### Synthesis and Characterization of BaBiO$_3$ Perovskite through Chemical Route

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**Abstract**

BaBiO$_3$ (perovskite) polycrystalline semiconducting material was synthesized by sol-gel chemical method. Structure of the sample was characterized by X-Ray Diffraction (XRD). Grain, Grain boundary topography and chemical composition of the sample studied by using Scanning Electron Microscope (SEM) and Energy Dispersive X-Ray Spectrometry (EDS). Fourier transform-Infrared spectroscopy (FT-IR) was used for the study of band structure. The result of XRD characterization was indicated as the BaBiO$_3$ is monoclinic perovskite and crystalline size is 85 nm. SEM image of the BaBiO$_3$ showed the grain size of 85 nm. The FT-IR spectroscopy study showed that, the BaBiO$_3$ has absorbent peak at 1420 cm$^{-1}$. The high temperature super conductivity of the K$_x$Bi$_{1-x}$O$_3$ is close to 30 K (for $x = 0.4$), one of the highest among materials without copper or iron. Unlike copper- and iron based superconductors, Ba$_{1-x}$K$_x$BiO$_3$ is nonmagnetic and its electrons are likely paired by a more conventional electron-phonon coupling mechanism (Timur Bazhirov et al., 2013). Super conductivity in Ba(Pb,Bi)O$_3$ over a composition range $0.1 < x < 0.3$ was discovered in 1975 by Sleight et al with a maximum $T_c$ of 13.5K. Superconductivity in the (Ba,K)BiO$_3$ was discovered in 1988 by Matthes and his colleagues (Grumann et al. 1994).

The crystal structure of BaBiO$_3$ was determined to be monoclinic at room temperature in 1976, 1979 by Cox and Sleight using powder neutron diffraction. This result was supported by neutron diffraction studies and x-ray absorption studies (Akhitar et al., 1993). In this compound, two different BiO$_6$ octahedral are connected alternatively by edge-sharing mode along the crystallographic directions. One octahedron is tilted from the vertical c-axis and the next one is tilted in opposite direction to construct a zigzag structure with the angle of 159.9$^\circ$ (Dongwoon Jung et al., 1999).

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### MATERIALS AND METHODS

The sol–gel method widely used to produce nano crystalline BaBiO$_3$ powders and films. This process involved dissolving the metal-containing compounds in the solvent, hydrolyzing to polymeric condensation, drying the resulting solution into various gels, and, finally, annealing...
An energy-dispersive (EDS) detector is used to separate the characteristic X-rays of different elements into an energy spectrum, and EDS system software is used to analyze the energy spectrum in order to determine the abundance of specific elements. EDS can be used to find the chemical composition of materials down to a spot size of a few microns, and to create element composition maps over a much broader raster area.

In figure 3 each energy peak of the EDS pattern corresponds to elements in the sample i.e. Ba, Bi and Au. The showing up of gold in the pattern is because the sample was coated with gold before its characterization of SEM.

The EDS does not only tell us the elemental composition of the sample but also shows the relative abundance of each chemical element in the sample (Table 1).

Table 1: elemental weight of BaBiO$_3$

<table>
<thead>
<tr>
<th>Elements</th>
<th>O</th>
<th>Ba</th>
<th>Bi</th>
<th>Au</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weight</td>
<td>11.81</td>
<td>21.07</td>
<td>49.78</td>
<td>12.33</td>
</tr>
</tbody>
</table>

Micro Structural Properties of BaBiO$_3$ Ceramics

The close observation at the micrograph of BaBiO$_3$ figure 2 taken from SEM showed large grain size at the boundary this is expected to be due to existence Bi ions in the sample (Sreenu et al., 2014) with same porosity and scratches. The grain size was around 4 µm in uniform as calculated using line intercept method.

Compositional Distribution Study

An interaction of an electron beam with a sample target produces a variety of emissions, including x-rays. An energy-dispersive (EDS) detector is used to separate the characteristic X-rays of different elements into an energy spectrum, and EDS system software is used to find the chemical composition of materials down to a spot size of a few microns, and to create element composition maps over a much broader raster area.

In figure 3 each energy peak of the EDS pattern corresponds to elements in the sample i.e. Ba, Bi and Au. The showing up of gold in the pattern is because the sample was coated with gold before its characterization of SEM.

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Fourier Transform Infrared Spectroscopy (FTIR)

A molecule absorbs radiation at certain frequency, which cause a quantum change in its energy. The IR radiation has correct frequency to cause a quantum jump in the vibration energy of the molecule. The vibrations of a molecule absorb the radiation of IR radiation, which the oscillations cause a change in the dipole moment. The frequency at which the absorption takes place is equal to frequency of oscillations of the dipole and falls in the region. IR spectra of all the samples are recorded in the range 4000-400 cm$^{-1}$ (Figure 4). From this FTIR pattern it is seen that pure BaBiO$_3$ shows as absorption at 1420 cm$^{-1}$ which are considered to be a characteristic feature of the sample and are attributed to Ba–O band bending vibrations. Even though some ions are different, the absorption peak in the vicinity of 540 cm$^{-1}$ is assigned to the vibration of O–M (M=ion at B-site) bond i.e. O-Bi (Table 2).

Table 2: Infrared band positions (cm$^{-1}$) of BaBiO$_3$

<table>
<thead>
<tr>
<th>Band position</th>
<th>Wave No(cm$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ba-O</td>
<td>1420</td>
</tr>
<tr>
<td>Bi-O</td>
<td>702, 520</td>
</tr>
</tbody>
</table>

Figure 2: the micrograph of BaBiO$_3$ taken by SEM

Figure 3: EDS pattern of BaBiO$_3$

Figure 4: Infrared spectra of barium bismuthate
CONCLUSIONS

BaBiO$_3$ polycrystalline material is synthesized by sol-gel method having the crystallite size of 85nm and the x-ray characterization with lattice parameters $a = 6.33\,\text{Å}$, $b = 6.12\,\text{Å}$ and $c = 8.62\,\text{Å}$ and unit volume is $334\,\text{cm}^3$ indicates that BaBiO$_3$ is monoclinic perovskite at room temperature with percentage of density 94 $(\text{gm/cm}^3)$. SEM results reveal that the grain size is large because of the Bi-ion. The EDS analyze of sintered pellet of BaBiO$_3$ reviled that the sample was pure. From the detailed FTIR spectra analysis, it was observed that the pronounced peak at 1420cm$^{-1}$, where a metallic bond is observed, considered being a characteristic feature of BaBiO$_3$.

Conflict of Interest
Conflict of interest none declared.

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