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COMPARATIVE STRUCTURAL ANALYSIS OF β-Ga_2O_3 THIN FILMS DEPOSITED ON p-TYPE Si(111) AND Si(100) SUBSTRATES VIA SOL-GEL SPIN COATING

Annotation

β-Gallium oxide (β-Ga_2O_3) thin films were successfully synthesized on p-type Si(111) and Si(100) substrates using the sol-gel spin-coating technique followed by thermal annealing. X-ray diffraction (XRD) analysis confirmed the formation of monoclinic β-Ga_2O_3 on both substrates. The influence of substrate orientation on crystallite size, lattice strain, and dislocation density was systematically examined. The crystallite size of β-Ga_2O_3 deposited on Si(100) (34.2 nm) was larger than that on Si(111) (31.7 nm), while both strain and dislocation density decreased with Si(100), indicating improved crystal quality. The results demonstrate that substrate orientation plays a crucial role in determining the structural properties of β-Ga_2O_3 films, which is essential for optimizing their performance in optoelectronic and power device applications.

Key words: β-Ga_2O_3 thin films; sol–gel spin coating; Si(111) substrate; Si(100) substrate; substrate orientation; crystallite size; X-ray diffraction (XRD); Williamson–Hall analysis; lattice strain; dislocation density; annealing; wide bandgap semiconductor

СРАВНИТЕЛЬНЫЙ СТРУКТУРНЫЙ АНАЛИЗ ТОНКИХ ПЛЁНОК β-Ga_2O_3, ОСАЖДЁННЫХ НА p-ТИП SI(111) И SI(100) ПОДЛОЖКИ МЕТОДОМ ЗОЛЬ-ГЕЛЬ ЦЕНТРИФУГИРОВАНИЯ

Аннотация

Тонкие плёнки β-оксид галлия (β-Ga_2O_3) были успешно синтезированы на подложках p-типа Si(111) и Si(100) с использованием метода золь-гель центрифугирования, за которым следовал процесс термического отжига. Анализ рентгеновской дифракции (XRD) подтвердил образование моноклинной фазы β-Ga_2O_3 на обеих подложках. Влияние ориентации подложки на размер кристаллитов, решёточное напряжение и плотность дислокаций было систематически изучено. Размер кристаллитов β-Ga_2O_3, осаждённых на Si(100) (34,2 нм), оказался больше, чем на Si(111) (31,7 нм), при этом наблюдалось уменьшение как напряжения, так и плотности дислокаций, что указывает на улучшение кристаллического качества. Полученные результаты показывают, что ориентация подложки играет решающую роль в определении структурных свойств плёнок β-Ga_2O_3, что является важным для оптимизации их характеристик в оптоэлектронных и силовых приборах.

Ключевые слова: β-Ga_2O_3 тонкие плёнки; золь-гель центрифугирование; подложка Si(111); подложка Si(100); ориентация подложки; размер кристаллитов; рентгеновская дифракция (XRD); анализ Вильямсона–Холла; решёточное напряжение; плотность дислокаций; отжиг; полупроводник с широкой запрещённой зоной.

SOL–GEL SPIN-COATING USULI ORQALI p-TIPLI Si(111) VA Si(100) SUBSTRATLARIDA O‘STIRILGAN β-Ga_2O_3 YUPQA PLYONKALARINING STRUKTURAVIY TAHLILI

Annotatsiya

β-galliy oksid (β-Ga_2O_3) yupqa plyonkalari sol–gel aylantirish (spin-coating) usuli yordamida p-tipli Si(111) va Si(100) substratlarida muvaffaqiyatli sintez qilindi va keyinchalik issiqlik bilan pishirish (annealing) jarayoni o‘tkazildi. Rentgen difraksiyasi (XRD) tahlili ikkala substratda ham monoklinik β-Ga_2O_3 fazasining hosil bo‘lganligini tasdiqladi. Substrat yo‘nalishining kristallit o‘lchami, panjara deformatsiyasi va dislokatsiya zichligiga ta’siri tizimli ravishda o‘rganildi. Si(100) ustiga cho‘ktirib o‘stirilgan β-Ga_2O_3 plyonkasining kristallit o‘lchami (34,2 nm) Si(111) dagidan (31,7 nm) kattaroq bo‘lib, bunda deformatsiya va dislokatsiya zichligi kamaygani kuzatildi. Bu esa kristall sifatining yaxshilanganini ko‘rsatadi. Natijalar shuni

ko‘rsatadiki, substrat yo‘nalishi β-Ga_2O_3 plyonkalarining tuzilma xossalarini belgilashda muhim omil hisoblanadi, bu esa ularning optoelektron va quvvatli qurilmalardagi samaradorligini oshirish uchun zarurdir.
Kalit so‘zlar: β-Ga_2O_3 yupqa plyonkalar; sol–gel aylantirish usuli; Si(111) substrati; Si(100) substrati; substrat yo‘nalishi; kristallit o‘lchami; rentgen difraksiyasi (XRD); Williamson–Hall tahlili; panjara deformatsiyasi; dislokatsiya zichligi; issiqlik bilan pishirish; keng taqiqlangan zonali yarim o‘tkazgich.

Introduction. Gallium oxide (Ga_2O_3) is a rapidly emerging ultra-wide bandgap (UWBG) semiconductor with exceptional potential for applications in high-power electronics, deep-UV photodetectors, and transparent devices. Its wide bandgap energy (4.8–5.2 eV), high breakdown electric field (~8 MV/cm), and excellent chemical and thermal stability make it a superior alternative to conventional semiconductors such as Si, GaN, and SiC [1,2,3].

Among its five polymorphs (α, β, γ, δ, and ε), the β-phase is the most thermodynamically stable at ambient conditions and is therefore widely studied for electronic and optoelectronic devices [4].

In thin-film form, β-Ga_2O_3 can be synthesized by various techniques including molecular beam epitaxy (MBE), metal-organic chemical vapor deposition (MOCVD), pulsed-laser deposition (PLD), and the sol-gel spin-coating route. Among these, sol-gel spin coating has received special attention as a low-cost, scalable method capable of producing uniform and high-purity oxide films [5,6]. However, the final microstructural quality of sol-gel-derived Ga_2O_3 strongly depends on substrate orientation and post-annealing parameters**.**

Silicon substrates, especially Si(111) and Si(100), offer well-controlled surface symmetries that can influence nucleation behavior, strain relaxation, and grain boundary formation. Despite several reports describing β-Ga_2O_3 growth on different substrates, few studies have provided a systematic comparison between Si(111) and Si(100) for sol-gel growth. Therefore, this research focuses on the influence of substrate orientation on the structural characteristics of β-Ga_2O_3 thin films, analyzing crystallite size, microstrain, and dislocation density derived from X-ray diffraction (XRD) and Williamson–Hall (W–H) methods.

Literature Review. Extensive research has demonstrated the importance of optimizing β-Ga_2O_3 thin-film growth parameters to achieve high crystalline quality and low defect density. Pearton et al. [1] and Higashiwaki et al. [2] emphasized that β-Ga_2O_3’s ultra-wide bandgap and high breakdown field make it ideal for high-voltage device applications, yet its performance is highly dependent on film quality and defect concentration. Roy et al. [3] and Galazka [4] discussed the thermodynamic stability of β-Ga_2O_3, noting that its monoclinic phase is most favorable for epitaxial and sol-gel synthesis.

Lin et al. [5] reported that substrate type and annealing temperature strongly affect β-Ga_2O_3 grain size and lattice strain. Similarly, Kim et al. [6] demonstrated that sol-gel-derived β-Ga_2O_3 films can achieve excellent crystallinity when processed under optimized thermal conditions. Li et al. [7] found that Si(100) substrates provide better lattice matching and result in reduced dislocation density compared to Si(111), leading to improved crystalline orientation. Zhao et al. [8] also highlighted the role of precursor concentration and spin speed in determining surface morphology and phase purity.

While several studies have described the dependence of Ga_2O_3 film properties on deposition parameters, few have applied Williamson–Hall (W–H) analysis to deconvolute strain and size effects, particularly for sol-gel systems on different Si orientations. Therefore, the present study combines conventional Scherrer analysis with W–H analysis to present a more complete understanding of strain relaxation behavior in β-Ga_2O_3 thin films.

Experimental Method. Materials

Gallium nitrate hydrate ($Ga(NO_3)_3 \cdot xH_2O$, 99.9%) was used as the precursor material. 2-Methoxyethanol (2-MOE) served as the solvent, and ethanolamine (EA) acted as a stabilizing agent. P-type Si(111) and Si(100) wafers were used as substrates.

2.2. Solution Preparation

A 0.1 M gallium oxide precursor solution was prepared by dissolving $Ga(NO_3)_3 \cdot xH_2O$ in 2-methoxyethanol under constant stirring at 60 °C. A small amount of ethanolamine was added to stabilize the solution and prevent premature hydrolysis. The resulting transparent sol was aged for 24 h before deposition.

2.3. Thin Film Deposition

The cleaned Si(111) and Si(100) substrates were coated with the prepared sol using a spin-coater operating at 3000 rpm for 30 s. Multiple coatings were applied to achieve the desired thickness, with each layer dried at 150 °C for 10 min. The coated films were subsequently annealed in air at 1000 °C to promote crystallization of β-Ga_2O_3.

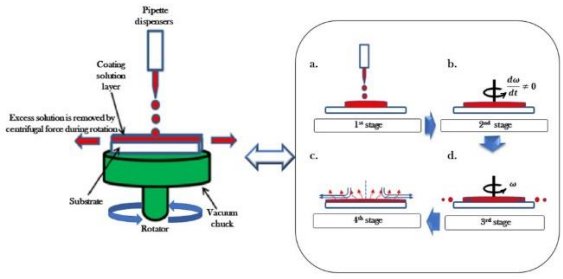

Fig.1. Ga_2O_3 film preparation process scheme. Spin coating steps: a) solution deposition, b) spinner acceleration, c) continuous solution spreading at constant angular speed, and d) solution evaporation and film thinning [9].

2.4. Characterization

The crystal structure and phase identification of the deposited films were analyzed by X-ray diffraction (XRD) using Cu Kα radiation (λ = 1.5406 Å). The average crystallite size (D) was calculated from the full width at half maximum (FWHM) of the diffraction peaks using the Scherrer equation [10,**Ошибка! Источник ссылки не найден.**1].

$$D = \frac{\kappa\lambda}{\beta cos\theta}$$

The dislocation density (δ)[11,12] and lattice strain (ε)[11,13,14] were estimated using:

$\delta = \frac{1}{D^2}$, $\varepsilon = \beta / (4 \tan\theta)$

3. Results and Discussion

3.1. XRD Analysis

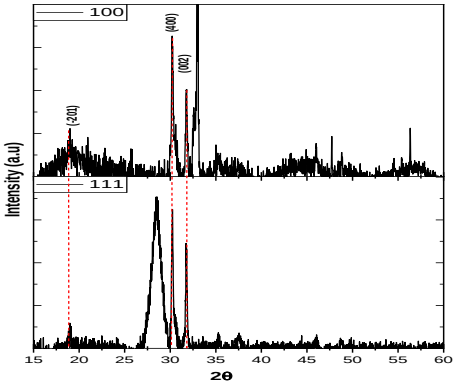

Fig.2. X-ray diffraction patterns of β-Ga_2O_3 thin films deposited on (a) Si (111) and (b) Si (100) substrates.

Figure 2 displays the XRD patterns of β-Ga_2O_3 thin films deposited on Si(111) and Si(100) substrates. Both samples exhibit distinct diffraction peaks at approximately 30.2° and 31.8°, corresponding to the (400) and (002) planes of monoclinic β-Ga_2O_3 (JCPDS No. 43-1012). The presence of these peaks confirms successful crystallization of β-Ga_2O_3 after annealing.

Table 1. Structural parameters of β-Ga_2O_3 thin films grown on Si(111) and Si(100) substrates.

Substrate	Peak (2θ)	Plane (hkl)	FWHM	D, average (nm)	δ (Dislocation Density, nm^{-2})	ε, strain
Si (111)	30.235°	(400)	0.2863	31.73	0.00099	−0.02575
	31.768°	(002)	0.2082			
Si (100)	30.242°	(400)	0.2464	34.24	0.00085	−0.01391
	31.775°	(002)	0.2046			

3.2. Effect of Substrate Orientation

A clear difference in crystallite size and microstrain is observed between the two samples. The β-Ga_2O_3 film deposited on Si(100) shows a larger crystallite size (34.2 nm) and smaller FWHM, indicating higher crystallinity and reduced defect density compared to the film on Si(111). The corresponding decrease in dislocation density and strain further suggests improved lattice ordering.

3.3. Structural Quality and Defect Control

The reduction in lattice strain and dislocation density on Si(100) implies that this orientation offers better lattice matching and stress accommodation during film growth. The observed negative strain values indicate compressive stress in both films, which arises due to differences in thermal expansion coefficients between Ga_2O_3 and silicon. The overall structural quality improvement on Si(100) highlights its potential for high-performance optoelectronic devices where defect minimization is essential.

3.4. Williamson-Hall plot analysis

The Williamson–Hall (W–H) method is a widely used approach to simultaneously evaluate crystallite size and lattice strain from XRD peak broadening. Unlike the Scherrer equation, which considers only size-induced broadening, the W–H model assumes that both crystallite size and strain contribute to the total peak broadening. The method is expressed by the equation [11,13**Ошибка! Источник ссылки не найден.**,14][Ошибка! Источник ссылки не найден.].

$$\beta \cos\theta = \frac{\kappa\lambda}{D} + 4\varepsilon \sin\theta$$

where β is the full width at half maximum (FWHM) in radians, θ is the Bragg angle, λ is the X-ray wavelength (1.5406 Å), D is the crystallite size, and ε represents lattice strain.

By plotting $\cos\theta$ versus $4\sin\theta$, a straight line is obtained in which the intercept corresponds to the crystallite size term (kλ/D) and the slope represents the lattice strain (ε).

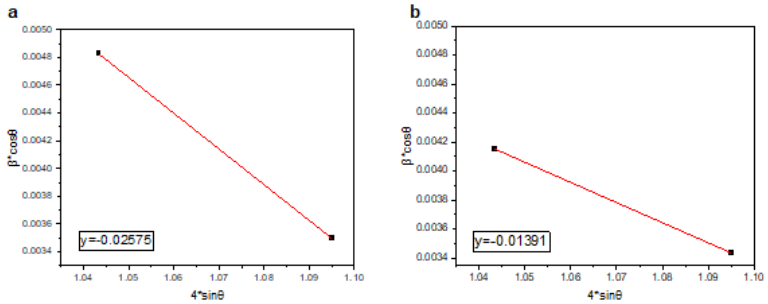

Fig.3 Plot of the Williamson-Hall formula for β-Ga_2O_3 thin films grown on (a) Si (111) and (b) Si (100) substrates where strain (ε) was determined.

In this study, the W–H plot analysis confirmed that the β-Ga_2O_3 films deposited on Si(100) exhibit a smaller positive slope, indicating lower lattice strain compared to the film on Si(111). The extrapolated intercept value corresponded to a larger crystallite size (~34 nm) for the Si(100) substrate versus ~32 nm for Si(111), consistent with the Scherrer results. This trend suggests that the Si(100) orientation provides a more favorable interface for strain relaxation and promotes grain coalescence, leading to improved film crystallinity.

Furthermore, the negative strain component obtained from the linear fit indicates the presence of compressive stress, likely caused by the thermal mismatch between β-Ga_2O_3 and the underlying silicon substrate during post-annealing. The combined W–H and Scherrer analyses confirm that the Si(100) substrate supports more uniform crystal growth, lower defect density, and enhanced structural integrity.

Conclusion. β-Ga_2O_3 thin films were synthesized on p-type Si(111) and Si(100) substrates via sol-gel spin-coating followed by annealing. XRD analysis confirmed the monoclinic β-phase on both substrates. Substrate orientation significantly influenced the structural parameters of the films. Films grown on Si(100) exhibited larger crystallite size (34.2 nm), lower dislocation density (0.00085 nm^{-2}), and reduced lattice strain (−0.0139) compared to those on Si(111). These findings indicate that Si(100) provides a more favorable surface for β-Ga_2O_3 growth, resulting in improved crystallinity and fewer structural defects.

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Author Contributions

The manuscript was written through contributions of all authors. All authors have given approval to the final version of the manuscript.

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