crystals

MDPI

SUPPLEMENTARY MATERIALS:

Article

Correlation between Crystal Structure and Thermoelectric Properties of $Sr_{1-x}Ti_{0.9}Nb_{0.1}O_{3-\delta}$ Ceramics

J. Prado-Gonjal [1,2,*], C. A. López [3], R. M. Pinacca [3], F. Serrano-Sánchez [1], N. M. Nemes [4], O. J. Dura [5], J.L. Martínez [1], M.T. Fernández-Díaz [6] and J.A. Alonso [1]

[1] Instituto de Ciencia de Materiales de Madrid (ICMM). Consejo Superior de Investigaciones Científicas (CSIC). Sor Juana Inés de la Cruz 3, E-28049 Madrid, Spain; j.prado@csic.es; fserrano@icmm.csic.es; martinez@icmm.csic.es, ja.alonso@icmm.csic.es

[2] Departamento de Química Inorgánica, Universidad Complutense de Madrid, E-28040 Madrid, Spain; jpradogo@ucm.es

[3] INTEQUI, Universidad Nacional de San Luis, CONICET, Fac. Qca., Bqca. y Far. (Chacabuco y Pedernera, 5700), San Luis, Argentine; calopez@unsl.edu.ar; rmp@unsl.edu.ar

[4] Departamento de Física de Materiales, Universidad Complutense de Madrid, E-28040 Madrid, Spain; nmnemes@fis.ucm.es

[5] Departamento de Física Aplicada, Universidad de Castilla-La Mancha, E-13071 Ciudad Real, Spain; Oscar.Juan@uclm.es

[6] Institut Laue Langevin, BP 156X, F-38042 Grenoble, France; ferndiaz@ill.fr

* Correspondence: jpradogo@ucm.es

Table S1. Structural parameters after the Rietveld refinement of $Sr_{0.9}(Ti_{0.9}Nb_{0.1})O_{3-\delta}$ from NPD data at 300 °C in the *Pm-3m* space group, a = 3.92942 (5) Å, with λ= 1.051 Å. Discrepancy factors: R_p = 2.36%, R_{wp} = 3.11%, R_{exp} = 2.03%, R_{Bragg} = 4.65, $\chi 2$ = 2.51.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Sr	0.50000	0.50000	0.50000	0.0137 (4)*	0.9
Ti	0.00000	0.00000	0.00000	0.0077 (5)*	0.88
Nb	0.00000	0.00000	0.00000	0.0077 (5)*	0.12
O1	0.50000	0.00000	0.00000	0.0147 (5)	0.947 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0056 (7)	0.0192 (4)	0.0192 (4)	0.00000	0.00000	0.00000

Table S2. Structural parameters after the Rietveld refinement of $Sr_{0.9}(Ti_{0.9}Nb_{0.1})O_{3-\delta}$ from NPD data at 600 °C in the *Pm-3m* space group, a = 3.94097 (8) Å, with λ= 1.051 Å. Discrepancy factors: R_p = 2.22%, R_{wp} = 2.78%, R_{exp} = 2.03%, R_{Bragg} = 6.70%, $\chi 2$ = 1.87.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sr	0.50000	0.50000	0.50000	0.0197 (6)*	0.9
Ti	0.00000	0.00000	0.00000	0.0112 (6)*	0.88
Nb	0.00000	0.00000	0.00000	0.0112 (6)*	0.12
O1	0.50000	0.00000	0.00000	0.0211 (6)	0.952 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0095 (8)	0.0268 (6)	0.0268 (6)	0.00000	0.00000	0.00000

Table S3. Structural parameters after the Rietveld refinement of $Sr_{0.9}(Ti_{0.9}Nb_{0.1})O_{3-\delta}$ from NPD data at 800 °C in the *Pm-3m* space group, a = 3.94935 (10) Å, with λ= 1.051 Å. Discrepancy factors: R_p = 2.08%, R_{wp} = 2.57%, R_{exp} = 2.04%, R_{Bragg} = 6.62%, $\chi 2$ = 1.65.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sr	0.50000	0.50000	0.50000	0.0225 (7)*	0.9
Ti	0.00000	0.00000	0.00000	0.0139 (8)*	0.87
Nb	0.00000	0.00000	0.00000	0.0139 (8)*	0.12
O1	0.50000	0.00000	0.00000	0.0253 (7)	0.950 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0114 (9)	0.0322 (6)	0.0322 (6)	0.00000	0.00000	0.00000

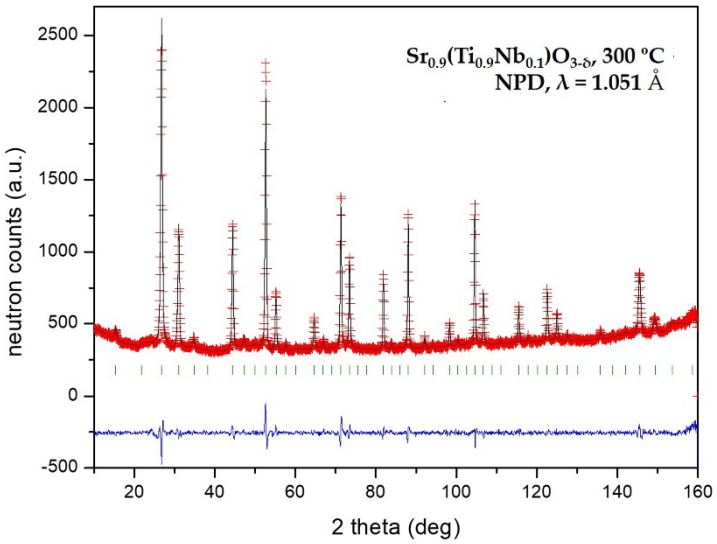

Figure S1. Observed (red crosses), calculated (black line), and difference (lower blue line) NPD profiles for $Sr_{0.9}(Ti_{0.9}Nb_{0.1})O_{3-\delta}$, at 300 °C. The allowed Bragg positions are shown as green vertical marks.

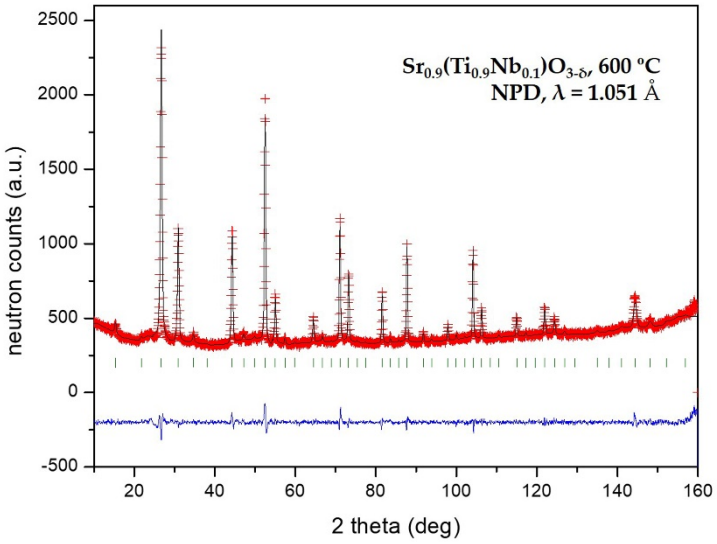

Figure S2. Observed (red crosses), calculated (black line), and difference (lower blue line) NPD profiles for $Sr_{0.9}(Ti_{0.9}Nb_{0.1})O_{3-\delta}$, at 600 °C. The allowed Bragg positions are shown as green vertical marks.