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The Structural Analysis Of Perovskite $(Ba_{0.8}Ca_{0.2})TiO_3$ Compound in A-site

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Abstract: Calcium doping material has been successfully doped to produce Barium Calcium Titanate ($Ba_{1-x}Ca_xTiO_3$) within the percentage of moles of calcium 20% that processed by the solid state reaction method. Firstly, compounds ($BaCO_3$, TiO_2, and $CaCO_3$) have mixed, grinding during the 7 hours to form of powder. Then after sample pellets were pressed by hydraulic press machine which have been Calcination in a furnace at 1100°c during 10 hours. The properties of sample were observed using X-ray diffraction.

Key Words: Barium Calcium Titanate, Solid state reaction, Calcination, x-ray diffraction.

1. Introduction:

The present work we have selected Ca ions to be doped at Ba site of YBaTiO3. The compounds were prepared by employing solid state reaction techniques. The 99.99% pure powders of different oxides were collected for purity of compound. The stoichiometric calculated amount of powders was mixed through wet mixing technique. Few drops of acetone were utilized for wet mixing medium. The powder was then compacted into circular pallets with very low pressure. These pallets were calcined in a furnace at 1100°c for 10 hours and then sintered for densification. The sintered samples were annealed in air for good quality of crystal formation.

2. Sample:

$Ba_{1-x}Ca_xTiO_3$ Where x = 0.2

3. Sample Preparation

For planning of the Perovskite compound of the $BaCaTiO_3$, we have taken the oxide type of the compound. For example, $BaCO_3$, TiO_2, and $CaCO_3$.The perovskite compound ($BaCaTiO_3$) plans to go through the way toward mixing, crushing, pelletization, sintering, Calcination and two fold time of annealing.

4. Structure

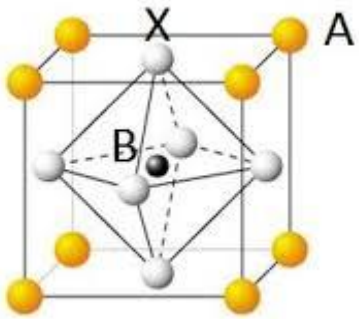

Figure 1 Perovskite Structure

Where,

- A ions
- B ions
- X ions

5. Calculation

5.1 Tolerance Factor (t) $(Ba_{0.8}Ca_{0.2})TiO_3$:

- Tolerance factor is an illustrate the stability and distortion of the crystal structure.
- Tolerance factor is generally used for perovskite material.
- The general formula of Goldschmidt tolerance factor is given below;

$$\text{Tolerance factor (t)} = \frac{ra+ro}{\sqrt{2}(ro+rb)}$$

Where,

- ra is the radius of the A cation
- rb is the radius of b cation
- ro is the radius of the anion

5.2 Ionic radii list:

Ca = 1 Å
Ba = 1.35 Å
Ti = 0.605 Å
O = 1.4 Å

- Average ionic radius = ionic radii of Ba* abundance + ionic radii of Ca* abundance
  = 1.35*0.80 + 1*0.20
  = 1.08 + 0.20
  = 1.28 Å

5.3 Goldschmidt Tolerance Factor (t) = $\frac{1.28+1.4}{1.41\ (1.4+0.605)}$

$= \frac{2.68}{1.41\ (2.005)}$

$= \frac{2.68}{2.827}$

(t) = 0.948

5.4 Range of Goldschmidt tolerance factor:

Goldschmidt tolerance factor	Structure	Explanation	Example
>1	Hexagonal/ Tetragonal	A ion too big and B ion is small	$BaNiO_3$
0.9-1	Cubic	A&B ion have ideal size	$SrTiO_3$ $BaTiO_3$
0.71-0.9	Orthorhombic / Rhombohedral	A ion too small to fit into B ion interstices	$GdFeO_3$ $CaTiO_3$
<0.71	Different structure	A ion and B ion have similar ionic radii	$FeTiO_3$

6. Stoichiometric Calculation

- The Goldschmidt tolerance factor , we defined the material structure is Chemical formula: $(Ba_{0.8}Ca_{0.2})TiO_3$

Chemical reaction:

$0.8\ BaCO_3 + TiO_2 + 0.2CaCO_3 \rightarrow (Ba_{0.8}Ca_{0.2})TiO_3 + CO_2$

- Molar Mass :

Ba = 137.327 g/mole
Ca = 40. 078 g/mole
O = 15.999 g/mole
Ti = 47.867 g/mole
C = 12.0107 g/mole

Molar mass of $BaCO_3$ = 197.334 g/mole
Molar mass of TiO_2 = 79.865 g/mole
Molar mass of $CaCO_3$ = 100.09 g/mole

Total molar mass of $(Ba_{0.8}Ca_{0.2})TiO_3$ = 213.7412 g/mole

Calculation for 1 gram $(Ba_{0.8}Ca_{0.2})TiO_3$

$\frac{0.80*197.334}{213.7412}$ g $BaCO_3$ = 0.7385 g $BaCO_3$

$\frac{1*79.865}{213.7412}$ g TiO_2 = 0.3736 g TiO_2

$\frac{0.20*100.09}{213.7412}$ g $CaCO_3$ = 0.09365 g $CaCO_3$

1 gram $Ba_{0.8}Ca_{0.2}TiO_3$

0.7385 $BaCO_3$ + 0.3736 TiO_2 + 0.0936 $CaCO_3$ ⟶ $Ba_{0.8}Ca_{0.2}TiO_3$

7. Result and Discussion

The structural characterisation of this perovskite $Ba_{0.8}Ca_{0.2}TiO_3$ compound is done by using the X-ray diffraction method. We get the information by X-ray plot, which is illustrate given below

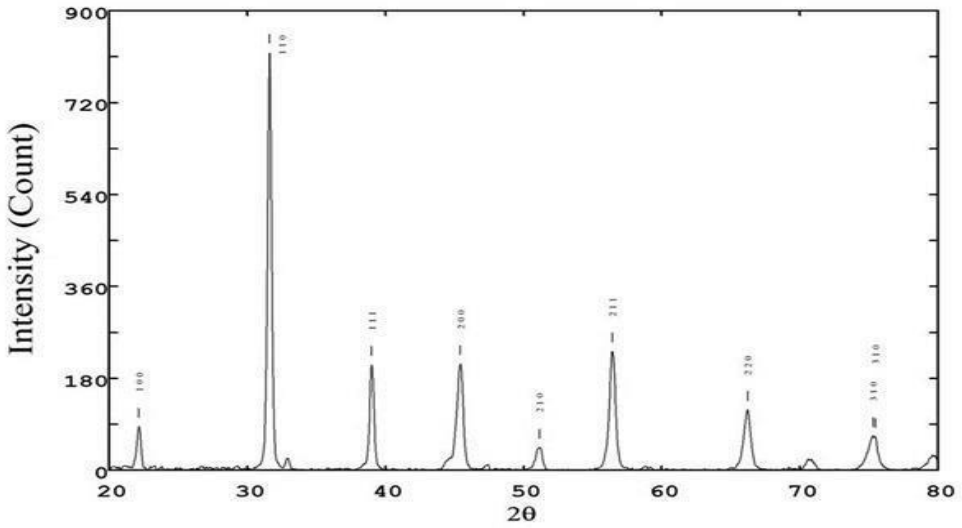

Figure 2 X-ray characterization plot

The x-ray analysis of the given perovskite compound is shown in the above plot. The plot shows the crystal structure. The peak illustrate that present of crystalline material. The x-ray characterisation of the given perovskite compound $Ba_{0.8}Ca_{0.2}TiO_3$ is done by powder- x software.

We find the a=3.998Å, b=3.998Å, and c= 4.089Å by using powder-x software.

FT-IR data

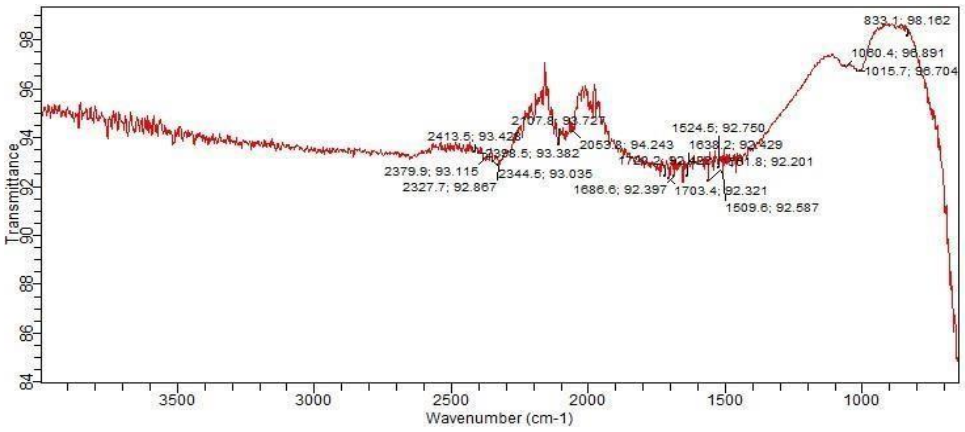

Figure 3 FT-IR plot

Confirmation of MNPs functionalization was carried out also by FT-IR spectroscopy. In this regard was recorded IR spectrum for hybrid material and for comparison are include also spectres of precursors. Investigation of IR spectra dates of final products showed presences of wavelength characteristics to Ti-O vibration , alkenes(C-H) peak at 833 cm^{-1} and 1080 cm^{-1},C=O bond at 1638 cm^{-1} and 1720 cm^{-1} and alkynes peak at 2107 cm^{-1} , 2413cm^{-1} , the peak at 3400 cm^{-1} corresponding for hydroxyl group –OH. According to these results the functionalism of MNPs with targeting dipeptide was successfully accomplished.

8. Conclusion:

The sample prepared by solid state reaction method. The analysis of XRD data using Powder X software shows that sample is tetragonal. For the $Ba_{0.8}Ca_{0.2}TiO_3$ XRD data is a=3.998Å, b=3.998Å, and c=4.089Å.

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