RIETVELD REFINEMENT OF BARIUM TITANATE STANNATE CRYSTAL STRUCTURE

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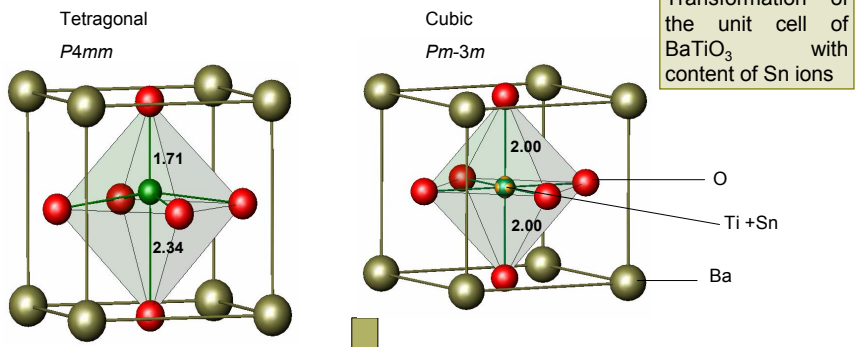
The barium titanates have wide application in electronic industry as a dielectric and ferroelectric materials. The $BaTiO_3$ doped with Sn is important for practical application in ceramic capacitors as well as in functionally graded materials. It is known that $BaTiO_3$ materials have the typical perovsikite crystal structural. Their ideal crystal structure is a centrosimetric cubic structure with space group. However, the changes in temperature, pressure, and composition lead to phase transitions and crystal structure transformations.

EXPERIMENTAL

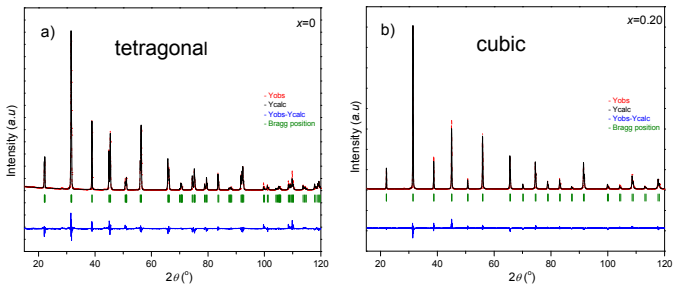
In this study the structure of barium titanate stannate (BTS) $BaTi_{1-x}Sn_xO_3$ (x = 0, 0.025, 0.05, 0.07, 0.10, 0.12, 0.15, 0.20) solid solutions was investigated. The BTS powders, with different Sn amount were synthesized by solid-state reaction technique. The structural investigations of the BTS samples were done at room temperature using an X-ray powder diffraction. The XRD patterns were obtained on a Philips PW-1050 automatic diffractometer using $CuK_{\alpha 1,2}$ radiation at 40 kV and 20 mA. The diffraction measurements were made over scattering angle 2θ from 20 to 120° with a step of 0.02° and a counting time of 15 s.

$$BaTiO_3 + Sn = BaTi_{1-x}Sn_xO_3$$

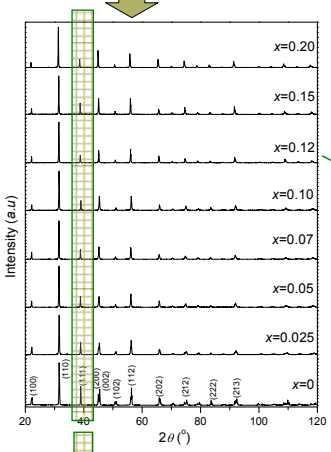


Transformation of the unit cell of $BaTiO_3$ with content of Sn ions

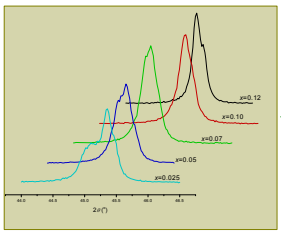
RESULTS



Final Rietveld refined plots of $BaTi_{1-x}Sn_xO_3$ (a) x = 0 and (b) x = 0.20



The changes in the (200) reflection with x =0.025, 0.05, 0.07, 0.10 (tetragonal phases) and 0.12, 0.15, 0.2 (cubic phase).

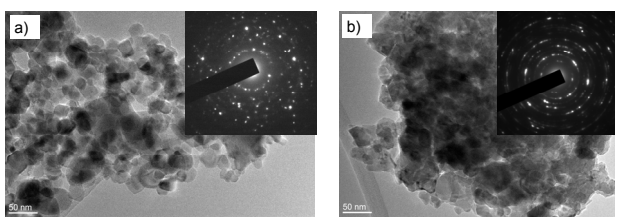


The nominal composition and unit cell contents obtained by Rietveld analysis

Notation	Nominal composition	Rietveld analysis
x=0	$BaTiO_3$	$BaTiO_3$
x=0.025	$BaTi_{0.975}Sn_{0.025}O_3$	$BaTi_{0.983}Sn_{0.017}O_3$
x=0.05	$BaTi_{0.95}Sn_{0.05}O_3$	$BaTi_{0.964}Sn_{0.036}O_3$
x=0.07	$BaTi_{0.93}Sn_{0.07}O_3$	$BaTi_{0.94}Sn_{0.06}O_3$
x=0.10	$BaTi_{0.90}Sn_{0.10}O_3$	$BaTi_{0.91}Sn_{0.09}O_3$
x=0.12	$BaTi_{0.88}Sn_{0.12}O_3$	$BaTi_{0.89}Sn_{0.11}O_3$
x=0.15	$BaTi_{0.85}Sn_{0.15}O_3$	$BaTi_{0.87}Sn_{0.13}O_3$
x=0.20	$BaTi_{0.80}Sn_{0.20}O_3$	$BaTi_{0.82}Sn_{0.18}O_3$

Unit cell parameters and cell volume for $BaTi_{1-x}Sn_xO_3$ (x = 0, 0.025, 0.05, 0.07, 0.10, 0.12, 0.15, 0.20) .

Notation	Space group	a (Å)	c (Å)	V (Å^3)
x=0	*P4mm*	3.9946(6)	4.0338(1)	64.37(2)
x=0.025	*P4mm*	4.0004(5)	4.0255(8)	64.42(2)
x=0.05	*P4mm*	4.0058(8)	4.0198(1)	64.044(2)
x=0.07	*P4mm*	4.0075(3)	4.0201(5)	64.56(3)
x=0.10	*P4mm*	3.9951(7)	4.0125(1)	64.044(2)
x=0.12	*Pm-3m*	4.0195(5)		64.94(1)
x=0.15	*Pm-3m*	4.0180(3)		64.87(3)
x=0.20	*Pm-3m*	4.0248		65.119(3)



The TEM images of $BaTi_{1-x}Sn_xO_3$ (a) x = 0 and (b) x = 0.20

CONCLUSION

The barium titanate stannate (BTS) $BaTi_{1-x}Sn_xO_3$ (x = 0, 0.025, 0.05, 0.07, 0.10, 0.12, 0.15, 0.20) solid solutions was investigated by X-ray powder diffraction and TEM microscopy. It was confirmed that increasing of Sn content in the perovskite structure results in transformation of the symmetry from tetragonal to cubic.