

## REFERENCES

- [1] S. Trolier-McKinstry, R.E. Newnham, Dielectrics and Ferroelectrics, Mater. Eng. (2018) 516–540. <https://doi.org/10.1017/9781316217818.029>.
- [2] Market Research Report, Piezoelectric Device Market, Report ID: PM2744 (2022).
- [3] S. Priya, H.C. Song, Y. Zhou, R. Varghese, A. Chopra, S.G. Kim, I. Kanno, L. Wu, D.S. Ha, J. Ryu, R.G. Polcawich, A Review on Piezoelectric Energy Harvesting: Materials, Methods, and Circuits, Energy Harvest. Syst. 4 (2019) 3–39. <https://doi.org/10.1515/ehs-2016-0028>.
- [4] F. Craciun, Dielectric, ferroelectric, antiferroelectric, relaxor, piezoelectric ceramics: Definitions and main applications, Elsevier Ltd., 2021. <https://doi.org/10.1016/B978-0-12-803581-8.12064-8>.
- [5] H. Jaffe, Piezoelectric Ceramics, J. Am. Ceram. Soc. 41 (1958) 494–498. <https://doi.org/10.1111/j.1151-2916.1958.tb12903.x>.
- [6] P.K. Panda, B. Sahoo, PZT to lead free piezo ceramics: A review, Ferroelectrics. 474 (2015) 128–143. <https://doi.org/10.1080/00150193.2015.997146>
- [7] K. Uchino, Glory of piezoelectric perovskites, Sci. Technol. Adv. Mater. 16 (2015). <https://doi.org/10.1088/1468-6996/16/4/046001>
- [8] R.K. Pandey, Fundamentals of electroceramics: materials, devices, and applications, John Wiley & Sons, 2019.
- [9] F. Cordero, Elastic properties and enhanced piezoelectric response at morphotropic phase boundaries, 2015. <https://doi.org/10.3390/ma8125452>.
- [10] G.A. Rossetti, A.G. Khachaturyan, G. Akcay, Y. Ni, Ferroelectric solid solutions with morphotropic boundaries: Vanishing polarization anisotropy, adaptive, polar glass, and two-phase states, J. Appl. Phys. 103 (2008). <https://doi.org/10.1063/1.2930883>.
- [11] D. Vanderbilt, M.H. Cohen, Monoclinic and triclinic phases in higher-order Devonshire theory, Phys. Rev. B. 63 (2001) 1–9. <https://doi.org/10.1103/PhysRevB.63.094108>.
- [12] A.K. Singh, S.K. Mishra, Ragini, D. Pandey, S. Yoon, S. Baik, N. Shin, Origin of high piezoelectric response of  $Pb(Zr_xTi_{1-x})O_3$  at the morphotropic phase boundary: Role of elastic instability, Appl. Phys. Lett. 92 (2008) 022910. <https://doi.org/10.1063/1.2836269>.
- [13] A.S. Bhalla, G. Ruyan, R. Rustum, The perovskite structure – a review of its role in ceramic science and technology, Mater. Res. Innov. (2000) 3–26.
- [14] T. Shi, G. Li, J. Zhu, Compositional design strategy for high performance ferroelectric oxides with perovskite structure, Ceram. Int. 43 (2017) 2910–2917. <https://doi.org/10.1016/j.ceramint.2016.11.085>.
- [15] N.K. Verma, A.K. Singh, Discovery of Ordered Tetragonal and Cubic Phases in the Morphotropic Phase Boundary Region of  $(1-x)Bi(Mg_{3/4}W_{1/4})O_3-xPbTiO_3$  Piezoceramics, Ceram. Int. 45 (2019) 17395–17408. <https://doi.org/10.1016/j.ceramint.2019.05.300>.
- [16] M. Singh, A.K. Singh, Studies on structural, morphological, and electrical properties of  $Ga^{3+}$  and  $Cu^{2+}$  co-doped ceria ceramics as solid electrolyte for IT-SOFCs, Int. J. Hydrogen Energy. 45 (2020) 24014–24025. <https://doi.org/10.1016/j.ijhydene.2019.09.084>.
- [17] J. Frantti, Notes of the Recent Structural Studies on Lead Zirconate Titanate, J.

- Phys. Chem. B. 112 (2008) 6521–6535. <https://doi.org/10.1021/jp711829t>.
- [18] B. Noheda, D.E. Cox, Bridging phases at the morphotropic boundaries of lead oxide solid solutions, Phase Transitions. 79 (2006) 5–20. <https://doi.org/10.1080/01411590500467262>.
- [19] S. Cheng, B. Zhang, S. Ai, H. Yu, X. Wang, J. Yang, C. Zhou, J. Zhao, G. Rao, Enhanced piezoelectric properties and thermal stability of  $\text{Bi}_{0.5}\text{Na}_{0.5}\text{TiO}_3$  modified  $\text{BiFeO}_3\text{-BaTiO}_3$  ceramics with morphotropic phase boundary, J. Mater. 93 (2023). <https://doi.org/10.1016/j.jmat.2023.01.001>.
- [20] F. Li, S. Zhang, D. Damjanovic, L.Q. Chen, T.R. Shroud, Local Structural Heterogeneity and Electromechanical Responses of Ferroelectrics: Learning from Relaxor Ferroelectrics, Adv. Funct. Mater. 28 (2018) 1–21. <https://doi.org/10.1002/adfm.201801504>.
- [21] A.K. Singh, S.K. Mishra, Ragini, D. Pandey, S. Yoon, S. Baik, N. Shin, Origin of high piezoelectric response of  $\text{Pb}(\text{Zr}_x\text{Ti}_{1-x})\text{O}_3$  at the morphotropic phase boundary: Role of elastic instability, Appl. Phys. Lett. 92 (2008) 1–4. <https://doi.org/10.1063/1.2836269>.
- [22] R.S. Solanki, S.K. Mishra, C. Moriyoshi, Y. Kuroiwa, I. Ishii, T. Suzuki, D. Pandey, Origin of high piezoelectricity at the morphotropic phase boundary (MPB) in  $(\text{Pb}_{0.94}\text{Sr}_{0.06})(\text{Zr}_x\text{Ti}_{1-x})\text{O}_3$ , (2017). <https://doi.org/10.48550/ARXIV.1703.02259>.
- [23] J. Fu, H. Qi, A. Xie, A. Tian, R. Zuo, Understanding the correlation between intermediate monoclinic phase (Cc) and piezoelectric properties in  $\text{NaNbO}_3\text{-BaTiO}_3\text{-CaZrO}_3$  ternary system with octahedral tilt, Acta Mater. 215 (2021) 117100. <https://doi.org/10.1016/j.actamat.2021.117100>.
- [24] M.J. Zou, Y.L. Tang, Y.L. Zhu, Y.J. Wang, L.X. Yang, X.L. Ma, Deterministic contribution of low symmetry phases to piezoresponse in oxide ferroelectrics, Acta Mater. 205 (2021) 116534. <https://doi.org/10.1016/j.actamat.2020.116534>.
- [25] Y.M. Jin, Y.U. Wang, A.G. Khachaturyan, J.F. Li, D. Viehland, Conformal miniaturization of domains with low domain-wall energy: Monoclinic ferroelectric states near the morphotropic phase boundaries, Phys. Rev. Lett. 91 (2003) 1–4. <https://doi.org/10.1103/PhysRevLett.91.197601>.
- [26] Y. Yan, L.D. Geng, L.F. Zhu, H. Leng, X. Li, H. Liu, D. Lin, K. Wang, Y.U. Wang, S. Priya, Ultrahigh Piezoelectric Performance through Synergistic Compositional and Microstructural Engineering, Adv. Sci. 9 (2022) 1–10. <https://doi.org/10.1002/advs.202105715>.
- [27] B. Noheda, D.E. Cox, G. Shirane, S.E. Park, L.E. Cross, Z. Zhong, Polarization rotation via a monoclinic phase in the piezoelectric 92% $\text{PbZn}_{1/3}\text{Nb}_{2/3}\text{O}_3$ -8% $\text{PbTiO}_3$ , Phys. Rev. Lett. 86 (2001) 3891–3894. <https://doi.org/10.1103/PhysRevLett.86.3891>.
- [28] E. Buixaderas, D. Nuzhnny, J. Petzelt, L. Jin, Polar lattice vibrations and phase transition dynamics in  $\text{Pb}(\text{Zr}_{1-x}\text{Ti}_x)\text{O}_3$ , 184302 (2011) 1–12. <https://doi.org/10.1103/PhysRevB.84.184302>.
- [29] F. Cordero, F. Craciun, F. Trequattrini, C. Galassi, P.A. Thomas, D.S. Keeble, A.M. Glazer, Splitting of the transition to the antiferroelectric state in  $\text{PbZr}_{0.95}\text{Ti}_{0.05}\text{O}_3$  into polar and antiferrodistortive components, Phys. Rev. B. 094107 (2013) 1–6. <https://doi.org/10.1103/PhysRevB.88.094107>.
- [30] G. Arlt, Domain contributions to piezoelectricity in ceramics, Proc. IEEE Ultrason. Symp. (1990) 733–742.
- [31] A.G.S. Filho, K.C. V Lima, A.P. Ayala, I. Guedes, P.T.C. Freire, F.E.A. Melo, J.M. Filho, Raman scattering study of the  $\text{PbZr}_{1-x}\text{Ti}_x\text{O}_3$  system : Rhombohedral-

- monoclinic-tetragonal phase transitions, (2002) 16–19. <https://doi.org/10.1103/PhysRevB.66.132107>.
- [32] I.H. Kim, I.H. Kim, S.G. Im, K.O. Jang, A phenomenological study on temperature-concentration-electric field phase diagram of relaxor ferroelectrics PMN-PT single crystals, *Phys. B Condens. Matter.* 639 (2022) 413961. <https://doi.org/10.1016/j.physb.2022.413961>.
- [33] A.K. Singh, D. Pandey, O. Zaharko, Powder neutron diffraction study of phase transitions in and a phase diagram of  $(1-x)[\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3] -x\text{PbTiO}_3$ , *Phys. Rev. B.* 74 (2006) 1–18. <https://doi.org/10.1103/PhysRevB.74.024101>.
- [34] D.M. Smyth, Defect structure in perovskite titanates, *Curr. Opin. Solid State Mater. Sci.* 1 (1996) 692–697. [https://doi.org/10.1016/S1359-0286\(96\)80053-2](https://doi.org/10.1016/S1359-0286(96)80053-2).
- [35] B. Noheda, D.E. Cox, G. Shirane, J. Gao, Z.G. Ye, Phase diagram of the ferroelectric relaxor  $(1-x)\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3-x\text{PbTiO}_3$ , *Phys. Rev. B - Condens. Matter Mater. Phys.* 66 (2002) 541041–5410410. <https://doi.org/10.1103/PhysRevB.66.054104>.
- [36] D.E. Cox, B. Noheda, G. Shirane, Y. Uesu, K. Fujishiro, Y. Yamada, Universal phase diagram for high-piezoelectric perovskite systems, *Appl. Phys. Lett.* 79 (2001) 400–402. <https://doi.org/10.1063/1.1384475>.
- [37] J. Hao, W. Li, J. Zhai, H. Chen, Progress in high-strain perovskite piezoelectric ceramics, *Mater. Sci. Eng. R Reports.* 135 (2019) 1–57. <https://doi.org/10.1016/j.mser.2018.08.001>.
- [38] G. Flora, D. Gupta, A. Tiwari, Toxicity of lead: A review with recent updates, *Interdiscip. Toxicol.* 5 (2012) 47–58. <https://doi.org/10.2478/v10102-012-0009-2>.
- [39] O.A. Ogunseitan, Public health and environmental benefits of adopting lead-free solders, *Jom.* 59 (2007) 12–17. <https://doi.org/10.1007/s11837-007-0082-8>.
- [40] C. Li, B. Xu, D. Lin, S. Zhang, L. Bellaiche, T.R. Shrout, F. Li, Atomic-scale origin of ultrahigh piezoelectricity in samarium-doped PMN-PT ceramics, *Phys. Rev. B.* 101 (2020) 1–7. <https://doi.org/10.1103/PhysRevB.101.140102>.
- [41] A. Upadhyay, H.A. Cha, J.H. Jeon, Stabilities and piezoelectric properties of morphotropic phase boundary composition  $0.2\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3-0.38\text{PbZrO}_3-0.42\text{PbTiO}_3$  ternary piezoceramics, *J. Mater. Sci.* 54 (2019) 6799–6806. <https://doi.org/10.1007/s10853-019-03365-3>.
- [42] D. Wang, Z. Fan, G. Rao, G. Wang, Y. Liu, C. Yuan, T. Ma, D. Li, X. Tan, Z. Lu, A. Feteira, S. Liu, C. Zhou, S. Zhang, Ultrahigh piezoelectricity in lead-free piezoceramics by synergistic design, *Nano Energy.* 76 (2020) 104944. <https://doi.org/10.1016/j.nanoen.2020.104944>.
- [43] H. Naganuma, Y. Inoue, S. Okamura, Evaluation of electrical properties of leaky  $\text{BiFeO}_3$  films in high electric field region by high-speed positive-up-negative-down measurement, *Appl. Phys. Express.* 1 (2008) 0616011–0616013. <https://doi.org/10.1143/APEX.1.061601>.
- [44] X. Li, Z. Chen, L. Sheng, L. Li, W. Bai, F. Wen, P. Zheng, W. Wu, L. Zheng, Y. Zhang, Remarkable piezoelectric activity and high electrical resistivity in Cu/Nb co-doped  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  high temperature piezoelectric ceramics, *J. Eur. Ceram. Soc.* 39 (2019) 2050–2057. <https://doi.org/10.1016/j.jeurceramsoc.2019.01.042>.
- [45] S. Harada, Y. Takagi, H. Nagata, T. Takenaka, Quenching effects on electrical properties of Cu-doped  $(\text{Bi}_{1/2}\text{Na}_{1/2})\text{TiO}_3$ -based solid solution ceramics, *J. Mater. Res.* 36 (2021) 1097–1104. <https://doi.org/10.1557/s43578-020-00048-7>.
- [46] Q. Gu, W.F. Liu, W. Wong-Ng, X.X. Wu, C. Wang, W. Zhou, S.Y. Wang, Modulation on the electrical and optical properties of Na and Rh co-doped Ruddlesden-Popper layered  $\text{Ca}_3\text{Ti}_2\text{O}_7$ , *J. Electroceramics.* 47 (2021) 42–50.

- https://doi.org/10.1007/s10832-021-00261-8.
- [47] S. Priya, A. Ando, Y. Sakabe, Nonlead perovskite materials:  $\text{Ba}(\text{Li}_{1/4}\text{Nb}_{3/4})\text{O}_3$  and  $\text{Ba}(\text{Cu}_{1/3}\text{Nb}_{2/3})\text{O}_3$ , *J. Appl. Phys.* 94 (2003) 1171–1177. https://doi.org/10.1063/1.1585121.
- [48] T.N. Nguyen, H.C. Thong, Z.X. Zhu, J.K. Nie, Y.X. Liu, Z. Xu, P.S. Soon, W. Gong, K. Wang, Review Hardening effect in lead - free piezoelectric ceramics, (2021). https://doi.org/10.1557/s43578-020-00016-1.
- [49] J. Hao, Z. Xu, R. Chu, Y. Zhang, G. Li, Q. Yin, Effects of  $\text{MnO}_2$  on phase structure, microstructure and electrical properties of  $(\text{K}_{0.5}\text{Na}_{0.5})_{0.94}\text{Li}_{0.06}\text{NbO}_3$  lead-free ceramics, *Mater. Chem. Phys.* 118 (2009) 229–233. https://doi.org/10.1016/j.matchemphys.2009.07.046.
- [50] C.S. Yu, H.L. Hsieh, Piezoelectric properties of  $\text{Pb}(\text{Ni}_{1/3},\text{Sb}_{2/3})\text{O}_3\text{-PbTiO}_3\text{-PbZrO}_3$  ceramics modified with  $\text{MnO}_2$  additive, *J. Eur. Ceram. Soc.* 25 (2005) 2425–2427. https://doi.org/10.1016/j.jeurceramsoc.2005.03.075.
- [51] D. Lin, K.W. Kwok, H.L.W. Chan, Effects of  $\text{MnO}_2$  on the microstructure and electrical properties of  $0.94(\text{K}_{0.5}\text{Na}_{0.5})\text{NbO}_3\text{-}0.06\text{Ba}(\text{Zr}_{0.05}\text{Ti}_{0.95})\text{O}_3$  lead-free ceramics, *Mater. Chem. Phys.* 109 (2008) 455–458. https://doi.org/10.1016/j.matchemphys.2007.12.015.
- [52] M. Zhang, X. Zhang, S. Das, Z.M. Wang, X. Qi, Q. Du, High remanent polarization and temperature-insensitive ferroelectric remanent polarization in  $\text{BiFeO}_3$ -based lead-free perovskite, *J. Mater. Chem. C.* 7 (2019) 10551–10560. https://doi.org/10.1039/c9tc02650a.
- [53] A.G. Kapyshev, V. V. Ivanova, Y.N. Venevtsev, New Perovskites, *Dokl. Akad. Nauk SSSR.* 167 (1966) 564–565.
- [54] H. Langbein, M. Bremer, I. Krabbes,  $\text{CuX}_2\text{O}_6$  and  $\text{Ba}_3\text{CuX}_2\text{O}_9$  ( $\text{X} = \text{Nb, Ta}$ ): Influence of the preparation conditions on phase formation and phase composition, *Solid State Ionics.* 101–103 (1997) 579–584. https://doi.org/10.1016/s0167-2738(97)00382-2.
- [55] M.E. Song, D. Maurya, Y. Wang, J. Wang, M.G. Kang, D. Walker, P.A. Thomas, S.T. Huxtable, R.J. Bodnar, N.Q. Vinh, S. Priya, Phase Transitions and Phonon Mode Dynamics of  $\text{Ba}(\text{Cu}_{1/3}\text{Nb}_{2/3})\text{O}_3$  and  $\text{Sr}(\text{Cu}_{1/3}\text{Nb}_{2/3})\text{O}_3$ for Understanding Thermoelectric Response, *ACS Appl. Energy Mater.* 3 (2020) 3939–3945. https://doi.org/10.1021/acsaem.0c00342.
- [56] W. Zhang, N. Kumada, Y. Yonesaki, T. Takei, N. Kinomura, T. Hayashi, M. Azuma, M. Takano, Ferroelectric perovskite-type barium copper niobate:  $\text{Ba}(\text{Cu}_{1/3}\text{Nb}_{2/3})\text{O}_3$ , *J. Solid State Chem.* 179 (2006) 4052–4055. https://doi.org/10.1016/j.jssc.2006.08.008.
- [57] A. Manavbasi, J.C. LaCombe, Dielectric Characteristics of Donor Doped Nonlead  $\text{Ba}(\text{Cu}_{1/3}\text{Nb}_{2/3})\text{O}_3$  Perovskite Material Synthesized by Microwave-assisted Citrate-nitrate Sol-gel Route, *MRS Online Proc. Libr.* 973 (2007) 8–13.
- [58] C. Starr, The copper oxide rectifier, *J. Appl. Phys.* 7 (1936) 15–19. https://doi.org/10.1063/1.1745338.
- [59] A. Ono, Preparation of new perovskite-type oxides  $\text{Ba}_{2.5}\text{Nb}_{1.5}\text{CuO}_{7.25}$  and  $\text{Sr}_3\text{Ta}_2\text{CuO}_9$ , *J. Mater. Sci. Lett.* 11 (1992) 114–115. https://doi.org/10.1007/BF00724616.
- [60] M. Kobune, K. Teraoka, H. Nishioka, H. Yamaguchi, K. Honda, Fabrication and characterization of binary piezoelectric  $(\text{Bi}_{1/2}\text{Na}_{1/2})\text{TiO}_3\text{-Ba}(\text{Cu}_{1/3}\text{Nb}_{2/3})\text{O}_3$  solid solutions, *Jpn. J. Appl. Phys.* 50 (2011). https://doi.org/10.1143/JJAP.50.09ND08.
- [61] D. Maurya, A. Kumar, V. Petkov, J.E. Mahaney, R.S. Katiyar, S. Priya, Local

- structure and piezoelectric instability in lead-free  $(1-x)\text{BaTiO}_3\text{-xA}(\text{Cu}_{1/3}\text{Nb}_{2/3})\text{O}_3$  ( $\text{A} = \text{Sr, Ca, Ba}$ ) solid solutions, *RSC Adv.* 4 (2014) 1283–1292. <https://doi.org/10.1039/c3ra44886j>.
- [62] C.W. Baek, N.K. Oh, G. Han, W.H. Yoon, J.W. Kim, J.J. Choi, B.D. Han, D.S. Park, K.D. Sung, J.H. Jung, D.Y. Jeong, J.J. Kim, J. Ryu, Effect of  $\text{Ba}(\text{Cu}_{1/3}\text{Nb}_{2/3})\text{O}_3$  content on multiferroic properties in  $\text{BiFeO}_3$  ceramics, *Mater. Sci. Eng. B* 177 (2012) 451–455. <https://doi.org/10.1016/j.mseb.2012.02.016>.
  - [63] D. Shen, X. Li, Z. Wang, Y. Liu, C. He, T. Li, X. Long, New binary  $(1-x)\text{Ba}(\text{Lu}_{1/2}\text{Nb}_{1/2})\text{O}_3\text{-xPbTiO}_3$  solid solution with morphotropic phase boundary, *J. Eur. Ceram. Soc.* 32 (2012) 1077–1083. <https://doi.org/10.1016/j.jeurceramsoc.2011.11.019>.
  - [64] X. Long, Z.G. Ye, Morphotropic phase diagram and dielectric and ferroelectric properties of  $(1-x)\text{Ba}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3\text{-xPbTiO}_3$  solid solution, *J. Appl. Phys.* 101 (2007) 3–8. <https://doi.org/10.1063/1.2747545>.
  - [65] X. Long, Z.G. Ye, New dielectric and ferroelectric solid solution of  $(1-x)\text{Ba}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3\text{-xPbTiO}_3$  with morphotropic phase boundary, *Chem. Mater.* 19 (2007) 1285–1289. <https://doi.org/10.1021/cm062733+>.
  - [66] Z. Wang, X. Li, Q. Wei, X. Long, Z.G. Ye, A ferroelectric solid solution of  $(1-x)\text{Ba}(\text{Yb}_{1/2}\text{Nb}_{1/2})\text{O}_3\text{-xPbTiO}_3$  with morphotropic phase boundary, *J. Appl. Phys.* 104 (2008) 1–4. <https://doi.org/10.1063/1.2969056>.
  - [67] Q. Wei, Z. Wang, X. Li, X. Long, Z.G. Ye, Morphotropic phase diagram and dielectric and ferroelectric properties of  $(1-x)\text{Ba}(\text{Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3\text{-xPbTiO}_3$  solid solution, *Chem. Mater.* 21 (2009) 506–510. <https://doi.org/10.1021/cm802734n>.
  - [68] Z. Wang, X. Li, C. He, X. Long, Relaxor behavior in the  $(1-x)\text{BaSnO}_3\text{-xPbTiO}_3$  solid solution, *Solid State Commun.* 151 (2011) 329–331. <https://doi.org/10.1016/j.ssc.2010.09.050>.
  - [69] M. Mhadhbi, Modelling of the High-Energy Ball Milling Process, *Adv. Mater. Phys. Chem.* 11 (2021) 31–44. <https://doi.org/10.4236/ampc.2021.111004>.
  - [70] H.M. Rietveld, Line profiles of neutron powder-diffraction peaks for structure refinement, *Acta Crystallogr.* 22 (1967) 151–152.
  - [71] H.M. Rietveld, A profile refinement method for nuclear and magnetic structures, *J. Appl. Crystallogr.* 2 (1969) 65–71.
  - [72] R.A. Young, The Rietveld method, 1993. <https://doi.org/10.1088/0031-8949/89/9/098002>.
  - [73] C.N.R. Rao, P. V. Vanitha, A.K. Cheetham, Phase separation in metal oxides, *Chem. - A Eur. J.* 9 (2003) 828–836. <https://doi.org/10.1002/chem.200390092>.
  - [74] D. Pandey, A.K. Singh, R. Ranjan, Ragini, Monoclinic phases in the  $\text{Pb}(\text{Zr}_x\text{Ti}_{1-x})\text{O}_3$  ceramics, *Ferroelectrics.* 325 (2005) 35–42. <https://doi.org/10.1080/00150190500326761>.
  - [75] C. Zhou, X. Ke, Y. Yao, S. Yang, Y. Ji, W. Liu, Y. Yang, L. Zhang, Y. Hao, S. Ren, L. Zhang, X. Ren, Evolution from successive phase transitions to ‘morphotropic phase boundary’ in  $\text{BaTiO}_3$ -based ferroelectrics, *Appl. Phys. Lett.* 112 (2018) 1–6. <https://doi.org/10.1063/1.5028302>.
  - [76] A.K. Singh, D. Pandey, On the discovery of two new monoclinic phases in the morphotropic phase boundary region of  $\text{Pb}[(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3]\text{-xPbTiO}_3$  ceramics, *Ferroelectrics.* 326 (2005) 91–99. <https://doi.org/10.1080/00150190500318370>.
  - [77] A. Upadhyay, A.K. Singh, Grain size dependent phase stabilities and presence of a monoclinic (Pm) phase in the morphotropic phase boundary region of  $(1-x)\text{Bi}(\text{Mg}_{1/2}\text{Ti}_{1/2})\text{O}_3\text{-xPbTiO}_3$  piezoceramics, *J. Appl. Phys.* 117 (2015). <https://doi.org/10.1063/1.4917211>.

- [78] R. Pandey, A. Tiwari, A. Upadhyay, A.K. Singh, Phase coexistence and the structure of the morphotropic phase boundary region in  $(1-x)\text{Bi}(\text{Mg}_{1/2}\text{Zr}_{1/2})\text{O}_3$ - $x\text{PbTiO}_3$  piezoceramics, *Acta Mater.* 76 (2014) 198–206. <https://doi.org/10.1016/j.actamat.2014.05.023>.
- [79] A.K. Singh, D. Pandey, Evidence for MB and MC phases in the morphotropic phase boundary region of  $(1-x)[\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3]$ - $x\text{PbTiO}_3$ : A Rietveld study, *Phys. Rev. B* 67 (2003) 064102. <https://doi.org/10.1103/physrevb.67.064102>.
- [80] W.F. Rao, Y.U. Wang, Microstructures of coherent phase decomposition near morphotropic phase boundary in lead zirconate titanate, *Appl. Phys. Lett.* 91 (2007) 15–18. <https://doi.org/10.1063/1.2767146>.
- [81] K. Shahzad, M.N. Khan, G. Shabbir, J. Bashir, Neutron and X-Ray Diffraction Crystal Structure Rietveld Analysis of  $\text{PbTiO}_3$  Ceramics, *Ferroelectrics* 414 (2011) 155–161. <https://doi.org/10.1080/00150193.2011.577332>.
- [82] H. Chen, J. Long, Z. Meng, Effect of Zr/Ti ratio on the properties of PMMN-PZT ceramics near the morphotropic phase boundary, *Mater. Sci. Eng. B* 99 (2003) 433–436. [https://doi.org/10.1016/S0921-5107\(02\)00448-8](https://doi.org/10.1016/S0921-5107(02)00448-8).
- [83] K. Pandya, R. Guo, A. Bhalla, Ferroelectric ceramics of  $2(\text{Pb},\text{Sr})\text{Nb}_2\text{O}_6:(\text{K},\text{Na})\text{NbO}_3$  tungsten bronze morphotropic phase boundary system, *Ferroelectr. Lett. Sect.* 25 (1999) 87–95. <https://doi.org/10.1080/0731517908204588>.
- [84] R. Pandey, A.K. Singh, Electric field induced cubic to monoclinic phase transition in multiferroic  $0.65\text{Bi}(\text{Ni}_{1/2}\text{Ti}_{1/2})\text{O}_3$ - $0.35\text{PbTiO}_3$  solid solution, *Appl. Phys. Lett.* 105 (2014) 1–5. <https://doi.org/10.1063/1.4899058>.
- [85] M. Ahart, M. Somayazulu, R.E. Cohen, P. Ganesh, P. Dera, H. Mao, R.J. Hemley, Y. Ren, P. Liermann, Z. Wu, Origin of morphotropic phase boundaries in ferroelectrics, *Nature* 451 (2008) 545–548. <https://doi.org/10.1038/nature06459>.
- [86] K. Roleder, A. Majchrowski, I. Lazar, R.W. Whatmore, A.M. Glazer, D. Kajewski, J. Koperski, A. Soszyński, Monoclinic domain populations and enhancement of piezoelectric properties in a PZT single crystal at the morphotropic phase boundary, *Phys. Rev. B* 105 (2022). <https://doi.org/10.1103/PhysRevB.105.144104>.
- [87] X. Zhang, Z. Fang, H. Yang, P. Zhao, X. Zhang, Y. Li, Z. Xiong, H. Yang, S. Zhang, B. Tang, Lattice evolution, ordering transformation and microwave dielectric properties of rock-salt  $\text{Li}_{3+x}\text{Mg}_{2-2x}\text{Nb}_{1-x}\text{Ti}_{2x}\text{O}_6$  solid-solution system: A newly developed pseudo ternary phase diagram, *Acta Mater.* 206 (2021) 116636. <https://doi.org/10.1016/j.actamat.2021.116636>.
- [88] T. Suzuki, T. Fujita, Anomalous Change in Crystalline Structure of  $(\text{La}_{1-x}\text{Ba}_x)_2\text{CuO}_{4-\gamma}$ , *J. Phys. Soc. Japan.* 58 (1989) 1883–1886. <https://doi.org/10.1143/JPSJ.58.1883>.
- [89] N.J. Donnelly, C.A. Randall, Pb loss in  $\text{Pb}(\text{Zr},\text{Ti})\text{O}_3$  ceramics observed by in situ ionic conductivity measurements, *J. Appl. Phys.* 109 (2011). <https://doi.org/10.1063/1.3585831>.
- [90] S. Pöykkö, D.J. Chadi, First principles study of Pb vacancies in  $\text{PbTiO}_3$ , *Appl. Phys. Lett.* 76 (2000) 499–501. <https://doi.org/10.1063/1.125800>.
- [91] Z. Zhang, P. Wu, L. Lu, C. Shu, Ab initio study of formations of neutral vacancies in ferroelectric  $\text{PbTiO}_3$  at different oxygen atmospheres, *J. Alloys Compd.* 449 (2008) 362–365. <https://doi.org/10.1016/j.jallcom.2006.01.142>.
- [92] Y. Yan, J.E. Zhou, D. Maurya, Y.U. Wang, S. Priya, Giant piezoelectric voltage coefficient in grain-oriented modified  $\text{PbTiO}_3$  material, *Nat. Commun.* 7 (2016)

- 1–10. <https://doi.org/10.1038/ncomms13089>.
- [93] A. Mishra, D.K. Khatua, G. Das Adhikary, N. Kumar, A. Upadhyay, B. Mahale, S. Saha, B. Majumdar, A. Senyshyn, R. Ranjan, Effect of sintering temperature on the structural disorder and its influence on electromechanical properties of the morphotropic phase boundary composition  $0.94\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3\text{-}0.06\text{BaTiO}_3$  (NBT-6BT), *J. Mater. Sci. Mater. Electron.* 32 (2021) 16088–16103. <https://doi.org/10.1007/s10854-021-06157-1>.
- [94] V. Kothai, B. Narayan, K. Brajesh, S.D. Kaushik, V. Siruguri, R. Ranjan, Ferroelectric phase coexistence by crystallite size reduction in  $\text{BiFeO}_3\text{-PbTiO}_3$ , *Phys. Rev. B* 90 (2014) 1–6. <https://doi.org/10.1103/PhysRevB.90.155115>.
- [95] A. Upadhyay, A.K. Singh, Grain size dependent phase stabilities and presence of a monoclinic (Pm) phase in the morphotropic phase boundary region of  $(1-x)\text{Bi}(\text{Mg}_{1/2}\text{Ti}_{1/2})\text{O}_3\text{-xPbTiO}_3$  piezoceramics, *J. Appl. Phys.* 117 (2015) 144102. <https://doi.org/10.1063/1.4917211>.
- [96] W. Zeng, Q. Li, C. Zhou, J. Xu, C. Yuan, G. Chen, A new insight into structural complexity in ferroelectric ceramics, *J. Adv. Ceram.* 6 (2017) 262–268. <https://doi.org/10.1007/s40145-017-0237-1>.
- [97] C. Martin, A. Maignan, M. Hervieu, B. Raveau, Z. Jirák, M.M. Savosta, A. Kurbakov, V. Trounov, G. André, F. Bourée, Structural study of the electron-doped manganites  $\text{Sm}_{0.1}\text{Ca}_{0.9}\text{MnO}_3$  and  $\text{Pr}_{0.1}\text{Sr}_{0.9}\text{MnO}_3$ : Evidence of phase separation, *Phys. Rev. B* 62 (2000) 6442–6449. <https://doi.org/10.1103/PhysRevB.62.6442>.
- [98] K. Yoshimura, H. Kubota, H. Tanaka, Y. Date, M. Nakanishi, T. Ohmura, N. Saga, T. Sawamura, T. Uemura, K. Kosuge, Compositional Phase Separation in  $\text{La}_{2-x}\text{Ba}_x\text{CuO}_y$  near the Optimum Composition for Superconductivity, *J. Phys. Soc. Japan.* 62 (1993) 1114–1117. <https://doi.org/10.1143/JPSJ.62.1114>.
- [99] F. Li, D. Lin, Z. Chen, Z. Cheng, J. Wang, C. Li, Z. Xu, Q. Huang, X. Liao, L.Q. Chen, T.R. Shrout, S. Zhang, Ultrahigh piezoelectricity in ferroelectric ceramics by design, *Nat. Mater.* 17 (2018) 349–354. <https://doi.org/10.1038/s41563-018-0034-4>.
- [100] N. Zhang, H. Yokota, A.M. Glazer, Z. Ren, D.A. Keen, D.S. Keeble, P.A. Thomas, Z.G. Ye, The missing boundary in the phase diagram of  $\text{PbZr}_{1-x}\text{Ti}_x\text{O}_3$ , *Nat. Commun.* 5 (2014) 1–9. <https://doi.org/10.1038/ncomms6231>.
- [101] Y. Zhang, D. Xue, H. Wu, X. Ding, T. Lookman, X. Ren, Adaptive ferroelectric state at morphotropic phase boundary: Coexisting tetragonal and rhombohedral phases, *Acta Mater.* 71 (2014) 176–184. <https://doi.org/10.1016/j.actamat.2014.03.007>.
- [102] L. Chen, M. Zhao, J. Wang, S. Zhang, F. Sun, L. Zhao, Phase transition and piezoelectric property of  $(\text{Ag},\text{K})\text{NbO}_3$  ceramics, *J. Mater.* 8 (2022) 863–872. <https://doi.org/10.1016/j.jmat.2022.01.001>.
- [103] F. He, Z. Wang, Q. Wu, J. Li, J. Wang, C.T. Liu, Phase separation of metastable  $\text{CoCrFeNi}$  high entropy alloy at intermediate temperatures, *Scr. Mater.* 126 (2017) 15–19. <https://doi.org/10.1016/j.scriptamat.2016.08.008>
- [104] A.A. Kündig, M. Ohnuma, D.H. Ping, T. Ohkubo, K. Hono, In situ formed two-phase metallic glass with surface fractal microstructure, *Acta Mater.* 52 (2004) 2441–2448. <https://doi.org/10.1016/j.actamat.2004.01.036>.
- [105] A. Ricci, N. Poccia, B. Joseph, G. Arrighetti, L. Barba, J. Plaisier, G. Campi, Y. Mizuguchi, H. Takeya, Y. Takano, N.L. Saini, A. Bianconi, Intrinsic phase separation in superconducting  $\text{K}_{0.8}\text{Fe}_{1.6}\text{Se}_2$  ( $T_c = 31.8\text{K}$ ) single crystals, *Supercond. Sci. Technol.* 24 (2011). [201](https://doi.org/10.1088/0953-201</a></p>
</div>
<div data-bbox=)

- [106] A. Ricci, N. Poccia, G. Campi, B. Joseph, G. Arrighetti, L. Barba, M. Reynolds, M. Burghammer, H. Takeya, Y. Mizuguchi, Y. Takano, M. Colapietro, N.L. Saini, A. Bianconi, Nanoscale phase separation in the iron chalcogenide superconductor  $K_{0.8}Fe_{1.6}Se_2$  as seen via scanning nanofocused x-ray diffraction, *Phys. Rev. B.* 84 (2011). <https://doi.org/10.1103/PhysRevB.84.060511>.
- [107] S. Buta, D. Morgan, A. Van der Ven, M.K. Aydinol, G. Ceder, Phase Separation Tendencies of Aluminum-Doped Transition-Metal Oxides ( $LiAl_{1-x}M_xO_2$ ) in the  $\alpha$ - $NaFeO_2$  Crystal Structure, *J. Electrochem. Soc.* 146 (1999) 4335–4338. <https://doi.org/10.1149/1.1392639>.
- [108] A. Moreo, S. Yunoki, E. Dagotto, Phase Separation Scenario for Manganese Oxides and Related Materials, *Science* (80-.) 283 (1999) 2034–2040. <https://doi.org/10.1126/science.283.5410.2034>.
- [109] P.M. Woodward, D.E. Cox, T. Vogt, C.N.R. Rao, A.K. Cheetham, Effect of compositional fluctuations on the phase transitions in  $(Nd_{1/2}Sr_{1/2})MnO_3$ , *Chem. Mater.* 11 (1999) 3528–3538. <https://doi.org/10.1021/cm990281d>.
- [110] J. Brookeman, A. Rigamonti, Pretransitional clusters and heterophase fluctuations at first-order phase transitions in crystals, *Phys. Rev. B.* 24 (1981) 4925–4930. <https://doi.org/10.1103/PhysRevB.24.4925>.
- [111] Y. Yamada, T. Iwase, K. Fujishiro, Y. Uesu, Y. Yamashita, I. Tomono, S. Shimanuki, Relaxor as heterophase fluctuation, *Ferroelectrics*. 240 (2000) 1629–1636. <https://doi.org/10.1080/00150190008227991>.
- [112] V.Y. Topolov, Heterogeneous Ferroelectric Solid Solutions, Springer International Publishing, Cham, 2018. <https://doi.org/10.1007/978-3-319-75520-5>.
- [113] W.R. Burack, A.R.G. Dibble, R.L. Biltonen, The relationship between compositional phase separation and vesicle morphology: Implications for the regulation of phospholipase A2 by membrane structure, *Chem. Phys. Lipids.* 90 (1997) 87–95. [https://doi.org/10.1016/S0009-3084\(97\)00084-4](https://doi.org/10.1016/S0009-3084(97)00084-4).
- [114] H.Z. Jin, J. Zhu, S. Miao, X.W. Zhang, Z.Y. Cheng, Ordered domains and polar clusters in lead magnesium niobate  $Pb(Mg_{1/3}Nb_{2/3})O_3$ , *J. Appl. Phys.* 89 (2001) 5048–5052. <https://doi.org/10.1063/1.1334369>.
- [115] D. Maurya, C.W. Ahn, S. Zhang, S. Priya, High dielectric composition in the system Sn-modified  $(1-x)BaTiO_3-xBa(Cu_{1/3}Nb_{2/3})O_3$ ,  $x=0.025$  for multilayer ceramic capacitors, *J. Am. Ceram. Soc.* 93 (2010) 1225–1228. <https://doi.org/10.1111/j.1551-2916.2009.03523.x>.
- [116] F. Li, S. Zhang, T. Yang, Z. Xu, N. Zhang, G. Liu, J. Wang, J. Wang, Z. Cheng, Z.G. Ye, J. Luo, T.R. Shrout, L.Q. Chen, The origin of ultrahigh piezoelectricity in relaxor-ferroelectric solid solution crystals, *Nat. Commun.* 7 (2016) 1–9. <https://doi.org/10.1038/ncomms13807>.
- [117] I. Levin, E. Cockayne, V. Krayzman, J.C. Woicik, S. Lee, C.A. Randall, Local structure of  $Ba(Ti,Zr)O_3$  perovskite-like solid solutions and its relation to the band-gap behavior, *Phys. Rev. B.* 83 (2011) 1–8. <https://doi.org/10.1103/PhysRevB.83.094122>.
- [118] X. Long, Z.-G. Ye, New Dielectric and Ferroelectric Solid Solution of  $(1-x)Ba(Mg_{1/3}Nb_{2/3})O_3-xPbTiO_3$  with Morphotropic Phase Boundary, *Chem. Mater.* 19 (2007) 1285–1289. <https://doi.org/https://doi.org/10.1021/cm062733+>.
- [119] A.A. Bokov, Z.G. Ye, Recent progress in relaxor ferroelectrics with perovskite structure, *J. Mater. Sci.* 41 (2006) 31–52. <https://doi.org/10.1007/s10853-005-5915-7>.

- [120] N. Setter, L.E. Cross, The role of B-site cation disorder in diffuse phase transition behavior of perovskite ferroelectrics, *J. Appl. Phys.* 51 (1980) 4356–4360. <https://doi.org/10.1063/1.328296>.
- [121] Y.U. Wang, Three intrinsic relationships of lattice parameters between intermediate monoclinic MC and tetragonal phases in ferroelectric Pb [(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)<sub>1-x</sub>Ti<sub>x</sub>]O<sub>3</sub> and Pb[(Zn<sub>1/3</sub>Nb<sub>2/3</sub>)<sub>1-x</sub>Ti<sub>x</sub>]O<sub>3</sub> near morphotropic phase boundaries, *Phys. Rev. B.* 73 (2006) 1–13. <https://doi.org/10.1103/PhysRevB.73.014113>.
- [122] D.D. Viehland, E.K.H. Salje, Domain boundary-dominated systems: Adaptive structures and functional twin boundaries, *Adv. Phys.* 63 (2014) 267–326. <https://doi.org/10.1080/00018732.2014.974304>.
- [123] J.A. Liu, C.H. Li, Y. Zou, A.N. Chen, L. Hu, Y.S. Shi, Effect of ball milling on the sintering performance of indium-gallium-zinc oxide ceramics: The diffusion mechanism and lattice distortion of milled powders, *Ceram. Int.* 47 (2021) 15682–15694. <https://doi.org/10.1016/j.ceramint.2021.02.138>.
- [124] C. Pavithra, W. Madhuri, S. Roopas Kiran, Effects of synthesis and sintering temperature in BCT-BST ceramics, *Mater. Chem. Phys.* 258 (2021) 123921. <https://doi.org/10.1016/j.matchemphys.2020.123921>.
- [125] R. Pramanik, M.K. Sahukar, Y. Mohan, B. Praveenkumar, S.R. Sangawar, A. Arockiarajan, Effect of grain size on piezoelectric, ferroelectric and dielectric properties of PMN-PT ceramics, *Ceram. Int.* 45 (2019) 5731–5742. <https://doi.org/10.1016/j.ceramint.2018.12.039>.
- [126] T. Li, M. Xu, K. Peng, Y. Sun, M. Wang, H. Dai, D. Liu, R. Xue, Z. Chen, Evolution of microstructure, defect, optoelectronic and magnetic properties of Cu<sub>1-x</sub>Ca<sub>x</sub>FeO<sub>2</sub> ceramics, *J. Phys. Chem. Solids.* 151 (2021) 109910. <https://doi.org/10.1016/j.jpcs.2020.109910>.
- [127] K. Prajapati, A.K. Singh, Improved ferroelectric and piezoelectric properties and structural correlations in a new ceramic 0.38Ba(Cu<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub>–0.62PbTiO<sub>3</sub> by MnO<sub>2</sub> additive, *J. Mater. Res.* 18 (2023). <https://doi.org/10.1557/s43578-023-00940-y>.
- [128] W.A. Goddard, On the wrong assignment of the XPS O-1s signal at 531–532 eV attributed to oxygen vacancies in photo- and electro-catalysts for water splitting and other materials applications, *Surf. Sci.* 284 (2021) 1119–1125. [https://doi.org/10.1007/978-3-030-18778-1\\_51](https://doi.org/10.1007/978-3-030-18778-1_51).
- [129] S. Poulston, P.M. Parlett, P. Stone, M. Bowker, Surface oxidation and reduction of CuO and Cu<sub>2</sub>O studied using XPS and XAES, *Surf. Interface Anal.* 24 (1996) 811–820. [https://doi.org/10.1002/\(SICI\)1096-9918\(199611\)24:12<811::AID-SIA191>3.0.CO;2-Z](https://doi.org/10.1002/(SICI)1096-9918(199611)24:12<811::AID-SIA191>3.0.CO;2-Z).
- [130] M. Aufray, S. Menuel, Y. Fort, J. Eschbach, D. Rouxel, B. Vincent, New Synthesis of Nanosized Niobium Oxides and Lithium Niobate Particles and Their Characterization by XPS Analysis, *J. Nanosci. Nanotechnol.* 9 (2009) 4780–4785. <https://doi.org/10.1166/jnn.2009.1087>.
- [131] M.C. Biesinger, B.P. Payne, B.R. Hart, A.P. Grosvenor, N.S. McEntryre, L.W.M. Lau, R.S.C. Smart, Quantitative chemical state XPS analysis of first row transition metals, oxides and hydroxides, *J. Phys. Conf. Ser.* 100 (2008). <https://doi.org/10.1088/1742-6596/100/1/012025>.
- [132] U. Diebold, T.E. Madey, TiO<sub>2</sub> by XPS, *Surf. Sci. Spectra.* 4 (1996) 227–231. <https://doi.org/10.1116/1.1247794>.
- [133] J.A.T. Verhoeven, H. van Doveren, XPS studies on Ba, BaO and the oxidation of Ba, *Appl. Surf. Sci.* 5 (1980) 361–373. <https://doi.org/10.1016/0378>

- 5963(80)90101-4.
- [134] S. Rondon, P.M.A. Sherwood, Core Level and Valence Band Spectra of PbO<sub>2</sub> by XPS, *Surf. Sci. Spectra.* 5 (1998) 104–110. <https://doi.org/10.1116/1.1247867>.
- [135] K. Xi, Y. Li, Z. Zheng, L. Zhang, Y. Liu, Y. Mi, Study on phase transitions and temperature stability of (1-x)K<sub>0.5</sub>Na<sub>0.5</sub>NbO<sub>3</sub>-xBi(Zn<sub>0.5</sub>Zr<sub>0.5</sub>)O<sub>3</sub> lead-free ceramics, *Mater. Chem. Phys.* 250 (2020) 123032. <https://doi.org/10.1016/j.matchemphys.2020.123032>.
- [136] A. Schönhals, F. Kremer, Analysis of Dielectric Spectra, in: Broadband Dielectric Spectroscopy, 2003. [https://doi.org/10.1007/978-3-642-56120-7\\_3](https://doi.org/10.1007/978-3-642-56120-7_3).
- [137] P. Kumar, B.P. Singh, T.P. Sinha, N.K. Singh, AC conductivity and dielectric relaxation in Ba(Sm<sub>1/2</sub>Nb<sub>1/2</sub>)O<sub>3</sub> ceramic, *Phys. B.* 406 (2011) 139–143. <https://doi.org/10.1016/j.physb.2010.09.019>.
- [138] H. Yan, F. Inam, G. Viola, H. Ning, H. Zhang, Q. Jiang, T. Zeng, Z. Gao, M.J. Reece, The Contribution of Electrical Conductivity, Dielectric Permittivity and Domain Switching in Ferroelectric Hysteresis Loops, *J. Adv. Dielectr.* 01 (2011) 107–118. <https://doi.org/10.1142/s2010135x11000148>.
- [139] V. Koval, G. Viola, Y. Tan, Biasing Effects in Ferroic Materials, in: *Ferroelectr. Mater. - Synth. Charact.*, 2015. <https://doi.org/10.5772/60764>.
- [140] A.J. Bell, Factors influencing the piezoelectric behaviour of PZT and other “morphotropic phase boundary” ferroelectrics, *J. Mater. Sci.* 41 (2006) 13–25. <https://doi.org/10.1007/s10853-005-5913-9>.
- [141] J. Che, X. Yao, The effect of lead deficiency on the dielectric properties of 0.80Pb(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub>-0.20PbTiO<sub>3</sub> ceramics, *Ceram. Int.* 30 (2004) 1377–1381. <https://doi.org/10.1016/j.ceramint.2003.12.102>.
- [142] X. Li, J. Fu, Y. Yang, Z. Li, W. Song, R. Zuo, Ultrahigh electrostrains of lead-free (Ba,Ca)(Ti,Zr)O<sub>3</sub> piezoelectric ceramics via defect engineering, *J. Mater. Sci.* 57 (2022) 10233–10241. <https://doi.org/10.1007/s10853-022-07281-x>.
- [143] D. Lin, S. Zhang, C. Cai, W. Liu, Domain size engineering in 0.5%MnO<sub>2</sub>-(K<sub>0.5</sub>Na<sub>0.5</sub>)NbO<sub>3</sub> lead free piezoelectric crystals, *J. Appl. Phys.* 117 (2015) 3–8. <https://doi.org/10.1063/1.4913208>.
- [144] Y. Yan, A. Kumar, M. Correa, K.H. Cho, R.S. Katiyar, S. Priya, Phase transition and temperature stability of piezoelectric properties in Mn-modified Pb(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub>-PbZrO<sub>3</sub>-PbTiO<sub>3</sub> ceramics, *Appl. Phys. Lett.* 100 (2012) 1–5. <https://doi.org/10.1063/1.3703124>.
- [145] Y. Deng, J. Wang, C. Zhang, H. Ma, C. Bai, D. Liu, F. Wu, B. Yang, Structural and Electric Properties of MnO<sub>2</sub>-doped KNN-LT lead-free Piezoelectric Ceramics, *Crystals.* 10 (2020) 1–8. <https://doi.org/10.3390/crust10080705>.
- [146] Q. Liu, F.Y. Zhu, L. Zhao, K. Wang, L. Li, J.F. Li, W. Jo, Further Enhancing Piezoelectric Properties by Adding MnO<sub>2</sub> in AgSbO<sub>3</sub>-Modified (Li,K,Na)(Nb,Ta)O<sub>3</sub> Lead-Free Piezoceramics, *J. Am. Ceram. Soc.* 99 (2016) 3670–3676. <https://doi.org/10.1111/jace.14412>.
- [147] H. Liu, R. Nie, Y. Yue, Q. Zhang, Q. Chen, J. Zhu, P. Yu, D. Xiao, C. Wang, X. Wang, Effect of MnO<sub>2</sub> doping on piezoelectric, dielectric and ferroelectric properties of PNN-PZT ceramics, *Ceram. Int.* 41 (2015) 11359–11364. <https://doi.org/10.1016/j.ceramint.2015.05.094>.
- [148] S.J. Yoon, S.Y. Yoo, J.H. Moon, H.J. Jung, H.J. Kim, Effects of La<sub>2</sub>O<sub>3</sub> and MnO<sub>2</sub> on the piezoelectric properties of 0.02Pb(Y<sub>2/3</sub>W<sub>1/3</sub>)O<sub>3</sub>-0.98Pb(Zr<sub>0.52</sub>Ti<sub>0.48</sub>)O<sub>3</sub>, *J. Mater. Res.* 11 (1996). <https://doi.org/doi.org.10.1557/JMR.1996.0041>.
- [149] X. Wang, P. Liang, X. Chao, Z. Yang, Dielectric Properties and Impedance

- Spectroscopy of MnCO<sub>3</sub>-Modified (Ba<sub>0.85</sub>Ca<sub>0.15</sub>)(Zr<sub>0.1</sub>Ti<sub>0.9</sub>)O<sub>3</sub> Lead-Free Ceramics, J. Am. Ceram. Soc. 98 (2015) 1506–1514. <https://doi.org/10.1111/jace.13481>.
- [150] L.X. He, C.E. Li, Effects of addition of MnO on piezoelectric properties of lead zirconate titanate, J. Mater. Sci. 35 (2000) 2477–2480. <https://doi.org/10.1023/A:1004717702149>.
- [151] A. Bradeško, M. Vrabelj, L. Fulanović, Š. Svirskas, M. Ivanov, R. Katiliūte, D. Jablonskas, M. Šimėnas, G. Usevičius, B. Malič, J. Banys, T. Rojac, Implications of acceptor doping in the polarization and electrocaloric response of 0.9Pb(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub>-0.1PbTiO<sub>3</sub> relaxor ferroelectric ceramics, J. Mater. Chem. C. 9 (2021) 3204–3214. <https://doi.org/10.1039/d0tc05854h>.
- [152] T. Zheng, H. Deng, W. Zhou, X. Zhai, H. Cao, L. Yu, P. Yang, J. Chu, Bandgap modulation and magnetic switching in PbTiO<sub>3</sub> ferroelectrics by transition elements doping, Ceram. Int. 42 (2016) 6033–6038. <https://doi.org/10.1016/j.ceramint.2015.12.157>.
- [153] W. Peng, L. Li, S. Yu, P. Yang, K. Xu, Dielectric properties, microstructure and charge compensation of MnO<sub>2</sub>-doped BaTiO<sub>3</sub>-based ceramics in a reducing atmosphere, Ceram. Int. 47 (2021) 29191–29196. <https://doi.org/10.1016/j.ceramint.2021.07.083>.
- [154] K. Toshio, S. Toshimasa, T. Takkai, D. Masaki, Effects of manganese addition on piezoelectric properties of Pb(Zr<sub>0.5</sub>Ti<sub>0.5</sub>)O<sub>3</sub>, Japan Soc. Appl. Phys. 31 (1992) 3058–3060. <https://doi.org/10.1143/JJAP.31.3058>.
- [155] E. Brzozowski, M.S. Castro, Grain growth control in Nb-doped BaTiO<sub>3</sub>, 168 (2005) 464–470. <https://doi.org/10.1016/j.jmatprotec.2005.02.246>.
- [156] M.J. Brova, B.H. Watson, R.L. Walton, E.R. Kupp, M.A. Fanton, R.J. Meyer, G.L. Messing, Tempered grain growth of high coercive field CuO-doped textured PYN-PMN-PT ceramics, J. Am. Ceram. Soc. 103 (2020) 6149–6156. <https://doi.org/10.1111/jace.17349>.
- [157] C.E.B. Marino, P.A.P. Nascente, S.R. Biaggio, R.C. Rocha-Filho, N. Bocchi, XPS characterization of anodic titanium oxide films grown in phosphate buffer solutions, Thin Solid Films. 468 (2004) 109–112. <https://doi.org/10.1016/j.tsf.2004.05.006>.
- [158] V.R. Galakhov, M. Demeter, S. Bartkowski, M. Neumann, N.A. Ovechkina, E.Z. Kurmaev, N.I. Lobachevskaya, Y.M. Mukovskii, J. Mitchell, D.L. Ederer, Mn 3s exchange splitting in mixed-valence manganites, Phys. Rev. B. 65 (2002) 1–4. <https://doi.org/10.1103/PhysRevB.65.113102>.
- [159] A.J. Nelson, J.G. Reynolds, J.W. Roos, Core-level satellites and outer core-level multiplet splitting in Mn model compounds, J. Vac. Sci. Technol. A Vacuum, Surfaces, Film. 18 (2000) 1072–1076. <https://doi.org/10.1116/1.582302>.
- [160] Y. Kamimura, B.Y. Lee, K. Yazawa, H. Funakubo, T. Iijima, H. Uchida, Fabrication and evaluation of Mn-substituted Ba(Cu<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub> ceramics, IOP Conf. Ser. Mater. Sci. Eng. 18 (2011) 2–6. <https://doi.org/10.1088/1757-899X/18/9/092038>.
- [161] R.D. Shannon, C.T. Prewitt, Effective ionic radii in oxides and fluorides, Acta Crystallogr. Sect. B Struct. Crystallogr. Cryst. Chem. 25 (1969) 925–946. <https://doi.org/10.1107/s0567740869003220>.
- [162] F.A. Kröger, H.J. Vink, Relations between the Concentrations of Imperfections in Crystalline Solids, Solid State Phys.-Adv. Res. Appl. 3 (1956) 307–435. [https://doi.org/10.1016/S0081-1947\(08\)60135-6](https://doi.org/10.1016/S0081-1947(08)60135-6).
- [163] G.R. Gajula, L.R. Buddiga, M. Dasari, Influence of Gd/Nb on activation energy,

- relaxation response, impedance, Nyquist plots and dielectric studies at high frequency of BaTiO<sub>3</sub>-Li<sub>0.5</sub>Fe<sub>2.5</sub>O<sub>4</sub> solid compounds, *Results Phys.* 18 (2020) 103196. <https://doi.org/10.1016/j.rinp.2020.103196>.
- [164] L. Liu, C. Wang, X. Sun, G. Wang, C. Lei, T. Li, Oxygen-vacancy-related relaxations of Sr<sub>3</sub>CuNb<sub>2</sub>O<sub>9</sub> at high temperatures, *J. Alloys Compd.* 552 (2013) 279–282. <https://doi.org/10.1016/j.jallcom.2012.10.081>.
- [165] M. Coskun, O. Polat, F.M. Coskun, Z. Durmus, M. Çaglard, A. Turut, The electrical modulus and other dielectric by the impedance spectroscopy of LaCrO<sub>3</sub> and LaCr<sub>0.90</sub>Ir<sub>0.10</sub>O<sub>3</sub> perovskites, *RSC Adv.* 8 (2018) 4634–4648. <https://doi.org/10.1039/c7ra13261a>.
- [166] K. Abd elmadjid, F. Gheorghiu, M. Zerdali, M. Kadri, S. Hamzaoui, Preparation, structural and functional properties of PbTiO<sub>3-δ</sub> ceramics, *Ceram. Int.* 45 (2019) 9043–9047. <https://doi.org/10.1016/j.ceramint.2019.01.240>
- [167] R.R. McQuade, P. Mardilovich, N. Kumar, D.P. Cann, Conduction properties of acceptor-doped BaTiO<sub>3</sub>–Bi(Zn<sub>1/2</sub>Ti<sub>1/2</sub>)O<sub>3</sub>-based ceramics, *J. Mater. Sci.* 55 (2020) 16290–16299. <https://doi.org/10.1007/s10853-020-05175-4>.
- [168] T.M. Kamel, G. de With, Poling of hard ferroelectric PZT ceramics, *J. Eur. Ceram. Soc.* 28 (2008) 1827–1838. <https://doi.org/10.1016/j.jeurceramsoc.2007.11.023>.

## LIST OF PUBLICATIONS

### PUBLICATIONS IN INDEXED JOURNALS

1. Unusual Crystal Structure Evolution, Multiple Morphotropic Phase Boundaries and Phase separation in  $(1-x)\text{Ba}(\text{Cu}_{1/3}\text{Nb}_{2/3})\text{O}_3-(x)\text{PbTiO}_3$  Perovskite Solid Solution, Krishna Prajapati and Akhilesh Kumar Singh, *Dalton Transactions, RSC*, doi-10.1557/s43578-023-00940-y, SJR-0.79, Q1, Citescore- 6.7, I.F. – 4.6
2. Improved Ferroelectric, Piezoelectric Properties and Structural Correlations in a New Ceramic  $0.38\text{Ba}(\text{Cu}_{1/3}\text{Nb}_{2/3})\text{O}_3-0.62\text{PbTiO}_3$  by  $\text{MnO}_2$  Additive, Krishna Prajapati and Akhilesh Kumar Singh, (2023) *Journal of Materials Research, Springer*, doi-10.1557/s43578-023-00940-y. SJR-0.7, Q1, Citescore- 3, I.F. - 3.0
3. Solution Processed  $\text{Li-Al}_2\text{O}_3/\text{LiNbO}_3/\text{Li-Al}_2\text{O}_3$  Stacked Gate Dielectric for a Non-volatile Ferroelectric Thin Film Transistor, Nila Pal, Rajarshi Chakraborty, Anand Sharma, Utkarsh Pandey, Vishwas Acharya, Krishna Prajapati, Akanksha Gupta, Swati Suman, Parasuraman Swaminathan, Akhilesh Singh, Pradip Roy and Bhola Nath Pal, *Journal of Alloys and Compounds, Elsevier*, 960 (2023)
4. Challenging Fabrication and Characterization of a New Ferroelectric Solid-Solution composition  $0.30\text{Bi}(\text{Cu}_{1/2}\text{Ti}_{1/2})\text{O}_3-0.70\text{PbTiO}_3$  , Krishna Prajapati, Satnam Singh Khanuja, (Accepted in Ferroelectrics, Taylor and Francis Ltd) SJR-0.21, Q4, Citescore-1.1, I.F. - 0.69
5. Piezoelectric, Ferroelectric and Dielectric characterization of a New Solid Solution  $(1-x)\text{Ba}(\text{Cu}_{1/3}\text{Nb}_{2/3})\text{O}_3-x\text{PbTiO}_3$ , Krishna Prajapati, Monika Singh and Akhilesh Kumar Singh, (under review in Solid state sciences, Elsevier) SJR- 0.62, Q2, Citescore-4, I.F. – 3.7
6. Phase Diagram of a New Phase Separated  $(1-x)\text{Ba}(\text{Cu}_{1/3}\text{Nb}_{2/3})\text{O}_3-x\text{PbTiO}_3$  Solid Solution with Multiple Morphotropic Phase Boundaries, Krishna Prajapati, Goranga Manna and Akhilesh Kumar Singh, (To be communicated in ACS Applied Materials and Interfaces, ACS) SJR-1.03, Q1, Citescore- 14.4, I.F. - 10.3
7. 170691, doi.org/10.1016/j.jallcom.2023.170691, SJR-1.03, Q1, Citescore- 9.6, I.F. - 6.3
8. Enhanced Ferroelectric, Piezoelectric and Dielectric Properties in Pb/Nb co-Doped  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ , Krishna Prajapati and Akhilesh Kumar Singh, (To be Communicated)
9. High-Temperature Ferroelectricity in Sb-doped  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ , Krishna Prajapati, Pragyanand Prajapati, Srishti Paliwal and Akhilesh Kumar Singh, (To be Communicated)

### PUBLICATIONS IN CONFERENCE PROCEEDINGS

10. Enhanced High-Temperature Dielectric and Ferroelectric Properties of  $\text{Sb}_2\text{O}_5$  Modified  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ . Krishna Prajapati, Srishti Paliwal and Akhilesh Kumar Singh, AIP proceeding. (Accepted Manuscript) SJR-0.16, Citescore-0.7, I.F.- 0.41

## **CONFERENCES AND WORKSHOPS ATTENDED**

1. National Seminar on Ferroelectrics and Dielectrics at **Vellore Institute of Technology, AP**, Virtual Conference (Dec 2022). (Oral presentation).
2. International Union of Materials Research Society, International Conference in Asia – 2022, (IUMRS-ICA) at **IIT Jodhpur** (Dec 2022). (Poster presentation).
3. National Seminar on Crystallography at **IIT Roorkee** (2021). (Oral presentation).
4. International Conference on Advanced Materials and Mechanical Characterization (2021) Virtual Conference. (Poster presentation).
5. International Conference on Advanced Material for Better Tomorrow, **IIT-BHU** (2021). (Poster presentation)
6. 6th International Conference on Nanoscience and Nano-technology, **SRM Institute of Science and Technology**, (2021). Virtual Conference, (Poster presentation)
7. Online workshop on Rietveld Refinement Methods by **UGC-DAE Consortium of Scientific Research** (2020).
8. National Seminar on Crystallography at **BARC**, Mumbai (2018). (Poster presentation).
9. Magneto-electric Composites Workshop at **IIT-Bombay**, Mumbai (2017).