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Thesis title:

Investigation on the Electrical and Cold Emission Properties of Wide Band Gap Perovskite Oxide $BaSnO_3$

Abstract

Ternary metal oxides with the chemical formula ABO_3 and crystal structure resembling $CaTiO_3$ are typically referred as perovskite oxide in the honor of Russian scientist L. A. Perovski. Perovskite oxides have received tremendous attention in recent years from both theoretical and practical perspectives due to their fascinating characteristics, such as their high energy storage capacity, visible light transparency, ferroelectricity etc. In this family, the interplay among structural, optical and transport properties are noted frequently which helps to integrate a number of intriguing features. Recently a lot of interest on wide band gap perovskite oxides especially on barium stannate ($BaSnO_3$) has grown due to its exciting optical, thermal and electrical properties. $BaSnO_3$ is visibly transparent having a wide band gap of ~3.1 eV and high thermal stability (>1000 °C). By simply changing the processing temperature and doping with right cation, it is possible to readily modify the electrical properties of $BaSnO_3$, as example dielectric permittivity, electrical conductivity etc. Aditionally, in the display sectors, $BaSnO_3$ in nano/micro form can be used to design numerous electronic devices, including flexible screens and other forms of field emission display units due to its desirable work function, electron affinity and tunable electrical property.

Even though there have been numerous studies on barium stannate and its properties published in the literature, there are still certain issues remain unresolved. The aim of this doctoral thesis, "**Investigation on the Electrical and Cold Emission Properties of Wide Band Gap Perovskite Oxide $BaSnO_3$**," is to investigate the synthesis methods, various properties, and different uses of both pure and doped barium stannate. Another important objective is to fabricate $BaSnO_3$/polymer nanocomposite and exploring their structural and electrical characteristics to improve their multipurpose performances. This dissertation firstly describes the synthesis process to prepare barium stannate and then modify the pure system to study different properties of the altered system.

Aiming to this, the nanocrystalline barium stannate powder was synthesized following traditional solid-state reaction route. The grain size as well as the density (or in other word, porosity) of the samples were varied by varying synthesis temperature. With routine structural, morphological, compositional and optical characterizations, the effects of grain size and density alteration on the electrical properties of the system were analyzed. It was found that the overall polarization *i.e.* the dielectric permittivity was increased with the grain size and the density of the sample. Also, the conductivity was enhanced due to the grain size increment which provides better ordered path in order to transport the charge carriers. Hence, the nanocrystalline $BaSnO_3$ is inferred as potential candidate for thermally stable ceramic capacitor.

Encouraged by the results, investigations were done to study the changes in the electrical properties of transition metal ion doped $BaSnO_3$, due to an alteration in external DC bias. Although, due to the smaller grain size and higher porosity, the room temperature permittivity and the conductivity were decreased for

the doped sample, but the application of DC bias was more prominent for the doped samples. Being smaller in size, vanadium plays important role in formation of lighter dipoles which helps in dipolar polarization in presence of external DC bias. The dielectric permittivity was increased with DC bias, whereas the grain and grain boundary resistances were reduced resulting an indirect enhancement in conductivity. Thus, the vanadium doped $BaSnO_3$ can serve as a tuning capacitive material at room temperature.

The suitable work function (3.04 eV), tunable electrical property, visible light transparency motivated us to find out whether the material can be used in a true multipurpose way. Aiming to this, simulation-based field electron emission was carried out using ANSYS-MAXWELL software. Encouraged by the positive results, the actual field emission experiment was investigated for pure and vanadium doped barium stannate nanocubes. The particle size variation has a significant impact on improving the emission efficiency of the doped samples. The turn on field was reduced and the enhancement factor was elevated for the vanadium doped $BaSnO_3$. For practical use in microelectronics, the optimum device condition was achieved by analyzing the effect of inter-electrode separation on the emission properties. Also, the doped sample showed a high temporal stability which is another important factor to consider.

The easily tunable electrical properties, as observed from the above studies, can further be extended in fulfilling the need for lead free peroskite/polymer nanocomposite with high dielectric permittivity, superior flexibility, large breakdown strength and low loss, $BaSnO_3$/PVDF nanocomposite films were prepared. Targeting this, $BaSnO_3$ nanorods were purposely synthesized for less agglomeration and easy achievement to the percolation threshold. The electrical properties were enhanced for the hybrid films along with an enhancement in electroactive phase of the polymer. Additionally, the composite films exhibited high transparency in visible region. These highly flexible, transparent hybrid films with high permittivity, better conductivity and low loss showed an enhanced open circuit voltage and short circuit current under free hand hammering. This work opens up newer possible applications for $BaSnO_3$ based composites beyond the traditional applications like sensors, ceramic capacitors etc.

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