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Optical Properties of Ferroelectric Thin Film Prepared by PLD Technique

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Abstract: Polycrystalline SrTiO3 is synthesized from a stoichiometric combination of metallic oxides by standard ceramic synthesis methods. SrTiO3 thin film X-ray diffraction examination confirmed the cubic structure phase. Strontium Titanate was deposited on the glass substrate. Studying the effect of annealing temperature on the structural properties of the glass of substrate, it is clear that increasing the annealing temperature can improve the crystallinity of SrTiO3 thin films. The surface morphology of the deposited thin films was studied using Scanning Electronic macroscopy; it is observed that the grain size increases with increasing the annealing temperature. The transitions of SrTiO3 films show high transmittance within the wavelength range (300-800nm), making them suitable for antireflection coating in this region. The optical energy gap of SrTiO3 films at various annealing temperatures was measured. It decreases as the annealing temperature of the coatings increases.

Keywords: Strontium Titanate oxide, annealing temperature, Transmittance of SrTiO3.

1 Introduction

Ferroelectrics are crucial for capacitors, sensors, actuators, electro-optics, and nonvolatile memory from a technological standpoint [1,2,3]. As electronic materials, these materials possess numerous advantageous qualities. For instance, its strong dielectric constant across a wide temperature range is what makes capacitors such a promising technology [4,3,5] .These materials are advantageous as actuators and sensors because to their extremely high piezoelectric coefficients [6]. Due to the high, low hysteresis displacements that ferroelectric films can achieve with relatively low electric fields, they are frequently utilized as actuators in micro-electromechanical systems (MEMS). Inkjet printers, fuel injectors, and high-speed valves are all examples of applications in the automobile industry that make use of bulk ferroelectrics [7,8,9]. Similarly, ferroelectrics are common in sensors, such as sonar systems and ultrasound sensors [10]. At ambient temperature, nominally pure SrTiO3 acts as an electrical insulator. Free charge carriers or charged ionic species can be produced by incorporating point defects into the lattice [11,12]. At ambient temperature, the charge carriers in ferroelectric SrTiO3 are predominantly electrons introduced by donor impurity doping or heating in a reducing atmosphere [13,14].

The latter treatment introduces an essentially comparable density of oxygen vacancies, which are known to have extremely high lattice mobility, especially at high temperatures. SrTiO$_3$ is thus considered a mixed electronic. In addition to their practical importance, STO film represents a good model system for paraelectric, tunable dielectric thin films [15,16,17]. Several methods are used to prepare STO thin films, including RF magnetron sputtering, metal-organic chemical vapour deposition (MOCVD), Molecular beam epitaxial (MBE, pulsed laser deposition (PLD), Sol-gel and hydrothermal synthesis [18,19,20]. The main objective of this work is to prepare the SrTiO3 compound using the stoichiometric ratio of compositions. Thin films of SrTiO3were deposited by Pulse Laser Deposition Technique on the glass substrate under different conditions, like annealing temperature, and studying these conditions and their

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influences on the structural morphology, roughness and grain size using X-ray diffraction (XRD) and Scanning Electronic Macroscope, as well as optical and electrical properties. Also, SrTiO3 films were deposited on the glass substrate to study the paraelectric behavior of the films. This work studied the effect of annealing temperature density of film, grain size and optical properties.

2 Theoretical parts

The absorption associated with the electronic transition between V.B and C.B in the material commencing at the absorption edge corresponds to a minimal energy differential (Eg) between the lowest minimum of the C.B. and the greatest maximum of the V.B[74].

The absorption coefficient (α) is defined as the relative number of photons absorbed per unit distance between energy states. It can be deduced from the absorption or transmission spectra using the Lambert Law.

$$I=I_o\ e^{(-\alpha t)}\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

“Where (I) is the transmitted intensity and I0 is the incident intensity of the light, and t is the thickness”

$$\alpha=2.303\ A/t\ldots\ldots\ldots\ldots\ldots\ldots\ (2)$$

“The energy of the incident photon (hυ) can be determined from the equation where υ is the incident photon frequency”

$$h\nu=\ 1240/\lambda\ldots\ldots\ldots\ldots\ldots\ldots\ldots(3)$$

In order to calculate the breadth of the absorption edge energy, or the width of the tails of localized states in the band gap, the Urbach equation can be used:

$$\alpha=\exp h\nu/E_t\ \ldots\ldots\ldots\ldots\ldots\ (4)$$

The equation (4) can be written in the new form because the term (Log I0/I) represents the absorption for the film material (A). Near the edge of absorption, the rate of absorption can be written as:

$$\alpha h\nu=[\![A((h\nu-E_g)]\!]^r\ldots\ldots\ldots\ldots\ldots..(5)$$

“Where (hυ)is the photon energy, E is the band gap, and r is a constant equals 1/2 and 3/2for allowed direct transitions”.

As a result of the averaged interaction of light and matter over multiple unit cells, the optical properties inside each layer can be defined macroscopically in terms of phenomenological parameters, the so-called optical constant or optical parameter.

$$n=n-ik\ldots\ldots\ldots\ldots\ldots\ldots\ldots(6)$$

$$v=c/n_c\ \ldots\ldots\ldots\ldots\ldots\ldots\ (7)$$

3 Experimental part

Pure Titanate dioxide(TiO2)supplied by (Haen,German Company), purity of 99.5%, also strontium carbonate (SrCO3),supplied by (BDH chemical Ltd (England)with a purity>98%, were used as raw materials to prepare strontium titanate (SrTiO3)by the conventional technique. The stoichiometric ratio (1:1) of these materials was mixed in gate mortar for one hour; after that, the mixture was fired in an electrical furnace at the ambient condition at 1200oC at a heating rate of 3ºC min-1 and soaked for 2 hours, then cooled to room temperature. The prepared powder was examined using the x-ray diffraction method. After that, SrTiO3 powder was pressed at 4 Ton to form a target with 1.2 cm diameter and 2.5 mm thickness.”The target should be as dense and homogenous as possible to ensure the good quality of the deposit. The focused Nd:YAG SHG Q-switching laser beam coming through a window falls on the target surface with an angle of 45°. The substrate is placed in front of the target, with its surface parallel to that of the target. Sufficient distance is kept between the target and the substrate so that the substrate holder does not obstruct the incident laser beam. The plasma evaporated towards the fixed substrate to deposit on it. Through this process, many investigators modify the deposition technique occasionally to obtain better-quality films. These include rotation of the target, the position of the substrate with respect to the target. “A double–beam UV-VIS-NIR 210A Spectrophotometer (VRIAN, made in Australia) was used to measure the transmittance and absorption of SrTiO3 films deposited at different conditions in the range of (200-800) nm. Background correction was taken for each scan. Transmittance and reflectance data can be used to calculate the absorption coefficients of the films at different wavelengths, which have been used to determine the band gap”.

4 Results and Discussion

4.1 X-Ray Diffraction Results of SrTiO3 Thin Films

SrTiO3 thin films prepared in this work by pulsed laser deposition technique were examined by x-ray diffraction pattern at 2° intervals from 20o to 80o. The Scherrer equation can be used to determine d-spacing by comparing the resulting spectra and tabulated data of SrTiO3, d-spacing, peak intensity, and Miller Indices values as in table (1) for peaks of (110). Some peaks have low crystallinity at room temperature; in other words, the intensity of these peaks reflected from the planes is very low, as shown in Fig.1. The analysis demonstrates that the reflection planes are (100), (110), (111), (200), (210), (211), (220), and (301). The peak (110) at (d=2.761Ao, 2θ=32.06) is the major peak with the highest degree of crystallinity. Table (1) shows the full width at half maximum (FWHM) of (110) peak at different annealing temperatures. The FWHM of High annealing temperatures can offer more kinetic energy for the mobility of the particles on the surface to achieve better crystalline growth. The intensity of SrTiO3 (110) peak at a substrate temperature of 973k is the highest, which indicates improvement in the SrTiO3 film crystallinity.

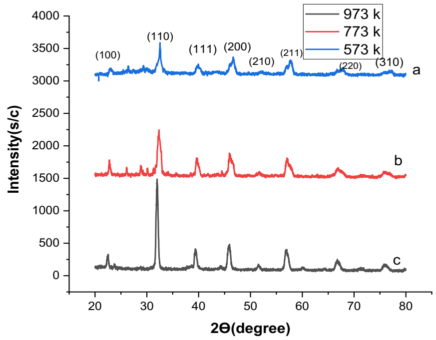

Fig. 1: X-ray Diffraction Pattern for SrTiO3 Thin Film at (a) Room temperature and different annealing temperatures (a) 573k,(b)773k, (c) 973k.

Table 1: Effect of Annealing Temperature on the Grain Size for SrTiO3 /Glass Thin Films.

Annealing Temperature K	2θ (110) reflection	d-space	FWHM	grain size (nm)
573k	32.409	2.76106	0.192	7.2998
773k	32.391	2.76198	0.181	7.5316
823k	32.382	2.76204	0.144	9.2560

4.2 Surface Morphology

Three dimension view surface morphology of 190 nm thickness prepared films under different annealing temperatures (723,773,823 k was studied using SEM. Fig. 2 shows that the film consists of nanocrystalline grains of randomly oriented morphology with uniform substrate surface coverage. It is also observed that the average grain size increases with the annealing temperature. This could be because as the temperature goes up, the atoms move around more easily. This makes the films recrystallize and grow grains more effectively, which makes the grains bigger. As the heating temperature goes up, the surface roughness goes down.

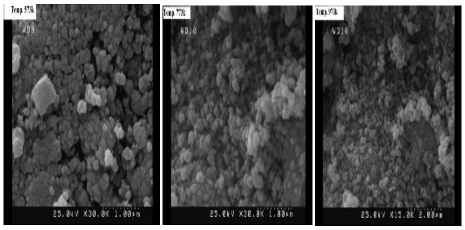

Fig. 2: The SEM Images of SrTiO3/glass Thin Films with thickness 190nmat different annealing temperatures (a) 573k (b) 773k (c) 873k.

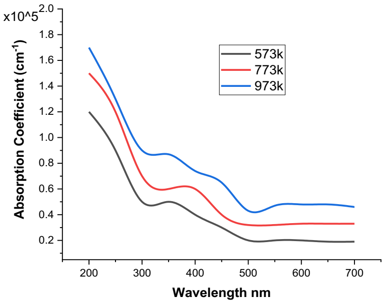

Fig. 3: The Variation of the Transmittance with Wavelength of the SrTiO3/Glass at 190nm thickness Films with Different Annealing Temperature

4.3 Optical properties

The optical properties of SrTiO3 thin films prepared, by pulsed laser deposition (PLD) technique, on glass substrate at different annealing temperatures have been investigated using UV- Visible transmission and absorbance spectrum. The optical energy gap Eg and optical constant, which includes the extinction coefficient k and refractive index (n), were calculated. Fig. 3 shows the transmission spectra of SrTiO3 films at the thickness of 190 nm with different annealing temperatures (723,773,823) k. It is observed that the film which has a higher temperature displayed lower transmittance because of the improved structure of the film and large grain size, which both cause an increase in absorption.

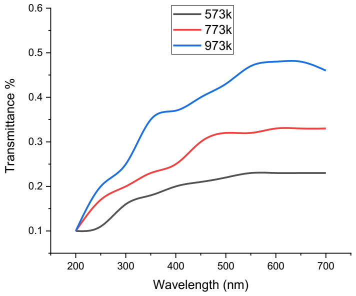

Fig. 4: The Variation of Absorption Coefficient with Wavelength of the SrTiO3/Glass Films with Thickness 190nm at Different Annealing Temperature**.**

Fig. 4 shows the variation of absorption coefficient with wavelength at different annealing temperatures (723,773,823) K with a thickness of 190 nm. It is seen that the absorption coefficient decreases with increasing the annealing temperature. The decrease in absorption coefficient with annealing temperatures decreases the energy gap due to the decrease of the localized state.

The optical energy gap values (Eg) for SrTiO3 film are calculated by graphing the direct energy gap relations (h)2 versus h(eV), as shown in Fig. 5. The Eg of SrTiO3 films deposited on a glass base at different annealing temperatures (573, 773, and 973) k is shown in the first figure.The quantum-size effect, which occurs when a film contains massive crystallites, can be used to explain the shift in optical energy gap energy. Figure 5 shows how the optical energy gap changes with heating temperature for a 190-nm-thick film. Eg drops from (3.7-3.2) eV as annealing temperature increases because more energy is available for crystallite development, resulting in an improvement in the crystalline of SrTiO3 films and consequently a decrease in the density of localized states. This is consistent with the experimental results of XRD analysis, indicating that annealing improves the optical quality of SrTiO3 films.

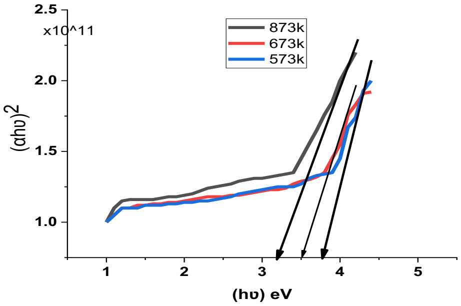

Fig. 5: The Variation of (αhυ) 2 with Photon Energy (hυ) of the SrTiO3/Glass Films at Different Annealing Temperatures.

5 Conclusions

Ferroelectric materials are promising materials with versatility, especially in optoelectronic devices and storage devices. Therefore, the materials can be converted into thin films to be easy to use in terms of weight and size. What is vital in the matter is that preparation parameters can control the properties of the film. The structural characteristics of the deposit SrTiO3 films on the glass substrate show that the films have low crystallinity at room temperature with a cubic structure. The XRD pattern revealed the topography surface of the film; the roughness of the film increased with increasing annealing temperatures. The transmittance decreases with increasing both annealing temperature and film thickness. The energy gap decreases with increasing annealing temperatures.

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Conflict of Interest
The authors declare no competing financial interest; there is no funding for the project.

Availability of data materials:
Data will not be shared because these data help study the correct choice of correct form for suitable applications.

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