

Supporting information for

Spinodal decomposition in lead-free piezoelectric BaTiO₃-CaTiO₃-BaZrO₃ crystals

Gabriel Buse^{1,2}, Cong Xin^{1,2,3}, Pascal Marchet⁴, Ana Borta-Boyón⁵, Mai Pham-Thi⁵, Hughes Cabane⁶, Emmanuel Veron⁷, Michael Josse^{1,2}, Matias Velazquez^{1,2}, Michel Lahaye⁸, Eric Lebraud^{1,2}, Mario Maglione^{1,2}, Philippe Veber^{1,2,9,}*

¹ CNRS, ICMCB, UMR 5026, Pessac F-33600, France

² Université de Bordeaux, ICMCB, UMR 5026, Pessac F-33600, France

³ Materials, Research and Technology Department, Luxembourg Institute of Science and Technology-University of Luxembourg, 41 Rue du Brill, 4422 Belvaux, Luxembourg

⁴ Université de Limoges, IRCER, UMR 7315, Limoges F-87068, France

⁵ Thales Research and Technology, 1, av. Fresnel, Campus de l'Ecole Polytechnique – 91767 PALAISEAU Cedex, France

⁶ CristallInnov, Cleanspace , Parc d'Activités Alpespace, 354 voie Magellan, F-73800 Sainte Hélène du Lac, France

⁷ Conditions Extrêmes et Matériaux : Haute Température et Irradiation, Site Haute Température, CS 90055, 1D avenue de la Recherche Scientifique, 45071 Orléans cedex 2, France

⁸ Placamat, UMS 3626, CNRS, Université de Bordeaux, 87 avenue Albert Schweitzer, 33600 Pessac, France

⁹ Université Lyon, Université Claude Bernard Lyon 1, CNRS, Institut Lumière Matière UMR 5306, F-69100, Villeurbanne, France

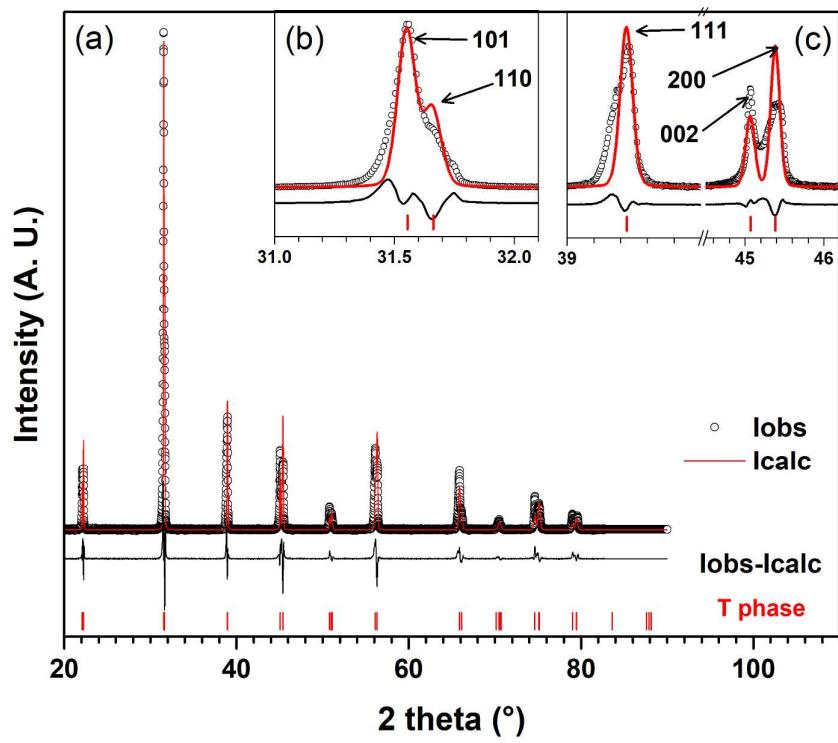


Figure S1. Results of the Rietveld refinement for annealed BCTZ6 crushed single crystal using the global composition $(\text{Ba}_{0.905}\text{Ca}_{0.0095})(\text{Ti}_{0.943}\text{Zr}_{0.057})\text{O}_3$ determined by EPMA, (a) 20–90° pattern refinement fit using tetragonal P4mm structure (space group #99), (b) and (c) details for selected peaks (the Miller indices are for tetragonal phase): GOF = 4.79, Rp = 16.04%, WRp = 23.94%

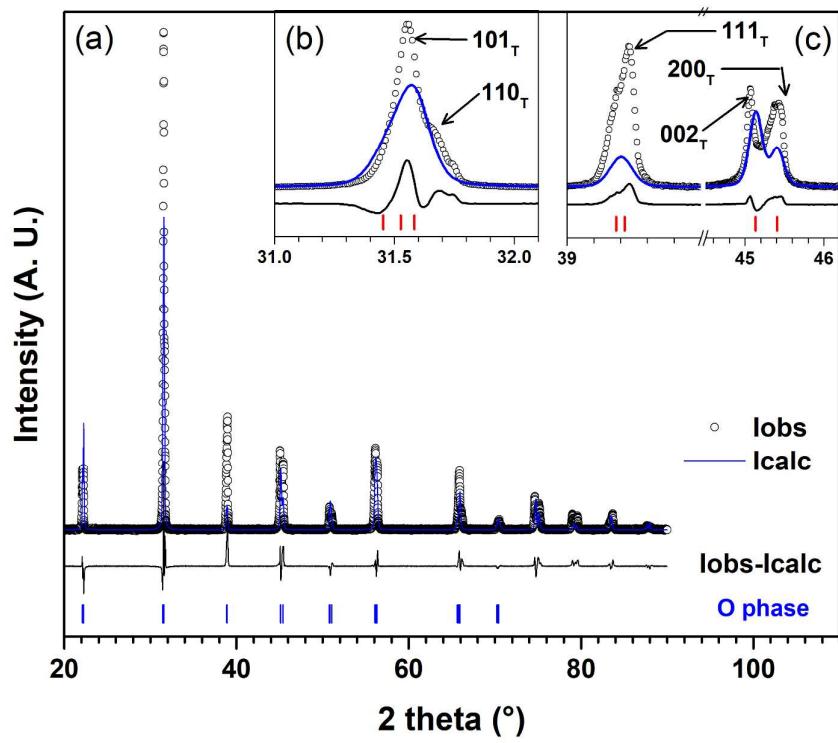


Figure S2. Results of the Rietveld refinement for annealed BCTZ6 crushed single crystal using the global composition $(\text{Ba}_{0.905}\text{Ca}_{0.0095})(\text{Ti}_{0.943}\text{Zr}_{0.057})\text{O}_3$ determined by EPMA, (a) 20–90° pattern refinement fit using orthorhombic Amm2 structure (space group #38), (b) and (c) details for selected peaks (the Miller indices are for tetragonal phase): GOF = 4.69, Rp = 16.35%, WRp = 24.69%

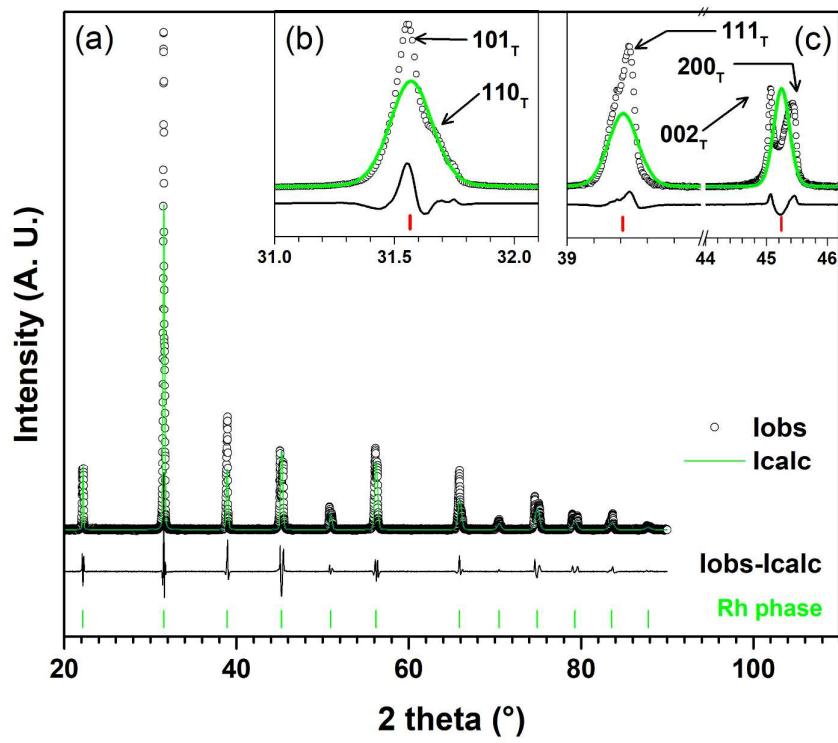


Figure S3. Results of the Rietveld refinement for annealed BCTZ6 crushed single crystal using the global composition $(\text{Ba}_{0.905}\text{Ca}_{0.0095})(\text{Ti}_{0.943}\text{Zr}_{0.057})\text{O}_3$ determined by EPMA, (a) 20–90° pattern refinement fit using rhombohedral R3m structure (space group #160), (b) and (c) details for selected peaks (the Miller indices are for tetragonal phase): GOF = 3.84, Rp = 13.43%, WRp = 20.19%