Synthesis, Structural and Morphological Property of $BaSnO_3$ Nanopowder Prepared by Solid State Ceramic Method

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Synthesis, Structural and Morphological Property of $BaSnO_3$ Nanopowder Prepared by Solid State Ceramic Method

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Abstract. $BaSnO_3$ is a cubic perovskite-type oxide that behaves as an n-type semiconductor with a wide band gap of 3.4 eV and remains stable at temperatures up to 1000^0C. It has wide applications such as thermally stable capacitors, humidity sensors, gas sensors, etc. Barium stannate has also been used in optical applications, in capacitors and ceramic boundary layers, and as a promising material to produce gas phase sensors for the detection of carbon monoxide and carbon dioxide. $BaSnO_3$ powder was prepared by solid state ceramic method. X-ray diffraction pattern of the prepared sample presents all the characteristic peaks of cubic phase of $BaSnO_3$ (JCPDScard no: 15 -0780). The lattice constant for the compound was calculated and found to be $4.101A^0$ which is in agreement with the reported value ($4.112A^0$). The average size of the crystallites estimated by Debye Scherrer's formula was found to be 49 nm shows the nanostructured nature. The Raman bands observed ~ 139, 833 and 1122 cm^{-1} can be assigned on the basis of the fundamental vibrations of SnO_6 octahedron which has Oh symmetry, in the distorted perovskite structure. The SEM image shows a porous surface morphology with grains of cuboidal structure with well-defined grain boundaries. UV-Visible spectra shows $BaSnO_3$ powder exhibit high reflectance in the 400-700 nm range.

1. Introduction

Alkaline earth stannates with the general formula $RSnO_3$(R = Ba,Sr and Ca) are important material systems inview of their interesting physical properties and perovskite structures.[1] Perovskite-type oxides have a simple and flexible structure that is easy for ionic substitution, carrier doping and oxygen non-stoichiometry, which can form a vast set of technologically important materials for a wide variety of industrial applications[2,3]. $BaSnO_3$ is a cubic perovskite-type oxide that behaves as an n-type semiconductor with a wide band gap of 3.4 eV and remains stable at temperatures up to 1000^0C. It has wide applications such as thermally stable capacitors, humidity sensors, gas sensors, etc[4-5]. Barium stannate has also been used in optical applications,[6] in capacitors and ceramic boundary layers, [7]and as a promising material to produce gas phase sensors for the detection of carbon monoxide[8] and carbon dioxide.[9] Lampe et al[8] proposed thin films of $BaSnO_3$ to be used as a NO sensor in the temperature

range of 450–550^{0}C, and as a material for CO sensor in the temperature range of 600–700^{0}C[10]. It is reported that $BaSnO_3$ doped with a few percent of La exhibits unusually high electrical mobility of 320 $cm^2(Vs)^{-1}$ at room temperature and superior thermal stability at high temperatures. Various techniques have been employed to synthesize, $BaSnO_3$ powder such as solid state method, self heat sustained method, co-precipitation method, hydrothermal synthesis method etc. This work reports the preparation and characterization of $BaSnO_3$ powder by solid state method and its structural, morphological and optical properties.

2. Experimental techniques

$BaSnO_3$ powder was prepared by solid state ceramic method[11]. Stoichiometric amount of commercially available high purity $BaCO_3$ and SnO_2 powders (Aldrich-purity 99.9%) were mixed in an agate motor for 6 hrs using acetone as the mixing medium. The homogeneous mixture thus obtained was heated in an alumina crucible up to temperature 1000^{o}C and kept at that temperature for 8 hrs. Polyvinyl alcohol was added to the calcined powder for the fabrication of pellets, which was burnt out during high-temperature sintering. Circular disc shaped pellets were prepared by applying a load of 5 ton. These pellets were crushed and sintered in a platinum crucible at temperature 1250°C for 6 hrs. The structural, morphological and optical properties of the material were investigated in detail. The crystalline quality and crystallographic orientation were investigated using X-ray diffraction analysis (XPERT-PRO X-ray diffractometer) using Cu Kα1 radiation of wavelength 1.54060Aº in the 2θ range 10-100º. The vibrational spectrum was recorded using micro-Raman spectrometer (Labram HR-800) using a laser radiation of wavelength 514 nm from an argon ion laser. The spectrum was recorded with a spectral resolution of $1cm^{-1}$. The morphology and elemental analysis of the compound were investigated using NOVA NANOSEM 450 (FEI,U.S.A) equipped with Quantax 200 Energy Dispersive X-ray spectrometer (Bruker).The absorbance and reflectance spectra of the material in the spectral range 200-900 nm were recorded using JASCO V-550 UV-visible double beam spectrometer. The TEM observation of the sample was carried out by using JEOL JEM -2100 electron microscope operating at 200keV.

3. Results and discussion

3.1. XRD analysis and Micro-RAMAN analysis

The XRD pattern of $BaSnO_3$ powder prepared by solid state reaction method and it presents a polycrystalline nature. X-ray diffraction pattern of the prepared sample presents all the characteristic peaks of cubic phase of $BaSnO_3$ (JCPDS card no: 15 -0780). The inter planar distance 'd' of the powder is calculated using Bragg's relation $2d\sin\theta = n\lambda$, where λ is the wavelength of the X-ray radiation and θ is the diffraction angle. The lattice constant for the compound was calculated and found to be 4.101A^0 which is in agreement with the reported value (4.112A^0)[1]. The average crystallite size (D_{hkl}) of the powder can be calculated using the Debye Scherrer's formula[12],

$$D_{hkl} = \frac{K\lambda}{\beta \cos\theta} \qquad \text{------- (1)}$$

where, λ is the wavelength of the X-ray and β is the FWHM in radians. The average size of the crystallites was found to be 49 nm. This shows the nanocrystalline nature of the powder.

Barium stannate in the cubic structure has space group Pm3m with 1 formula unit per Bravais lattice. The micro-Raman spectrum of the $BaSnO_3$ powder prepared in the present case by solid state reaction method presents a very intense band at 1054 , intense band at 560,139and weak intense band at 686,336,1130.The band at 1054 is due to$BaCO_3$. The Raman bands observed ~ 139, 833 and 1130 cm^{-1} can be assigned on the basis of the fundamental vibrations of SnO_6 octahedron which has O_h

symmetry, in the distorted perovskite structure. The Raman active mode observed at 139cm^{-1} can be assigned to v_5F_{2g} *mode*.[13]

3.2 SEM Analysis

Fig.1(a). shows the SEM micrograph of the $BaSnO_3$ sample. The SEM image shows a porous surface morphology with grains of cuboidal structure having well defined grain boundaries. The elemental analysis of the compound using EDS analysis supports the formation of the compound. Fig.1(b). shows the EDS spectra of the powder sample prepared by the solid state method. The EDS spectra also gives an evidence for the synthesis and formation of compound.

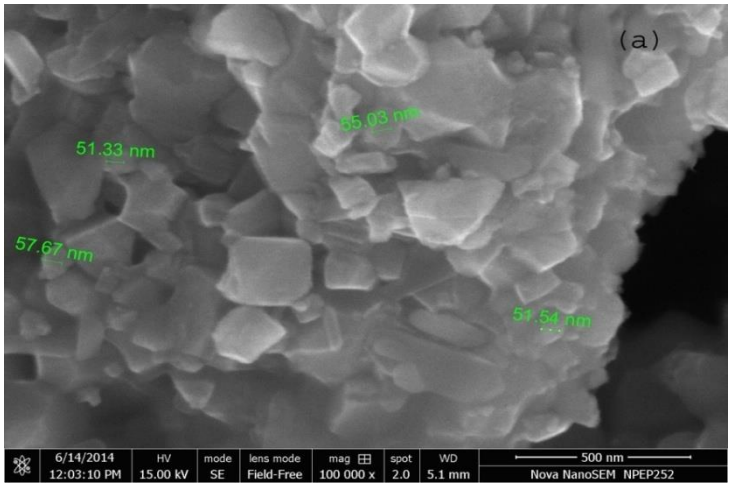

Fig.1(a):SEM images of $BaSnO_3$ prepared by solid state reaction method

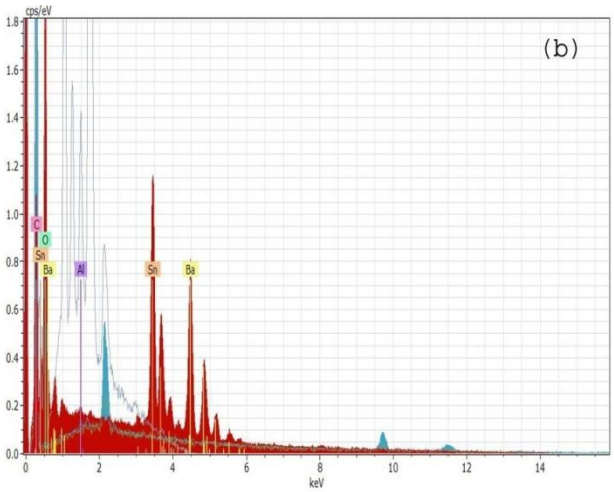

Fig. 1(b): EDS images of $BaSnO_3$ prepared by solid state reaction method

3.3. TEM Analysis

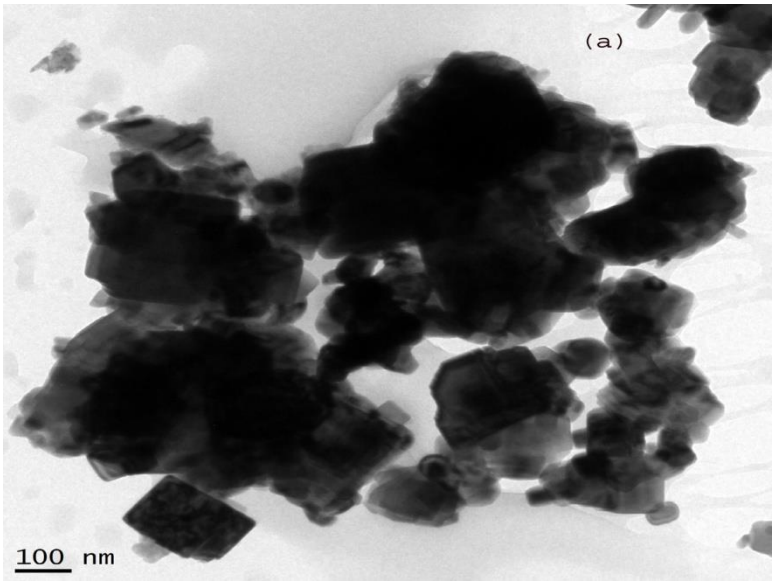

Fig 2: TEM image of $BaSnO_3$ prepared by solid state reaction method

A high resolution nanostructural and morphological characterization of powder were studied by using transmission electron microscopy The particle size of the powder calculated from *TEM analysis* is 55nm which is in agreement with XRD and SEM analysis. The TEM image also shows the porous surface morphology with grains of cuboidal structure.

3.4. UV-Visible Analysis

The reflectance and absorbance spectra of $BaSnO_3$ powder samples are recorded in the wavelength range 200-900 nm. The absorption spectrum and reflectance spectrum of the powder sample is shown in fig.3(a)and 3(b) respectively. The sample exhibit high reflectance in the 400-700 nm range. The band gap energy is found to be ~ 3.1eV which is in agreement with reported values. The band gap and the electronic structure depend primarily on the bond in within the corner-sharing octahedral network (SnO_6)[14].

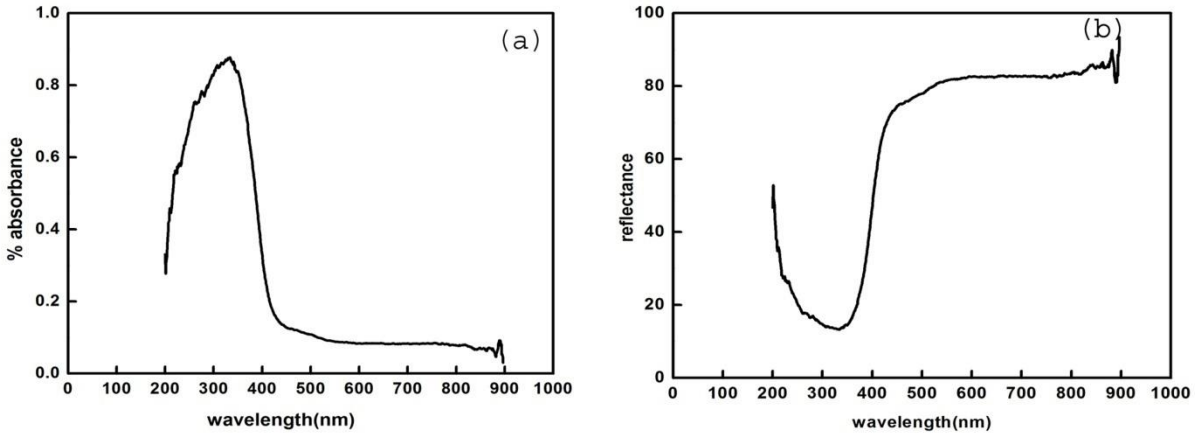

Fig.3(a):Absorption spectrum of $BaSnO_3$ and 3(b): Reflectance spectrum of $BaSnO_3$

4. Conclusion

The XRD and micro-Raman analysis suggest cubic crystalline structure supporting the formation of $BaSnO_3$ phase in the prepared sample. The SEM image shows a porous surface morphology with cuboidal grains with well- defined grain boundaries for the prepared sample. The sample exhibit high reflectance in the 400-700 nm range. The HRTEM image shows the nanocrystalline nature. The HRTEM image also supports the XRD and SEM analysis. The UV-visible analysis is carried out and the sample exhibit high reflectance in the 400-700 nm range. The band gap energy is found to be ~3.1eV which is in agreement with reported values.

5. References

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