

Structural Properties of Copper Doped Strontium Titanate

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Abstract

Strontium titanate (SrTiO_3 , STO) is an ABO₃-type perovskite and well-known incipient ferroelectric, characterized by a very high dielectric constant at low temperature. This perovskite, either in bulk or in thin films, is a favorite substrate (buffer layer) for the growth of high-T_c superconducting oxide layers. Important properties of these superconducting structures depend in an essential way on the substrate dielectric response which can be used as a convenient tuning mechanism. In this connection effect of copper doping into STO was taken for the present study and structural properties were investigated. $\text{Cu}_{1-x}\text{Sr}_x\text{TiO}_3$ ($x=0.1$ to 0.9) powders were prepared by conventional bulk preparation method. Structural properties of the prepared samples were investigated by X-ray diffraction SEM and EDAX. From XRD profiles, effect of Cu concentration on the crystal structure, average particle size and lattice parameter was investigated. At low Cu concentration a phase of $\text{Cu}_3\text{SrTi}_4\text{O}_{12}$ was identified from the XRD profiles which crystallizes into cubic structure with $a=7.426\text{\AA}$. The less solubility of Cu in STO was confirmed from XRD and EDAX profiles.

Introduction

Oxide ceramics such as SrTiO_3 (STO) are widely used for passive devices in high frequency systems such as filters and antennas, and also in active devices such as tunable rf filters and phase switchers. STO-based compounds are also used in grain boundary layer capacitors, in which conductivity differences increase the device performance. The electronic structure of strontium titanate can be changed by the introduction of dopants, e.g. changing it from insulator to metallic conductor. For applications in electronic devices, the contact between the ceramic and the electrode material plays an important role in device performance. In particular, band alignment at the metal-oxide interface can determine the electrical properties of the device [1].

High dielectric permittivity lead-free compositions are currently of great interest due to the need for environmental harmless applications.

The perovskite strontium titanate (SrTiO₃, ST) is an incipient ferroelectric material, i.e. it possesses polar soft modes but does not exhibit any ferroelectric phase transition down to 0 K. It is known that the dielectric response and other related properties of SrTiO₃ can be modified by controlling the Sr/Ti ratio and oxygen vacancy concentration, by oxygen isotope exchange and by doping and substituting Sr and/or Ti ions. In contrast, isovalent Sr-site dopants, such as Ca²⁺, Ba²⁺, Pb²⁺, Cd²⁺ and Mn²⁺ as well as heterovalent Bi³⁺ induce a dielectric anomaly [2]. There is considerable renewed interest in the low-temperature properties of SrTiO₃. This perovskite, either in bulk or in thin films, is a favorite substrate for the growth of high-T_c superconducting oxide layers. Important properties of these superconducting structures depend in an essential way on the substrate dielectric response which can be used as a convenient tuning mechanism. On the other hand, unusual phenomena were uncovered in recent low-T investigations of bulk SrTiO₃.

SrTiO₃ is generally considered as a textbook example of a quantum Para Electric (QPE). In the present study we confirm, as already suggested in, that the incipient ferroelectricity of the bulk material is first stabilized by the structural distortions induced by the AFD transition. If it were not for these distortions, SrTiO₃ would undergo a FE transition around 30 K. This conclusion is reached based on high-resolution hyper-Raman spectroscopy (HRS) results obtained from single crystals oriented in the tetragonal phase. The splitting of the TO frequencies is well described by the standard free-energy expansion, while the general T-dependence approximately follows the quantum mean-field treatment of QPE. The TO frequencies show no evidence for any anomaly at T_q [3-5].

Experimental Details

The present investigation involves the detailed study of structural properties of Copper doped SrTiO₃. The samples with varying Copper concentration were synthesized in air by the high temperature solid-state reaction method described by Anna E McHale (1). The purity of the materials was higher than 99%. The calcination of the samples was carried at 1350°C. Formation of the Cu_{1-x}Sr_xTiO₃ was confirmed from XRD profiles. The XRD studies at room temperature were carried out using SEIFERT X-ray powder diffractometer. The Cu K α radiation with a wavelength $\lambda = 1.54056\text{\AA}$ was used for recording X-ray diffraction patterns. Ni filter was used as the monochromatic. The X-ray machine was operated with 30 mA beam current and 40 kV of power. For phase identification and for the determination of unit cell parameters, the patterns were compared against standard patterns given in powder diffraction file (The J.C. PDS files). In order to obtain the accurate cell parameters, the data (2 θ and hkl values) were fed to a computer program EXPO2009 and the cell parameters obtained with an accuracy of >0.1%. Surface morphology of the samples was analyzed from SEM photographs. Composition studies were carried with EDAX.

Results and Discussion

Figures 1 show XRD profile of $\text{Cu}_{1-x}\text{Sr}_x\text{TiO}_3$ sample for Cu concentration of 0.1 weight percentage. Particle size was calculated from this profile and found that it decreases with the increase of copper concentration. The average particle size was found to be 600Å. At low Cu concentration a phase of $\text{Cu}_3\text{SrTi}_4\text{O}_{12}$ was identified from the XRD profiles which crystallizes into cubic structure with $a=7.426\text{Å}$. The less solubility of Cu [6] in STO was confirmed from XRD and EDAX profiles. At high Cu concentration (>0.2) no specific phase of $\text{Cu}_{1-x}\text{Sr}_x\text{TiO}_3$ was identified and separate CuO and TiO₂ (rutile) phases were identified. This makes $\text{Cu}_{1-x}\text{Sr}_x\text{TiO}_3$ a candid material as buffer layer in superconducting devices.

Figures 2 shows SEM photograph of $\text{Cu}_{1-x}\text{Sr}_x\text{TiO}_3$ samples for Cu concentration of 0.1 weight percentage. Grains are clearly visible in this photograph. Grain size was calculated from this photograph and found that it decreases with the increase of Cu concentration. Figures 3 shows EDAX Profile of $\text{Cu}_{1-x}\text{Sr}_x\text{TiO}_3$ sample for Cu concentration of 0.1 weight percentage. Compositional changes are clearly seen in this profile.

It is propped to carry electrical, thermoelectric and dielectric properties of these samples to investigate the conduction mechanism and dielectric response in these materials.

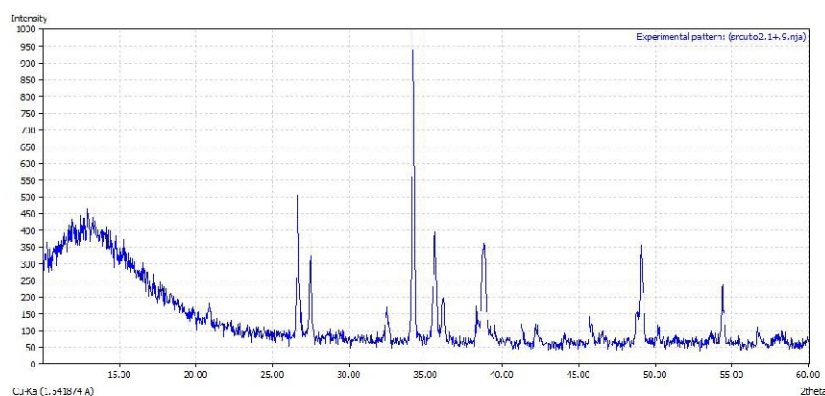


Figure 1: XRD profile of $\text{Cu}_{1-x}\text{Sr}_x\text{TiO}_3$ sample for Cu concentration of 0.1.

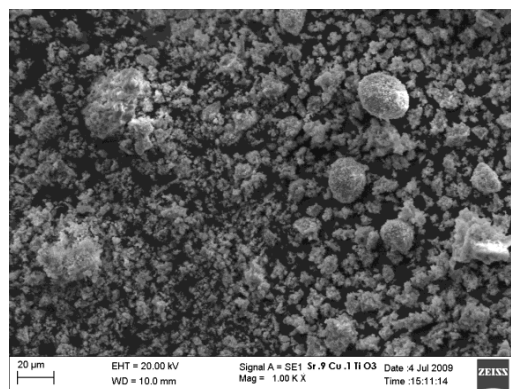


Figure 2: SEM photograph of $\text{Cu}_{1-x}\text{Sr}_x\text{TiO}_3$ sample for Cu concentration of 0.1.

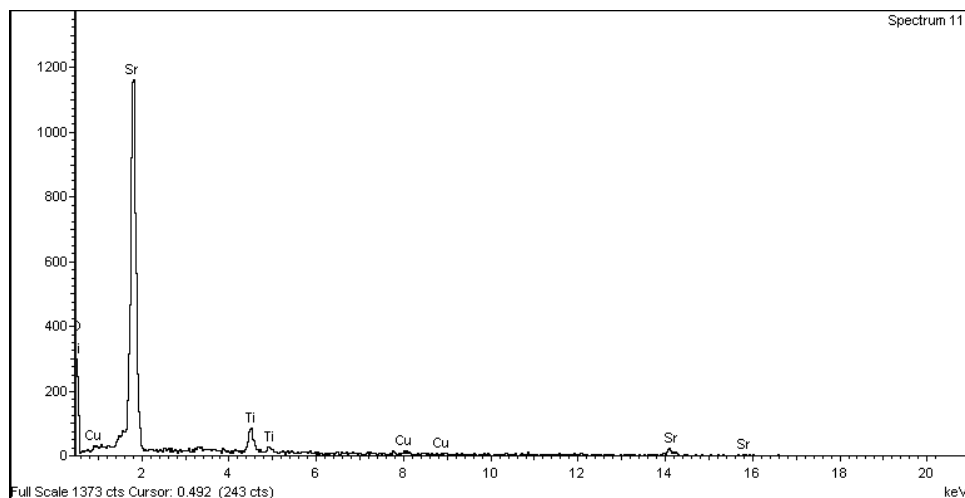


Figure 3: EDAX Profile of $\text{Cu}_{1-x}\text{Sr}_x\text{TiO}_3$ sample for Cu concentration of 0.1.

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