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ITO films as a functional material for THz radiation modulation

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Abstract. In this paper, we investigate the terahertz (THz) transmittance and band gap (BG) properties of magnetron sputtered indium tin oxide (ITO) thin films. The THz transmittance was measured using THz time domain spectroscopy, which provides insight into the interaction of terahertz radiation and free carriers inside the films. The band gap was determined from spectrophotometric data using Tauc diagrams, which allowed the analysis of both direct and indirect electron transitions. The results showed that the THz transmittance decreases with increasing film thickness, primarily due to the increase in free carrier absorption associated with higher conductivity and carrier concentration in thicker films. The observed optical band gap values depend on the Burstein–Moss effect caused by the filling of low-energy states in the conduction band with free electrons. The obtained results demonstrate a close relationship between the electronic structure and terahertz response in ITO films, confirming their potential for efficient control of terahertz radiation and application in optoelectronic devices.

Keywords: indium tin oxide, Terahertz transmittance, band gap, THz time-domain spectroscopy, spectrophotometry, Tauc plots

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ITO-пленки как функциональный материал для управления ТГц излучением

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Аннотация. В данной работе мы исследуем пропускание в терагерцовом (ТГц) диапазоне и ширину запрещенной зоны (ЗЗ) тонких пленок оксида индия-олова (ITO), полученных магнетронным распылением. Пропускание в ТГц диапазоне измерялось с помощью терагерцовой спектроскопии во временной области, что позволило изучить взаимодействие терагерцового излучения со свободными носителями заряда в пленках. Ширина запрещенной зоны определялась по спектрофотометрическим данным с использованием диаграмм Таука, что позволило проанализировать как прямые, так и непрямые электронные переходы. Результаты показали, что пропускание в ТГц диапазоне уменьшается с увеличением толщины пленки, в первую очередь из-за увеличения поглощения свободными носителями заряда, связанного с более высокой проводимостью и концентрацией носителей заряда в более толстых пленках. Наблюдаемые значения оптической ширины запрещенной зоны зависят от эффекта Бурштейна–Мосса, вызванного заполнением низкоэнергетических состояний в зоне проводимости свободными электронами. Полученные результаты демонстрируют тесную взаимосвязь между электронной структурой и терагерцовым откликом пленок ITO, подтверждая их потенциал для эффективного управления терагерцовым излучением и применения в оптоэлектронных устройствах.

Ключевые слова: оксид индия-олова, ТГц пропускание, запрещенная зона, ТГц спектроскопия временного разрешения, спектрофотометрия, диаграммы Таука

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Introduction

The terahertz (THz) range is regarded as one of the most promising and has seen significant development in recent years [1] for a wide range of applications, including wireless communications [2], spectroscopy [3], and biomedical diagnostics [4]. However, the effective shielding of THz radiation remains a challenge, especially in the development of functional coatings that are transparent in the visible range.

One of the most promising materials for THz radiation shielding is indium tin oxide (ITO) thin films. Thanks to their combination of high transparency in the visible range and excellent electrical conductivity [5], ITO films are widely used in display technologies [6], sensors [7], and solar cells [8]. Importantly, the optoelectronic performance of ITO can be significantly improved through post-deposition annealing, which enhances crystallinity, increases carrier mobility, and reduces the concentration of lattice defects, thereby simultaneously improving both conductivity and transparency.

In recent years, numerous studies have focused on the electrical and optical properties of ITO films across a broad spectral range, including the visible and THz regions. These investigations have addressed both as-deposited and annealed samples. However, most studies have focused on films thicker than 100 nm. For example, Sahoo et al. [9] examined the effect of annealing in a nitrogen atmosphere at 400–800 °C on the THz optical properties and their correlation with electrical characteristics of ITO films with a thickness of approximately 275 nm.

At the same time, ultrathin coatings with thicknesses below 100 nm remain largely unexplored. In this thickness range, carrier concentration, structural defects, and annealing conditions play a particularly significant role, directly affecting terahertz transmittance and the optical band gap.

In the present work, we investigate annealed ultrathin ITO films with thicknesses of 20–100 nm and demonstrate how thickness influences their terahertz transmittance and optical band gap. This approach allows us to establish the correlation between carrier concentration and the spectral properties of ITO.

Materials and Methods

ITO films of various thicknesses (20, 40, 60, and 100 nm) were deposited on glass substrates (25×25 mm) by magnetron sputtering using a VUP-11M vacuum system. The deposition was carried out in an argon atmosphere at a working pressure of 0.2 Pa and a DC power of 85 W. Prior to deposition, the substrates underwent ultrasonic cleaning.

To improve the structural and optoelectronic properties of ITO films, such as crystallinity, conductivity and transparency, post deposition annealing was performed. Thermal treatment helps to eliminate lattice defects, increase the mobility of charge carriers and reduce the resistance of the film, which is especially important for its use as a transparent conductive coating.

Annealing of ITO coated glass samples was performed in a nitrogen atmosphere at 200 °C for 1 hour using a CVDomna setup. The heating rate was 10 °C/min, and the nitrogen pressure was maintained at 20 kPa throughout the thermal cycle.

The THz transmittance of ITO thin films was characterized using terahertz time-domain spectroscopy (THz-TDS), which allows direct measurement of both the amplitude and phase of THz pulses passing through samples in the frequency range of 0.1–1.0 THz. The optical band gap (BG) of the films was determined using UV-visible spectrophotometric measurements. Transmission spectra were analyzed by the Tauc plot method, which involves plotting $(\alpha h\nu)^{1/n}$ versus photon energy where α is the absorption coefficient and n depends on the type of electronic transition.

Results and Discussion

The results of the transmittance coefficient study in the THz range for ITO films of different thicknesses are presented in Fig. 1. The decrease in transmittance with increasing thickness in the THz range is primarily due to the increase in the absorption of terahertz radiation in thicker ITO layers. This effect is associated with the high concentration of free charge carriers in ITO. The behavior can be described by the Drude model, which takes into account the dynamics of these free carriers. According to this model, the terahertz electromagnetic field causes oscillations of free electrons, which leads to a loss of field energy due to scattering and absorption processes.

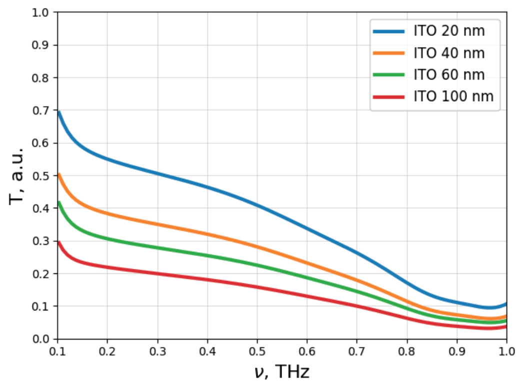

Fig. 1. Transmission spectra of ITO films with different thicknesses in the THz range

To gain a deeper understanding of the electronic properties of the ITO films, the optical band gap energy was investigated. The band gap was determined using the Tauc plot method, which is a widely used approach to extract optical band gap values from absorption spectra. Since ITO is an indirect bandgap semiconductor, Tauc plots were constructed for both direct and indirect electronic transitions. The parameter n in the Tauc equation determines the type of electronic transition, with $n = 1/2$ used for direct allowed transitions which are generally more probable, and $n = 2$ for indirect allowed transitions, which typically have lower probability due to the involvement of phonons. The corresponding Tauc diagrams for the films are shown in Fig. 2.

In ITO films, the optical band gap determined from direct transitions is approximately 3.86 eV for all film thicknesses. This wide band gap is attributed to the Burstein-Moss effect, where a

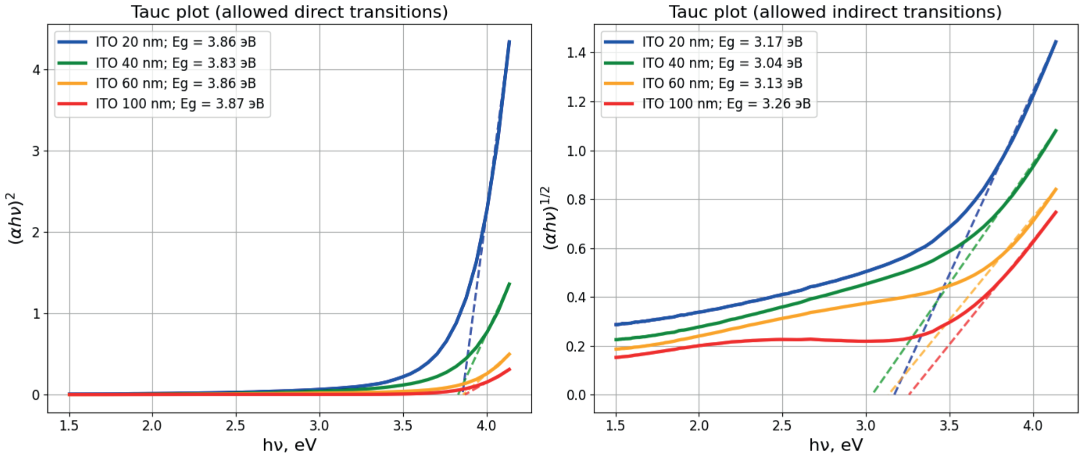

Fig. 2. Tauc plots used to determine the optical bandgap of the ITO films

high concentration of free carriers fills the low-energy states in the conduction band. As a result, electrons require higher energy to transition from the valence band to the conduction band, which shifts the absorption edge to higher energies, resulting in increased transmission in the visible range and higher electrical conductivity. Meanwhile, the lower-energy indirect band gap is due to defect states or localized structural disorder inside the films, which introduce absorption channels in the ultraviolet region due to below-bandgap transitions.

Conclusion

In this work, we investigated the spectral characteristics of annealed ultrathin ITO films deposited by magnetron sputtering in the terahertz range. It was shown that films with thicknesses below 100 nm can provide effective shielding, reducing the transmittance down to 0.1 at 1 THz. This behavior is attributed to the high concentration of free charge carriers, which also affects the optical band gap via the Burstein–Moss effect and ensures high transparency in the visible range. The interplay between carrier concentration, band structure, and scattering processes governs both THz absorption and the optical properties of the films.

However, a more precise correlation between the optical band gap and THz transmittance requires further investigation. In particular, additional measurements, including the determination of carrier mobility and concentration via the Hall effect, as well as the study of structural features of ultrathin films, will be essential for a comprehensive quantitative understanding of the relationship between free carrier dynamics, optical absorption, and electrical conductivity.

The present study provides a foundation for further research and the optimization of ultrathin ITO films for applications in transparent and flexible optoelectronic and terahertz devices.

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