Preparation and characterization of new perovskite compounds $(Na_{0.5}Sr_{0.5})(M_{0.5}N_{0.5})O_3$ (M=Ti,Zr N=Ta, Nb)

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I. Introduction

Most of the compounds with the general formular ABO_3 have the perovskite structure. Crystal structure and properties depends on the ions which resides on A and B-site. Therefore various perovskite-related structres have been studied to get the desired structure and properties. Typical types are represented as ternary perovskite-type oxides($A^{+1}B^{+5}O_3$, $A^{+2}B^{+4}O_3$, $A^{+3}B^{+3}O_3$ and oxygen- and cation-deficient phases) and complex perovskite type compounds($A(B'_{0.67}B''_{0.33})O_3$, $A(B'_{0.33}B''_{0.67})O_3$, $A(B'_{0.5}B''_{0.5})O_3$ and oxygen deficient phases $A(B'_xB''_y)O_{3-x}$). In this research, we will study the crystal structure and dielectric properties about the new $(A^{+1}_{0.5}A^{+2}_{0.5})$ $(B^{+4}_{0.5}B'^{+5}_{0.5})O_3$ type perovskite compound.

2. Experimental

The composition used in the present experiment were $(Na_{0.5}Sr_{0.5})(Ti_{0.5}Nb_{0.5})O_3$, $(Na_{0.5}Sr_{0.5})(Ti_{0.5}Ta_{0.5})O_3$ and $(Na_{0.5}Sr_{0.5})(Zr_{0.5}Nb_{0.5})O_3$. These composition were prepared from oxide powders $SrCO_3$, Na_2CO_3, TiO_2, ZrO_2, Nb_2O_5 and Ta_2O_5 . The mixed powders were calcined at 850℃ 10h. and the calcined powder was pressed into a disk measuring 10 mm diameter and 0.7 mm thick. Disk pellets were sintered at 1300℃ 1h. Dielectric properties were measured in the temperature range 22K~700K. The powder X-ray Rietveld analysis were carried out for 5000 diffraction data, which were recorded by MAC Science diffractometer. The data were taken from 20° to 120° (2θ) with 0.02° intervals.

3. Results and disscusion

Three compounds $(Na_{0.5}Sr_{0.5})(Ti_{0.5}Nb_{0.5})O_3$, $(Na_{0.5}Sr_{0.5})(Ti_{0.5}Ta_{0.5})O_3$ and $(Na_{0.5}Sr_{0.5})(Zr_{0.5}Nb_{0.5})O_3$ showed a single phase perovskite structure with small superstructure reflections of XRD. We found that these superlattice were induced by the distortions of oxygen octahedon not by the ordering of cations. So, following Glazer, the unitcell and space group of each compound were determined as shown in TABLE 1. The powder X-ray diffraction patterns were analyzed by the RIETAN powder X-ray Rietveld analysis program.

Fig.2 shows the dielectric constant variation with temperature. Usually dielectric anomaly have a relation with structure change and phase transition temperature increase with the distortion of structure. So it is expected to find a same realtion between the phase transition temperature and octahedron distortion for our samples.

4. Summary

New complex perovskite compounds $(Na_{0.5}Sr_{0.5})(Ti_{0.5}Nb_{0.5})O_3$, $(Na_{0.5}Sr_{0.5})(Zr_{0.5}Ta_{0.5})O_3$ and $(Na_{0.5}Sr_{0.5})(Ti_{0.5}Ta_{0.5})O_3$ have been prepared. The crystal structures of these compounds were determined by powder X-ray Rietveld analysis. The crystal structure of $(Na_{0.5}Sr_{0.5})$ $(Ti_{0.5}Nb_{0.5})O_3$ and $(Na_{0.5}Sr_{0.5})(Zr_{0.5}Ta_{0.5})O_3$ was Pmmn, and that of $(Na_{0.5}Sr_{0.5})(Ti_{0.5}Ta_{0.5})O_3$ was I4/mmm. All these compounds showed the superstructure due to the oxygen octahedron distortion. The selected bond distances and bond angles were calculated by the OFFER. The octahedron distortion for each sample, which was measured from the bond distances and bond angles, showed the following order: $(Na_{0.5}Sr_{0.5})(Zr_{0.5}Ta_{0.5})O_3$ > $(Na_{0.5}Sr_{0.5})$ $(Ti_{0.5}Nb_{0.5})O_3$ > $(Na_{0.5}Sr_{0.5})(Ti_{0.5}$ $Ta_{0.5})O_3$. Dielectric properties were measured for the samples. In this study, the crystal structure and dielectric properties of the new complex perovskite structures are duscussed.

References.

1. Hoon- Taek chung , "The relation of dielectric properties and structure change with temperature for $(Na_{0.5}Sr_{0.5})(Ti_{0.5}Nb_{0.5})O_3$", J. of Korean Association of Crystal Growth. 5(4) 394 - 399 (1995).

2. In-Seon Kim et al.,"Preperation and charateriation of new ruthenium compounds with perovskite structure", Mat. Res. Bul.,28 1029- 1039 (1993).

TABLE 1. Crystal data for $(Na_{0.5}Sr_{0.5})(Ti_{0.5}Nb_{0.5})O_3$, $(Na_{0.5}Sr_{0.5})(Ti_{0.5}Ta_{0.5})O_3$ and $(Na_{0.5}Sr_{0.5})(Zr_{0.5}Ta_{0.5})O_3$.

Empirical formula	$(Na_{0.5}Sr_{0.5})(Ti_{0.5}Nb_{0.5})O_3$	$(Na_{0.5}Sr_{0.5})(Ti_{0.5}Ta_{0.5})O_3$	$(Na_{0.5}Sr_{0.5})(Zr_{0.5}Ta_{0.5})O_3$
Cryatal system	orthorhombic	tetragonal	orthorhombic
Space group	Pmmn-No.59	I4/mmm-No.139	Pmmn-No.59
Cell constant	a = 7.8342(4) Å b = 7.8361(4) Å c = 7.8551(1) Å	a = 7.8367(1) Å c = 7.8537(1) Å	a = 8.0214(21) Å b = 8.0208(21) Å c = 8.0544(2) Å
Z	8	8	8
2θ range	20° -120°	20° -120°	20° -120°
No. of data point	5000	5000	5000
R factors(%)[a]			
R_{wp}	9.92	8.63	9.13
R_p	7.93	6.36	6.09
R_e	4.12	2.93	2.85
R_i	4.01	6.56	3.48
S	2.41	2.94	3.01

a) $R_{wp} = \{\sum_i w_i [y_i - f_i(x)]^2 / \sum w_i y_i^2\}^{1/2}$ $Rp = \{\sum_i | [y_i - f_i(x)] | / \sum y_i\}$

$R_e = \{N_p - N_r - N_c / \sum w_i y_i^2\}^2$ $R_i = \sum | I_k('O') - I_k(c) | / \sum I_k('O')$ $S = R_{wp} / R_e$

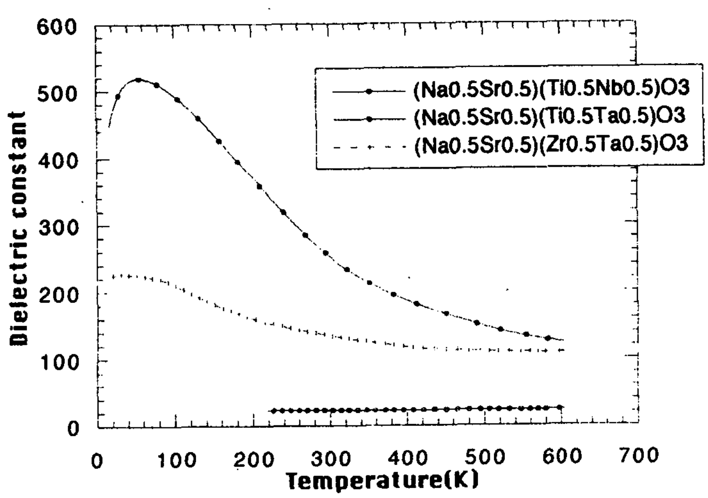

Fig.2 Dielectric constants as a funtion of temperature in the system.