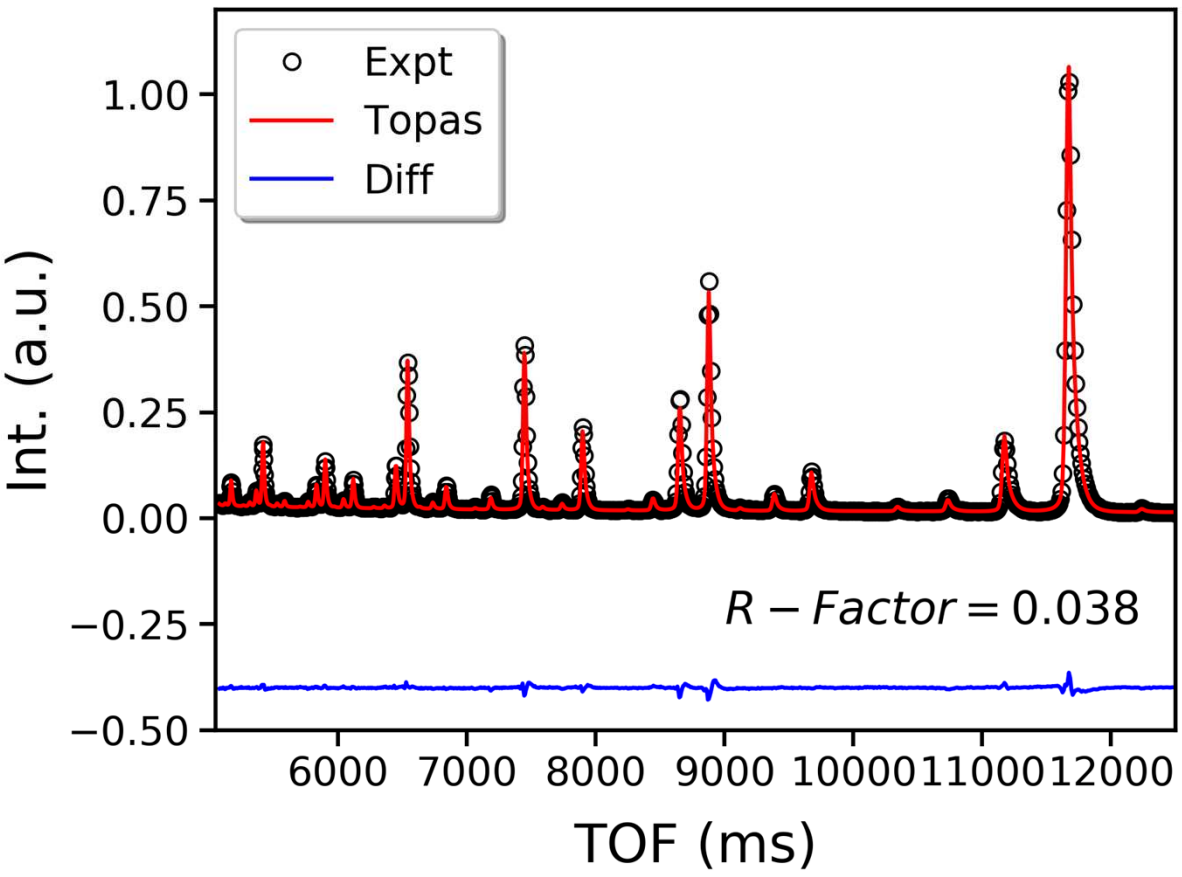
Expt
Topas
Diff
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
Int. (a.u.)
$R - Factor = 0.038$
6000
7000
8000
9000
10000
11000
12000
TOF (ms)

Fig. S1

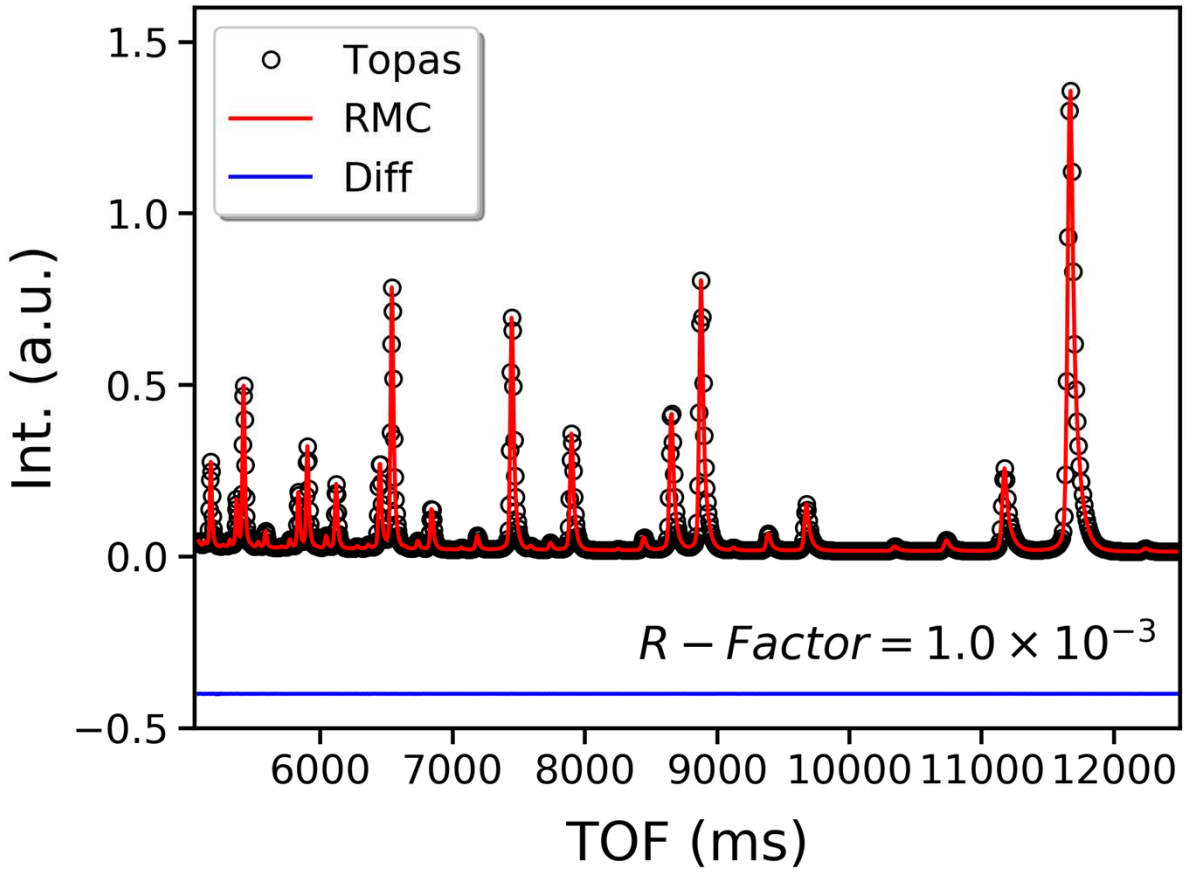
Topas
RMC
Diff
$R - Factor = 1.0 \times 10^{-3}$
Int. (a.u.)
TOF (ms)
1.5
1.0
0.5
0.0
−0.5
6000
7000
8000
9000
10000
11000
12000

Fig. S2

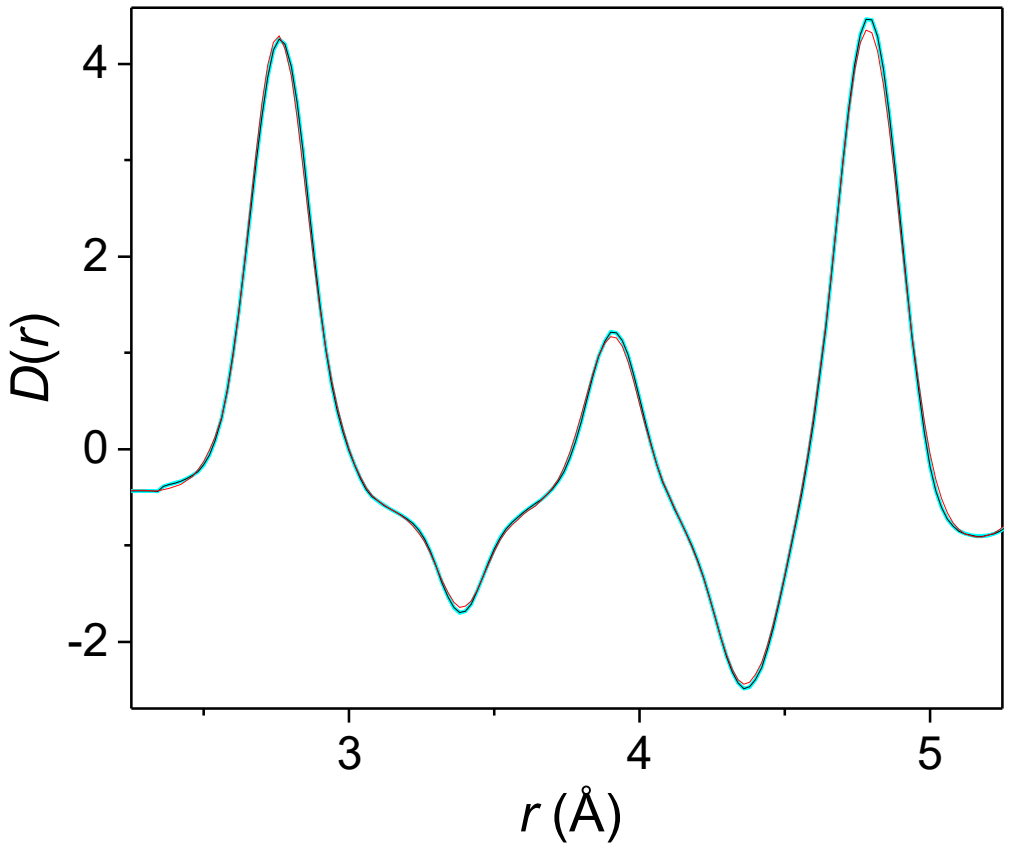

Fig. S3