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Effect of Oxygen Percentage on the Energy Band Gap of Ga_2O_3 Thin Films Deposited by RF Magnetron Sputtering Method

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In this study, Ga_2O_3 films were deposited on a sapphire substrate using the Radio Frequency (RF) magnetron sputtering technique. The films were produced at 100 W power and at different oxygen percentages of 0%, 2%, and 4%. Then, the films were annealed in air at 900°C. The transmittance measurements of all films were performed and the energy band gaps were calculated. The energy band gap between before and after annealing increased as the oxygen percentage increased. Based on these results, it was revealed that the O_2 concentration plays a crucial role in controlling the optical properties of Ga_2O_3, which can greatly affect the device performance.

1. Introduction

After the development and application of pure and compound semiconductors from the XX century, broadband-gap materials have pioneered the production of both electronic and optoelectronic devices. Current studies cover ultra-wide bandgap (UWBG) semiconductor materials with an energy band gap exceeding 4 eV. AlGaN, AlN, diamond and β-Ga_2O_3 semiconductors belonging to the class of materials called transparent semiconductor oxides (TSOs) are among the few UWBG materials of interest [1]. Among these materials, Gallium oxide (Ga_2O_3) has a wide band gap (~4.48-4.90 eV range) [2], high critical field strength [3], high thermal capacity [4], high breakdown field (~8 MV/cm) [5] and high Johnson and Baliga's figure-of merits (2844 and 3214) as compared to Silicon (Si) [6] has attracted great attention due to its chemical stability, low cost and high optical transparency [7-16] . Gallium oxide has a high electrical conductivity, which gives the material the advantage to outperform GaN and SiC in terms of low-resistance electrical contacts. This advantage is due to the point defects found in the structure of Ga_2O_3 [17-19]. Ga_2O_3 has five different phases, commonly referred to as α, β, γ, δ, and ε. Among them, the α and β phases are the most stable, and even the β phase is thermally and chemically more stable than any other phase. Therefore, studies on gallium oxide have focused on the β phase [7]. Deep ultraviolet light detectors [20, 21], photodiodes [22, 23], transparent field effect tubes [24, 25], drug carriers in the biomedical field due to its high luminescence feature [11,26], gas sensors [27], thin-film solar They are used in many fields such as batteries [28,29] and luminescent phosphors [30, 31]. Radio frequency (RF) magnetron deposition [32-35], pulsed laser deposition (PLD) [36,37], molecular beam epitaxy (MBE) [38,39], metal-organic chemical vapor deposition (MOCVD) [40, 41], atomic layer deposition (ALD) [42, 43], spray pyrolysis [44, 45] and sol-gel [46] are used to prepare Ga_2O_3 thin film. There are certain differences between the properties (structure, morphology and optical band gap) of thin films prepared with different growth methods. Among the growth methods, the RF magnetron sputtering technique has become important in the preparation of Ga_2O_3 thin films due to the high film quality of the prepared thin films, good adhesion to the substrate, low cost and rapid film formation [31].

In this study, RF magnetron sputtering method was used to grow Ga_2O_3 on sapphire substrate. The changes in optical properties of Ga_2O_3 thin films grown at different oxygen percentages before and after annealing were investigated using a UV-VIS-NIR spectrophotometer.

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2. Results and Discussion

The optical band gaps of the films were calculated using the Tauc formula, with the help of the transmittance curves measured with the Cary 5000 spectrophotometer [35]. First of all, the absorption coefficient (α) was found by using the transmittance values.

$$\alpha = {}^{1}/_{d} \ln(T) \qquad (1)$$

where T is the transmittance of the thin film and d is the thickness of the film.

The relationship between the absorption coefficient and the incident photon energy and the band gap of the material is given as:

$$(\alpha h\upsilon) = B(h\upsilon - E_g)^n \qquad (2)$$

where B is constant, $h\upsilon$ is photon energy and n is a constant equal to ½ for direct bandgap semiconductors.

In order to determine the optical properties of Ga_2O_3 thin films produced at different oxygen percentages, the transmittance ($T\%$) of the films was measured in the wavelength range of 250-400 nm at room temperature. In Fig.1, our transmittance was around 83% when no oxygen was given to the system, and around 84% when 2% oxygen was given. When we gave the oxygen percentage as 4%, our transmittance was measured at around 82.5%. In other words, as the percentage of oxygen increased, the transmittance first increased and then the transmittance decreased.

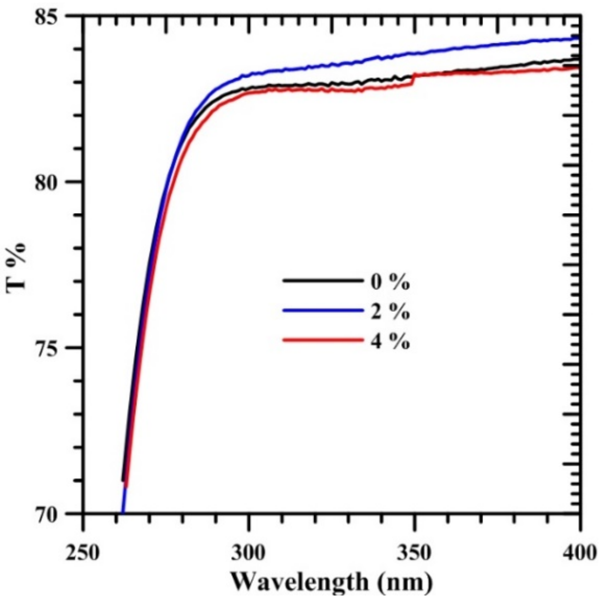

Figure 1. Variation of the transmittance of Ga_2O_3 thin films produced at different Oxygen percentages according to wavelength.

In Fig. 2, the variation of $(\alpha E)^2$ calculated with the help of the absorption coefficient calculated by using the transmittance values of the Ga_2O_3 thin films produced by giving different oxygen percentages, according to the energy is shown. Interference fringe is not observed in Fig. 2. The energy band gap was measured as 5.48 eV when no oxygen was supplied to the system, 5.52 eV when 2 % oxygen was given, and 5.52 eV when 4% oxygen was given. According to this graph, as the percentage of oxygen increased, the energy band gap increased.

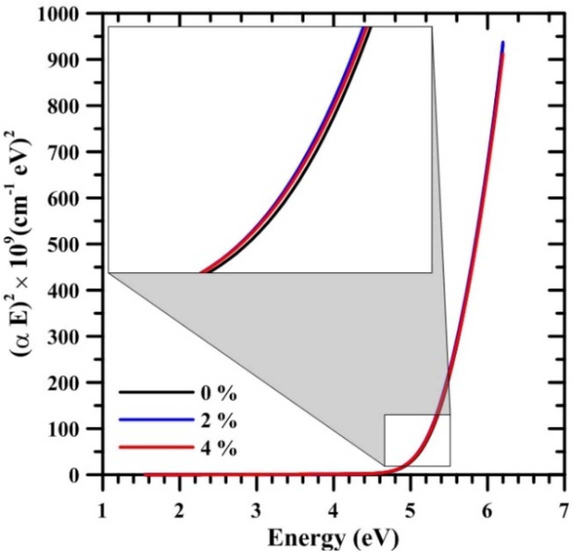

Figure 2. Variation of Ga_2O_3 thin films $(\alpha E)^2$ according to energy produced at different oxygen percentages.

Figure 3 shows the variation of the transmittance of Ga_2O_3 thin films produced at different oxygen percentages and then annealed at 900°C for 60 minutes in the air. In figure 3, our transmittance was around 83 % when no oxygen was given to the system, and around 84 % when 2 % oxygen was given. When we give the oxygen percentage as 4%, our transmittance is measured at around 86 %. As the percentage of oxygen increased, the transmittance first decreased and then the transmittance increased. The annealing process provides additional oxygen, which causes oxidation of the Ga_2O_3 thin films. As a result, interference fringes were observed in the films grown after annealing.

Figure 4 shows the variation of $(\alpha E)^2$ with energy, which is found with the help of the absorption coefficient calculated by utilizing the transmittance values of Ga_2O_3 thin films produced by giving different oxygen percentages and annealed at 900°C in the air for 60 minutes. The energy band gap was measured as 5.37 eV when no oxygen was supplied to the system, 5.37 eV when 2% oxygen was given, and 5.40 eV when 4% oxygen was given. According to this graph, as the percentage of oxygen increased, the energy band gap increased.

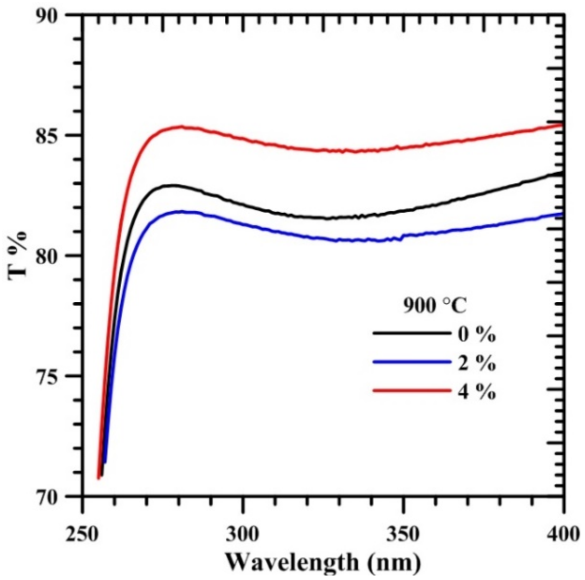

Figure 3. Variation of the transmittance of Ga_2O_3 thin films produced at different oxygen percentages and annealed at 900°C according to wavelength.

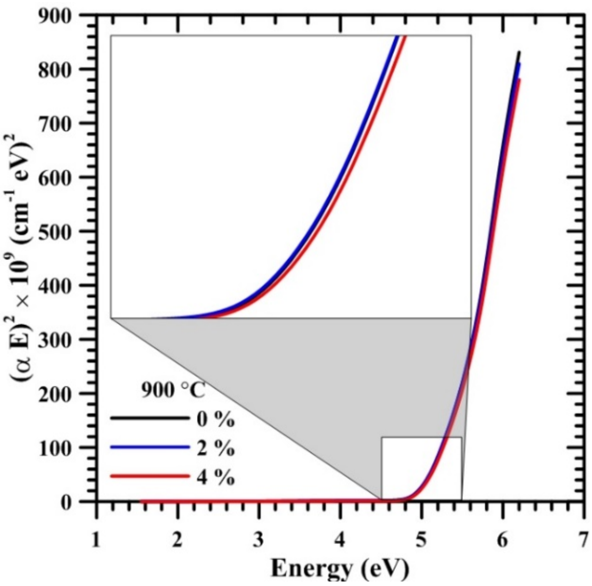

Figure 3. Variation of $(\alpha E)^2$ of thin films produced at different oxygen percentages and annealed at 900°C with respect to energy

3. Conclusion

Using the RF magnetron sputtering method, Ga_2O_3 thin films at different oxygen percentages were successfully grown on a sapphire substrate. The grown thin films were annealed in air at 900°C for 60 minutes. The effect of annealing on the optical properties of Ga_2O_3 thin films produced at different oxygen percentages was investigated. While the films grown before annealing are in amorphous form, it is thought that the structure shifts to crystal after annealing. The energy band gap of the Ga_2O_3 thin films was found by calculating the absorption coefficient using the transmittance curves. It was observed that the transmittance changed as the percentage of oxygen increased. It was observed that the energy band gap increased within itself as the oxygen percentage increased before and after annealing. It was seen that the energy band gap of the films after annealing was less than the energy band gap of the films before annealing. The reason for this change is thought to be due to oxygen defects in the Ga_2O_3 structure.

Method

In this study, the NANOVAK NVTS-400-2TH2SP Thermal and Sputter Combined System was used to produce the films. A gallium oxide target with 99.99% purity and 0.250-inch thickness and 2-inch diameter properties was used to grow gallium oxide films on the sapphire substrate. First, the substrates were placed in acetone filled in a small glass beaker. The surfaces were cleaned in acetone for 8-10 minutes and left to dry. The base pressure was set to 7.4×10^{-6} Torr, the working pressure was 7×10^{-3} Torr, the power was 100 W and the substrate rotation was 10 rpm. Ga_2O_3 films were grown at room temperature, with a thickness of 200 nm (the value entered in the thickness monitor) and at different oxygen percentages (0%, 2%, 4%).

After growing, the samples were placed in a furnace and annealed at 900 °C. In the annealing process, the samples were kept in an air atmosphere for 60 minutes. After annealing, the temperature was gradually lowered to room conditions. After annealing, the effect of annealing on the crystal quality of the films was investigated. Optical characterization of the samples was performed using a dual beam UV-Vis–NIR spectrophotometer (Cary 5000). Optical transmittance spectra were obtained in the wavelength range of 250-400 nm using the solid sample holder accessory.

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Authors’ contributions

H.H.: Sample preparation and experiments. H.S.A.: Sample preparation and experiments. E.Ş.T.: Methodology, Writing –original draft & review & editing, Formal analysis, Investigation.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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