Synthesis, Characterization, Structural and Phase Analysis of Novel Antiferroelectric Solid Solution

PRESENTER

Yihan Lin, yla496@sfu.ca

Department of Chemistry, Faculty of Science

BACKGROUND

Antiferroelectric materials have drawn attentions widely, as promising candidates for energy storage and other applications. In this work, a novel antiferroelectric perovskite solid solution system, (1-x) $AgNbO_3$-(x) $PbZrO_3$ will be introduced, along with its interesting phase transitions and relaxation behaviors.

METHOD

$$(1\text{-}x)[(0.5)Ag_2O + (0.5)Nb_2O_5] + x[PbO + ZrO_2] \longrightarrow Ag_{(1-x)}Pb_{(x)}Nb_{(1-x)}Zr_{(x)}O_3$$

Hand grinding mental oxides PbO, ZrO_2, Ag_2O and Nb_2O_5 raw powder

Press into large pellets

Calcine at 950ºC for 6 hours (under O_2 atmosphere)

Break pellet and grind again

Add PVA, press into small pellets

Sinter at 1100˚C for 10 hours (under O_2 atmosphere)

$$Ag_2O + Nb_2O_5 \rightarrow 2\,AgNbO_3$$

Place calcined $AgNbO_3$ powder into alumina crucible

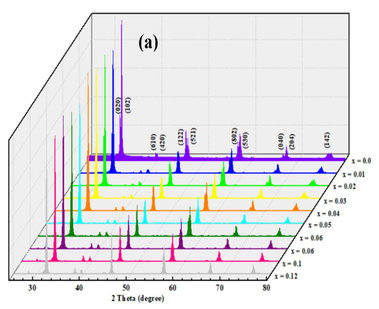
Heat furnace to 1300°C with rate 300°C/hr

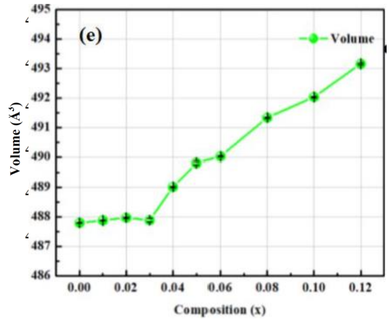
Keep temperature at 1300C° for 4 hours

Cool furnace to room temperature at 20°C/hr

RESULTS & DISCUSSION

Structural Analysis

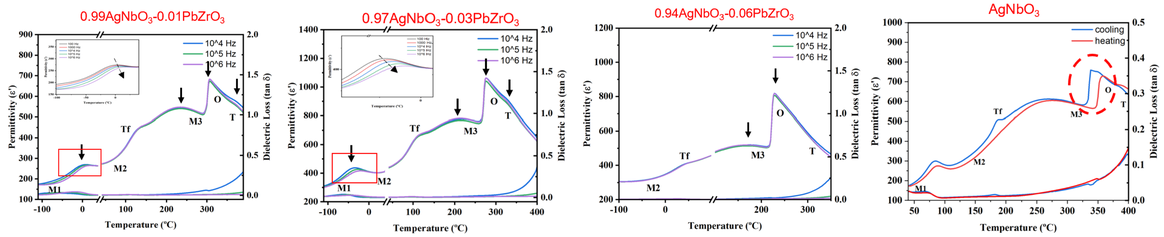


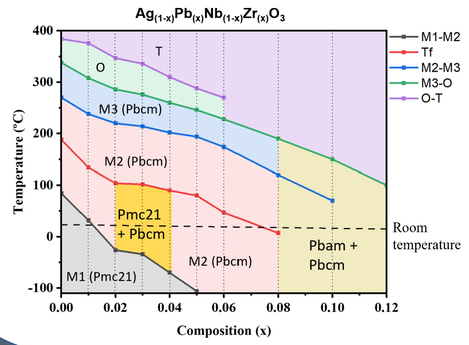


With the increase in concentration of lead zirconate $PbZrO_3$:

- The main symmetry of the solid solution remains orthorhombic but having different space groups.
- Cell volume increased

Dielectric Analysis

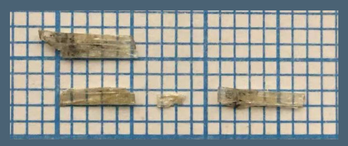


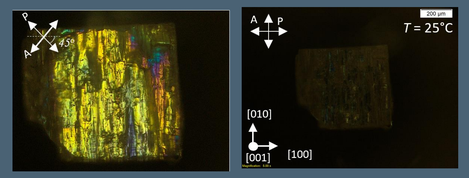


As the PbZrO3 concentration increases

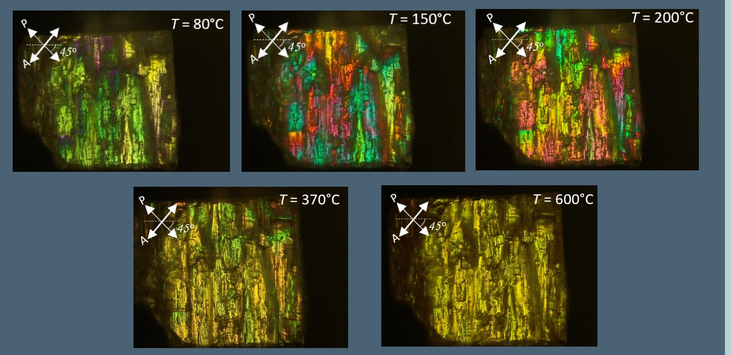
- All transition temperatures (as shown in arrows) shift lower
- Orthorhombic - Tetragonal (O-T) transition intensity diminished
- Dielectric thermal hysteresis behavior (circled in red) upon heating and cooling shown a first order phase transition

Single Crystals





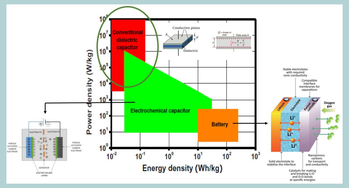
- Extinction of light at 0° proved orthorhombic phase symmetry at room temperature

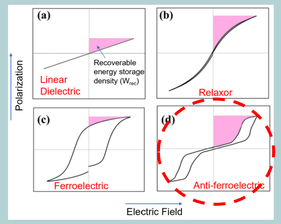


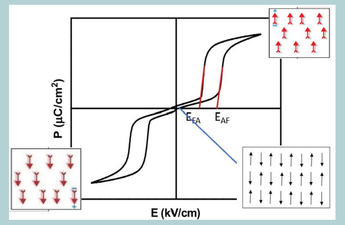
- As temperature increased, reflected color of crystal changed, indicating birefringence changes
- Moore study is needed to understand the optical properties

ADDITIOAL INFORMATION

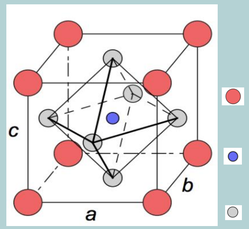
Types of dielectric materials







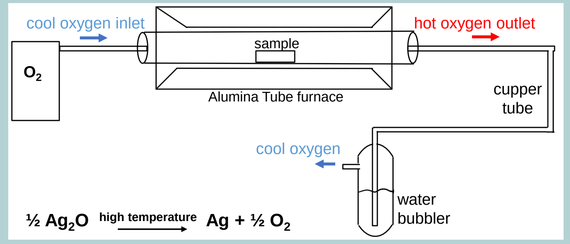
That is a perovskite structure



ABO_3

- A cations: large cations like Ag^+, Pb^{2+}…
- B cations: smaller cations like Nb^{5+}, Zr^{4+}…
- Oxygen anion: O^{2-}

Experimental setup



REFERENCES

1) J. Gao et.al., J. Am. Ceram Soc.101,5443–5450(2018)
2) 2) Z. Liu et.al., Adv. Mater. Technol. 3, 1800111(2018)
3) 3) P. Gao, Z.-G. Ye et. al., Chem. Mater. ,31, 979−990 (2019)
4) H. J. Goldschmidt AND J. R. Rait, Nature, 152, 356–356, (1943).

ACKNOWLEDGEMENTS

undergraduate research symposium

NSERC CRSNG

SFU SIMON FRASER UNIVERSITY

4D LABS