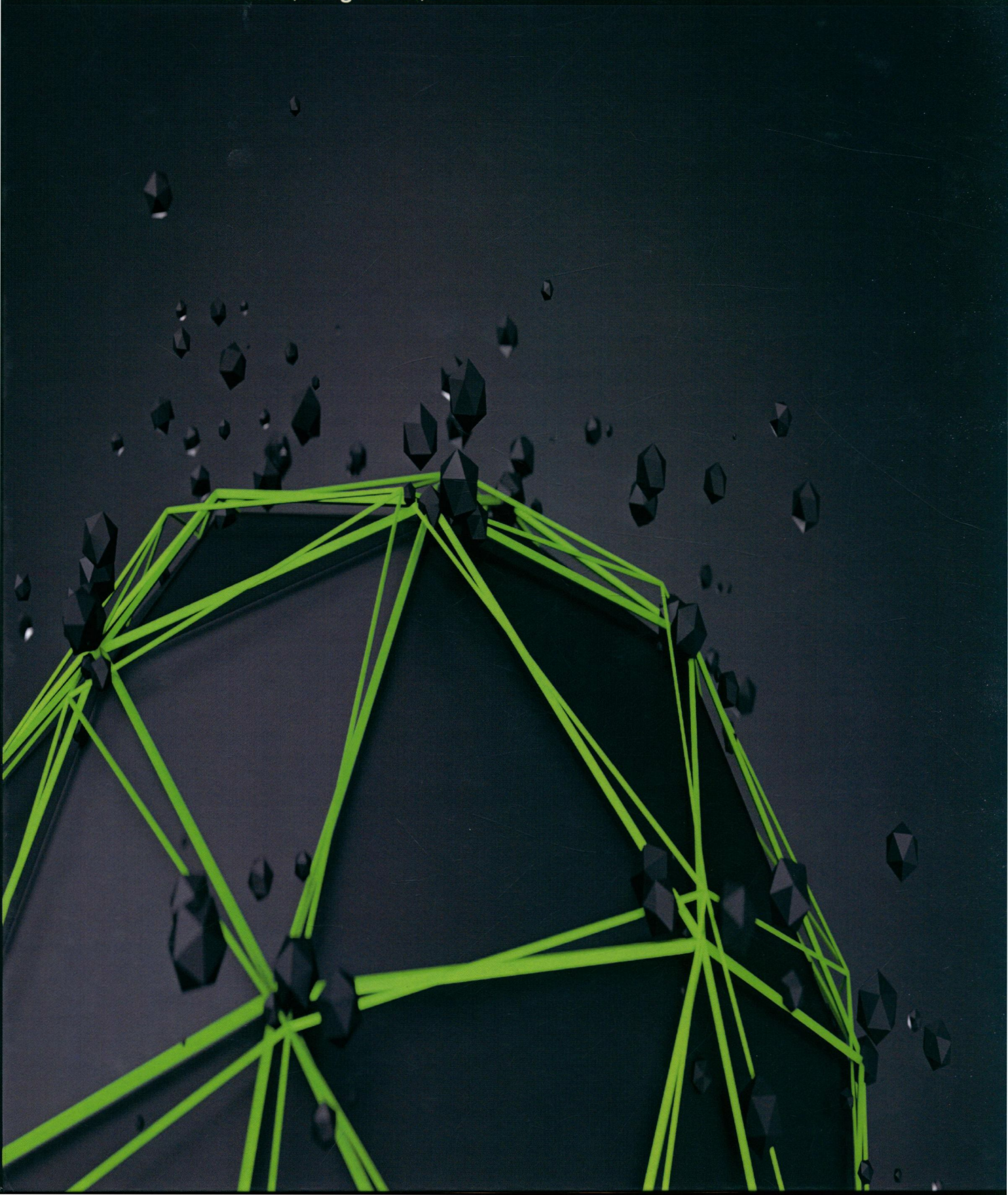


Electrical Conductivity in Polycrystalline Materials

Contributors: Yawei Li, Zhigao Hu, et al.



About the Book

Polycrystalline or multicrystalline materials, or polycrystals are solids that are composed of many crystallites of varying size and orientation. Most inorganic solids are polycrystalline, including all common metals, many ceramics, rocks and ice. The extent to which a solid is crystalline (crystallinity) has important effects on its physical properties. Sulfur, while usually polycrystalline, may also occur in other allotropic forms with completely different properties. Although crystallites are referred to as grains, powder grains are different, as they can be composed of smaller polycrystalline grains themselves. While the structure of a (monocrystalline) crystal is highly ordered and its lattice is continuous and unbroken. amorphous materials, such as glass and many polymers, are non-crystalline and do not display any structures as their constituents are not arranged in an ordered manner. Polycrystalline structures and paracrystalline phases are in between these two extremes.

Electrical Conductivity in Polycrystalline Materials examines the influence of composition, structure, and size factor on the dielectric permittivity and electrical conductivity of polycrystalline materials. The problem of the determination of the macroscopic conductivity of statistically homogeneous and isotropic polycrystalline materials in terms of the principal values of the conductivity tensor of the constituent crystals is considered. A perturbation expansion, in terms of correlation functions with an optimal value of the zeroth - order estimate of the effective conductivity, is derived in which a separation is established into texture dependent and independent quantities. Consistence with the analogous expansion for the effective resistivity is demonstrated. This Book is intended for students, post-graduate students, and scientists in the field of polycrystalline materials.



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Electrical Conductivity in Polycrystalline Materials

List of Contributors

- Yawei Li**
Key Laboratory of Polar Materials and Devices, Ministry of Education, Department of Electronic Engineering, East China Normal University, Shanghai, People's Republic China
- Zhigao Hu**
Key Laboratory of Polar Materials and Devices, Ministry of Education, Department of Electronic Engineering, East China Normal University, Shanghai, People's Republic China
- Junhao Chu**
Key Laboratory of Polar Materials and Devices, Ministry of Education, Department of Electronic Engineering, East China Normal University, Shanghai, People's Republic China
National Laboratory for Infrared Physics, Shanghai Institute of Technical Physics, Chinese Academy of Sciences, Shanghai, People's Republic China
- Mario Lanza**
Dept. Eng. Electrònica, Edifici Q, Campus UAB, 08193 Bellaterra, Spain
- Vanessa Iglesias**
Dept. Eng. Electrònica, Edifici Q, Campus UAB, 08193 Bellaterra, Spain
- Marc Porti**
Dept. Eng. Electrònica, Edifici Q, Campus UAB, 08193 Bellaterra, Spain
- Montse Nafria**
Dept. Eng. Electrònica, Edifici Q, Campus UAB, 08193 Bellaterra, Spain
- Xavier Aymerich**
Dept. Eng. Electrònica, Edifici Q, Campus UAB, 08193 Bellaterra, Spain
- Sanjaya Brahma**
Materials Research Centre, Indian Institute of Science, Bangalore, India
- Ram Naresh Prasad Choudhary**
Department of Physics, Institute of Technical Education and Research, Siksha O Anusandhan University, Bhubaneswar, India
- Awalendra Kumar Thakur**
Department of Physics and Meteorology, Indian Institute of Technology, Kharagpur, India
- Srinivasarao Ajjampur Shivashankar**
Materials Research Centre, Indian Institute of Science, Bangalore, India
- Lakshmi Vijayan**
Department of Physics, School of Physical, Chemical and Applied Sciences, Pondicherry University, R. V. Nagar, Kalapet India
- G. Govindaraj**
Department of Physics, School of Physical, Chemical and Applied Sciences, Pondicherry University, R. V. Nagar, Kalapet India
- Naoto Eguchi**
Faculty of Pure and Applied Sciences, Division of Material Sciences, University of Tsukuba, Tsukuba, Japan
- Kohsuke Kawabata**
Faculty of Pure and Applied Sciences, Division of Material Sciences, University of Tsukuba, Tsukuba, Japan
- Hiromasa Goto**
Faculty of Pure and Applied Sciences, Division of Material Sciences, University of Tsukuba, Tsukuba, Japan
- Vijendra A. Chaudhari**
Department of Physics, Dayanand Science College, Latur 413 531, India

Govind K. Bichile

Department of Physics, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad 431 004, India

Ayşegül Taşçıoğlu

Department of Biosystems Engineering, Faculty of Agriculture, Uludag University, 16059 Bursa, Turkey

Onur Taşkın

Department of Biosystems Engineering, Faculty of Agriculture, Uludag University, 16059 Bursa, Turkey

Ali Vardar

Department of Biosystems Engineering, Faculty of Agriculture, Uludag University, 16059 Bursa, Turkey

N V Melnikova

Ural Federal University, Lenina Avenue 51, Ekaterinburg 620000, Russia

K V Kurochka

Ural Federal University, Lenina Avenue 51, Ekaterinburg 620000, Russia

V E Zaikova

Ural Federal University, Lenina Avenue 51, Ekaterinburg 620000, Russia

A V Tebenkov

Ural Federal University, Lenina Avenue 51, Ekaterinburg 620000, Russia

A N Babushkin

Ural Federal University, Lenina Avenue 51, Ekaterinburg 620000, Russia

Teng Ma

Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, 72 Wenhua Road, Shenyang 110016, China

Zhibo Liu

Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, 72 Wenhua Road, Shenyang 110016, China

Jinxu Wen

State Key Laboratory of Optoelectronic Materials and Technologies, Guangdong Province Key Laboratory of Display Material and Technology, School of Physics and Engineering, Sun Yat-sen University, Guangzhou 510275, China

Yang Gao

Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, 72 Wenhua Road, Shenyang 110016, China

Xibiao Ren

State Key Laboratory of Silicon Materials, School of Materials Science and Engineering, Zhejiang University, Hangzhou 310027, China.

Huanjun Chen

State Key Laboratory of Optoelectronic Materials and Technologies, Guangdong Province Key Laboratory of Display Material and Technology, School of Physics and Engineering, Sun Yat-sen University, Guangzhou 510275, China

Chuanhong Jin

State Key Laboratory of Silicon Materials, School of Materials Science and Engineering, Zhejiang University, Hangzhou 310027, China.

Xiu-Liang Ma

Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, 72 Wenhua Road, Shenyang 110016, China

Ningsheng Xu

State Key Laboratory of Optoelectronic Materials and Technologies, Guangdong Province Key Laboratory of Display Material and Technology, School of Physics and Engineering, Sun Yat-sen University, Guangzhou 510275, China

Hui-Ming Cheng
Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, 72 Wenhua Road, Shenyang 110016, China

Wencai Ren
Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, 72 Wenhua Road, Shenyang 110016, China

Kevin Hammonds
Thayer School of Engineering at Dartmouth College, Hanover, NH, USA

IAN Baker
Thayer School of Engineering at Dartmouth College, Hanover, NH, USA

Bing Gu
Jiangsu Key Laboratory on Opto-Electronic Technology and Department of Physics, Nanjing Normal University, Nanjing 210097, China

Yang Wang
Department of Materials Science and Engineering, National University of Singapore, Singapore 117576, Singapore

John Wang
Department of Materials Science and Engineering, National University of Singapore, Singapore 117576, Singapore

Wei Ji
Department of Physics, National University of Singapore, 2 Science Drive 3, Singapore 117542, Singapore

Preface

Polycrystalline or multicrystalline materials, or polycrystals are solids that are composed of many crystallites of varying size and orientation. Most inorganic solids are polycrystalline, including all common metals, many ceramics, rocks and ice. The extent to which a solid is crystalline (crystallinity) has important effects on its physical properties. Sulfur, while usually polycrystalline, may also occur in other allotropic forms with completely different properties. Although crystallites are referred to as grains, powder grains are different, as they can be composed of smaller polycrystalline grains themselves. While the structure of a (monocrystalline) crystal is highly ordered and its lattice is continuous and unbroken, amorphous materials, such as glass and many polymers, are non-crystalline and do not display any structures as their constituents are not arranged in an ordered manner. Polycrystalline structures and paracrystalline phases are in between these two extremes.

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ELECTRICAL PROCESSES IN POLYCRYSTALLINE BIFEO₃ FILM

Yawei Li¹, Zhigao Hu¹ and Junhao Chu^{1, 2}

¹Key Laboratory of Polar Materials and Devices, Ministry of Education, Department of Electronic Engineering, East China Normal University, Shanghai, People's Republic China

²National Laboratory for Infrared Physics, Shanghai Institute of Technical Physics, Chinese Academy of Sciences, Shanghai, People's Republic China

INTRODUCTION

As an oxide with perovskite structure, Bismuth ferrite (BiFeO₃, BFO) has been studied from 1970s (Teague, et al. 1970; Kaczmarek, et al. 1975). The structure and magnetic properties of BFO were confirmed before 1970s. As reported, the crystal structure of BFO is perovskite with rhombohedral distortion and the space group is R3c. BFO is G-type antiferromagnetic. It was controversial about whether BFO was ferroelectrics until the hysteresis loop of single crystal BFO was measured in 1970 (Teague, et al. 1970). According to Teague's results, the single crystal BFO was anisotropy. The remnant polarizations (P_r) along the (100) and (111) direction were 3.5 $\mu\text{C}/\text{cm}^2$ and 6.1 $\mu\text{C}/\text{cm}^2$ at the temperature of liquid nitrogen, respectively. However, because of the higher leakage current in the bulk BFO, it was difficult to measure the ferroelectric properties of BFO at room temperature. The problem of higher leakage blocks not only the studies of the electrical properties of BFO, but also the application of BFO in electrical devices. In 2003, the epitaxial BFO films with higher electrical resistivity and higher remnant polarization was fabricated by pulsed laser deposition (PLD) method (J. Wang, 2003). The value of P_r of the epitaxial BFO films is about 50 $\mu\text{C}/\text{cm}^2$. This value is larger than that of the traditional ferroelectrics such as Pb(Zr,Ti)O₃ (PZT), BaTiO₃ (BTO). If the BFO film with larger P_r can be used in ferroelectric memory (FeRAM), the size of the storage cell can be reduced and the storage density can be increased (Maruyama, 2007). More studies on BFO films are carried out (Eerenstein, 2005; Zavaliche, 2005; Singh, 2007; Hauser, 2008; Liu, 2008; Yang, 2008). Even though the leakage mechanism in epitaxial BFO film has been studied (Pabst, 2007), the higher leakage current is still an obstacle for the study and application of polycrystalline BFO films. Compared to the epitaxial BFO films grown on perovskite structure substrate, the applications of polycrystalline BFO on silicon wafer are broader in the field of microelectronic devices. In this chapter, polycrystalline BFO films are fabricated by different physical and chemical methods on buffered silicon and perovskite structure substrate. The structural and electrical properties of these polycrystalline BFO films are investigated.

EXPERIMENTS

Considering the universality of our conclusion for different polycrystalline BFO films, the samples studied in this work are fabricated by two different methods, PLD and chemical solution deposition (CSD) methods. The former is a typical physical method of film deposition. The later is a chemical method. At the same time, different materials are used as substrate. For the samples prepared by PLD, n-type silicon covered by a layer of (La,Sr)CoO₃ (LSCO) is used as substrate. The layer of LSCO

acts as bufferlayer for the growth of BFO and bottom electrode for the electrical measurement. For the samples prepared by CSD, the single crystal SrTiO_3 (STO) covered by LaNiO_3 (LNO) is used as substrate.

The Fabrications of BFO Films by PLD Method

For the preparation of polycrystalline BFO films by PLD method, single-side polished silicon wafer is used as substrate. Before the deposition of BFO film, a layer of LSCO is deposited on the surface of silicon wafer by PLD. The component of the LSCO target is $(\text{La}_{0.5}\text{Sr}_{0.5})\text{CoO}_3$. The component of BFO target is $\text{Bi}_{1.05}\text{FeO}_3$. The excess bismuth is used to compensate the evaporation of bismuth at higher temperature during the growth of BFO films. The depositions of LSCO and BFO are carried out in a vacuum chamber with background pressure lower than 10^{-4} Pa. A KrF excimer laser with the wavelength of 248 nm is used for the deposition. During the deposition of LSCO layer, the oxygen pressure in the chamber is about 25 Pa. The temperature of the silicon wafer is 650°C (Li, 2009). Details about the deposition conditions are listed in table 1. The deposition of LSCO layer is carried out for 20 minutes. After the deposition, the oxygen pressure in the chamber increased to 50 Pa and maintained for 30 min. The thickness of the LSCO layer is about 200 nm obtained from the scanning electronic microscope.

Table 1: The deposition conditions of LSCO and BFO films grown on silicon wafer by PLD method

Target	LSCO	BFO
Frequency of pulse	5Hz	3Hz
Oxygen pressure	25Pa	3Pa
Substrate temperature	650°C	700°C
Deposition time	20min	90min
Holding temperature	650°C	495°C
Holding oxygen pressure	50 Pa	$3\text{Pa}/1.01\times10^5\text{Pa}$
Holding time	30min	30min

The oxygen pressure in the chamber during the deposition of the polycrystalline BFO films is 3 Pa. the temperature of the substrate is kept at 700°C . Details about the deposition conditions of BFO films are also listed in table 1. The deposition of BFO films is carried out for 90 minutes. After the deposition, the BFO films are cooled to 495°C slowly and held for 30 min in a certain oxygen pressure. In order to study the effect of oxygen vacancies, two kinds of BFO films are fabricated by PLD. For the BFO film containing less vacancy of oxygen, the oxygen pressure in the chamber is 1.01×10^5 Pa when the sample is held at 495°C for 30min. For the sample containing more vacancy of oxygen, the oxygen pressure in the chamber is just 3 Pa when the sample is kept at 495°C for 30min (Li, 2008).

The Fabrications of BFO Films by CSD Method

Regarding the preparation of polycrystalline BFO films by CSD method, single crystal STO is used as substrate. A layer of LNO is fabricated on the surface of STO before the preparation of BFO films. The layer of LNO is also fabricated by CSD method and is used as bottom electrode. Both STO and LNO are perovskite structure and smaller crystal constant than BFO. Therefore, the substrate and the LNO layer can induce the growth of BFO films. The fabrication of LNO layer by CSD method is same to the way has been reported in literature (Meng, 2001). For the synthesizing of LNO precursor, lanthanum nitrate and nickel acetate are used as starting materials. The mixture of acetic acid and water are used as solvent. Lanthanum nitrate and nickel acetate with a stoichiometric molar ratio of 1:1 are dissolved in the solvent. The concentration of the precursor is 0.3mol/L. For the preparation of the LNO layer, the LNO precursor is spin-coated on STO substrate at 3000rpm for 20 s. the wet film is dried at 180°C for 300s in a rapid thermal process furnace. Then the dried film is calcined at 380°C for 300s for the organic compound pyrolyzing. Finally, the amorphous film is annealed at 650°C for 300s for crystallization. The cycle of coating and thermal process are repeated six times to obtain LNO layer with expected thickness.

In regard to the synthesizing of BFO precursor, bismuth nitrate and nickel acetate are used as starting materials. Acetic acid is used as solvent (Li, 2005). The fabrication of BFO film is also contained two steps, spin-coating precursor on LNO covered STO substrate and rapid thermal process in furnace. The precursor is spin-coated at 4000rpm for 20 s. The film is dried at 180°C for 240s, pyrolyzed at 350°C for 240s, and annealed at 600°C for 240s. Two kinds of BFO films with different electrical resistivity are fabricated.