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# MODELING OF OPTICAL AND SURFACE PROPERTIES OF ALUMINUM THIN FILMS USING SPECTROSCOPIC ELLIPSOMETRY

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In this study, aluminum (Al) thin films deposited on soda lime glass substrates were investigated using spectroscopic ellipsometry with a focus on optical modeling and surface characteristics. The films were fabricated by thermal deposition under controlled vacuum conditions. A multilayer optical model, including Al, native oxide ($Al_2O_3$), and surface-roughness layers, was developed to accurately fit the experimental ellipsometric data. The analysis was performed in the photon energy range of 0.5–6 eV at multiple incidence angles. The Cauchy and Lorentz dispersion models were applied to represent the dielectric response of the oxide and metallic layers, respectively. The surface roughness was modeled using the effective medium approximation. The obtained results demonstrate that surface morphology and oxide layer formation play a significant role in determining the optical behavior of Al thin films. Variations in surface roughness and interface properties were found to influence the refractive index and extinction coefficient. The developed optical model showed good agreement with experimental data, confirming its reliability in describing complex thin-film systems. These findings highlight the importance of accurate optical modeling for the design and optimization of thin film materials in engineering and optoelectronic applications.

**Keywords:** *Spectroscopic ellipsometry; Optical model; Dielectric constants; Thin layers*

## 1. INTRODUCTION

The rapid development of modern nanotechnology has led to growing interest in thin-film materials due to their wide range of applications in electronics, photonics, and energy-related systems [1–3]. Among these materials, aluminum (Al) thin films are particularly attractive because of their favorable optical, electrical, and mechanical properties, as well as their technological compatibility with large-scale fabrication processes [4–6]. In thin-film systems, the physical and optical properties are strongly influenced not only by the intrinsic properties of the material but also by surface morphology and interfacial characteristics. In particular, the formation of a native oxide layer and surface roughness can significantly modify light–matter interactions, thereby altering optical constants such as the refractive index and extinction coefficient [7–10]. Therefore, accurate characterization of these effects is essential for designing and optimizing functional thin-film devices. Spectroscopic ellipsometry (SE) is a powerful and non-destructive optical technique widely used to investigate thin-film structures. It enables simultaneous determination of thickness, dielectric function, and surface properties with high sensitivity over a broad spectral range [11–14]. However, the reliability of the extracted parameters strongly depends on the adequacy of the optical model used to describe the system [15-17]. In this context, the development of appropriate multilayer optical models is crucial, especially for systems with multiple interfaces and surface effects. Incorporating layers such as native oxides and surface roughness into the model allows for a more realistic representation of the physical structure and improves the accuracy of the analysis [18–21]. In this work, aluminum thin films deposited on soda-lime glass substrates are investigated using spectroscopic ellipsometry. A multilayer optical modeling approach is employed to analyze the effects of surface roughness and oxide layer formation on the system's optical response.

The novelty of this work lies in the development of a comprehensive optical model for thermally deposited Al thin films on soda-lime glass substrates that simultaneously accounts for the metallic Al layer, the native $Al_2O_3$ overlayer, and surface-roughness effects within a unified spectroscopic ellipsometry framework. Such an approach provides a more realistic description of the films' physical structure and improves the accuracy of the extracted optical parameters. The proposed model can serve as a reliable tool for investigating thickness-dependent optical properties of Al thin films and for optimizing Al-based structures intended for photonic and optoelectronic applications.

## 2. MATERIALS AND METHODS

Two thin aluminum films with different thicknesses were fabricated from nanopowders via thermal deposition. The thermal evaporation was performed using a Leybold-Heraeus L-560 vacuum system. The working pressure in the vacuum chamber was maintained at 2×10-5 mbar. The substrates used were chemically cleaned 25×19 mm glass plates. Prior to thermal evaporation, the surfaces of the glass substrates were ionized at 800 W. To enhance the deposition

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process, the glass substrates were heated to 100°C in the vacuum chamber. The thermal evaporation process was conducted for 25 seconds. Although the nominal deposition time was identical for both samples, small variations in the evaporation rate, source material distribution, and local deposition conditions resulted in different film thicknesses (80 and 100 nm). Such variations are commonly observed in thermally evaporated thin films and can significantly influence the final film thickness.

The optical parameters of the two Al films obtained were examined by spectroscopic ellipsometry over a photon energy range of 0.5-6 eV. The incident angle during the ellipsometric measurements was varied at 60°, 65°, 70°, and 75°, and all measurements were performed at room temperature. The optical constants of the Al/SLG (soda lime glass) systems were retrieved through regression analysis of the obtained SE data. The ellipsometric parameters Ψ and Δ represent the amplitude ratio and phase shift of the parallel (p) and perpendicular (s) components of the reflected light, respectively. The complex reflectance ratio of the polarized light is given by:

$$\rho = \frac{r_p}{r_s} = tan\Psi e^{i\Delta} \quad (1)$$

where $r_p$ and $r_s$ are the Fresnel reflection coefficients of p- and s-polarized light, respectively. The measurements were performed using an M-2000 rotating compensator spectroscopic ellipsometer (RCE, J.A. Woollam Co., Inc.). The measured ellipsometric parameters were analyzed through regression fitting of the experimental data. The intensities Is and Ic recorded by the rotating compensator ellipsometer are expressed as [22]:

$$I_s = sin2\Psi sin\Delta, \; I_c = sin2\Psi cos\Delta \quad (2)$$

In Eq. (2), Is and Ic represent the experimentally measured intensity components obtained from the modulation of the polarization state of the reflected light. These quantities are directly related to the ellipsometric parameters Ψ and Δ and provide information about the optical properties and thicknesses of the individual layers that form the sample. Therefore, fitting the calculated $I_s$ and $I_c$ spectra to the experimental data enables a reliable determination of the optical constants and structural parameters of the multilayer system.

A four-layer optical model was used to reproduce the experimental $I_s$ and $I_c$ signals over the entire photon-energy range. This model consists of the substrate (SLG), thin film (Al), alumina ($Al_2O_3$), and surface roughness (Fig. 1).

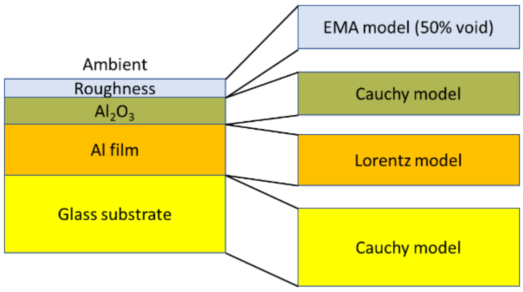


**Figure 1.** Theoretical model of the samples

In this model, the surface roughness was described using the Effective Medium Approximation (EMA) based on Bruggeman theory, modeled by Bruggeman's EMA (50% $Al_2O_3$ + 50% void). The Cauchy dispersion model was applied to the $Al_2O_3$ and SLG layers, as these transparent dielectric materials can be accurately described using this empirical relation:

$$n(E) = A+BE^2+CE^4 \quad (3)$$

where *A*, *B*, and *C* are fitting parameters.

The Al layer was fitted using the Lorentz model, which is particularly useful for metals and semiconductors. The physical basis for Lorentz oscillators has been extensively discussed in many textbooks [23,24]. The Lorentz layer can be described as a collection of absorption peaks that is Kramers-Kronig consistent:

$$\tilde{\varepsilon}(h\nu) \equiv \varepsilon_1 + i\varepsilon_2 = \varepsilon_{1\infty} + \sum_k \frac{A_k}{E_k^2 - (h\nu)^2 - iB_k h\nu} \quad (4)$$

where $k$ is the oscillator index, $A_k$ is the amplitude, $E_k$ is the center energy, $B_k$ is the broadening of each oscillator, $h\nu$ is the photon energy in eV, and $\epsilon_1$ is an additional offset.

## 3. OPTICAL MODELING

To accurately describe the optical response of aluminum thin-film systems, a multilayer optical model was developed using spectroscopic ellipsometry data. The model consists of four main layers: the glass substrate, the aluminum (Al) thin film, the native oxide layer ($Al_2O_3$), and a surface roughness layer. The substrate (soda lime glass) was considered optically homogeneous and isotropic. The aluminum thin film was treated as a metallic layer, while the oxide layer was assumed to be transparent within the investigated spectral range. The surface roughness was modeled using the Effective Medium Approximation (EMA), where the roughness layer was represented as a mixture of 50% void and 50% bulk material, following Bruggeman's theory. To describe the optical properties of each layer, appropriate dispersion models were applied. The dielectric response of the $Al_2O_3$ layer and the glass substrate was modeled using the Cauchy dispersion relation, which is suitable for transparent dielectric materials. In contrast, the aluminum layer was described using the Lorentz oscillator model, which effectively represents the absorption processes in metallic systems. The model parameters, including layer thicknesses, optical constants, and surface roughness, were determined through regression analysis by minimizing the difference between experimental and calculated ellipsometric data. The fitting procedure was carried out using a nonlinear optimization algorithm, ensuring high accuracy and reliability of the results. This modeling approach enables a comprehensive understanding of how surface morphology and interfacial properties influence the optical behavior of aluminum thin films.

## 4. RESULTS AND DISCUSSION

***4.1 Ellipsometric fitting.*** An optical model for isotropic media or isotropic thin-film/substrate systems was used to fit the calculated data to the experimental $\psi$ and $\Delta$ values. The Complete EASE software was employed for the ellipsometric data-fitting procedure, achieving a mean squared error (MSE) of less than 1.5 in the worst case. The experimental data were fitted using the Levenberg–Marquardt algorithm, applying parameterized model dielectric functions simultaneously for all data points measured in the UV/VIS ranges. The Lorentz oscillator model, available in the Complete EASE database, was used to describe the dielectric response of the aluminum layer across the investigated spectral range. This model is widely employed for metallic materials and provides a physically meaningful representation of their optical behavior. The measured ellipsometric parameters (full red and green curves) and their fits (dashed black curves) for incident angles of 60°, 65°, 70°, and 75° are presented in Fig. 2 and Fig. 3 for Al/SLG samples, respectively. A similarly good fit to the measured $\Psi$ and $\Delta$ was obtained for other incident angles. The quality of the obtained film surfaces is confirmed by the low MSE and roughness values (overlayer thickness).

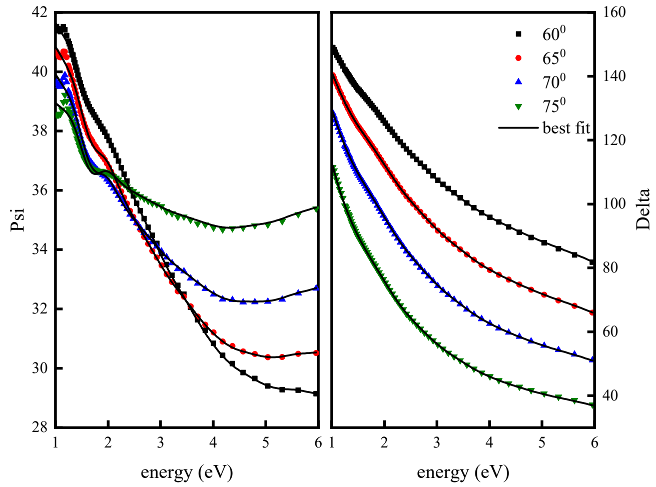


**Figure 2.** Experimental (dots) and fitted (lines) ellipsometric data of sample $d_1$ with 100 nm Al thin film

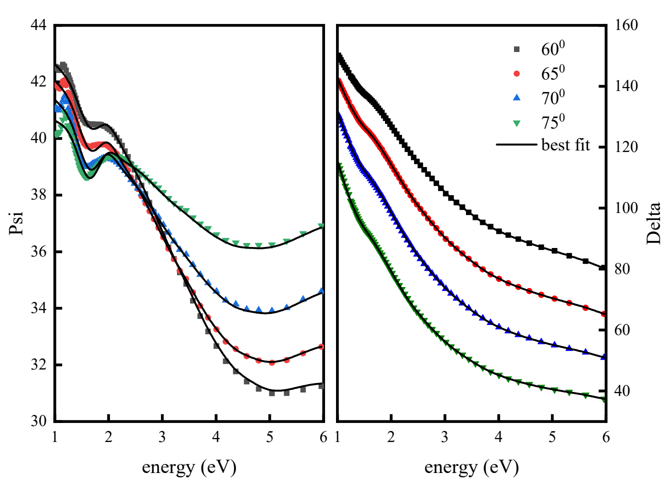


**Figure 3.** Experimental (dots) and fitted (lines) ellipsometric data of sample $d_2$ with 80 nm Al thin film

***4.2 Optical constants***. The optical constants of the aluminum thin films, including the refractive index (n) and extinction coefficient (k), were determined from the fitted ellipsometric data using the developed multilayer optical model. The analysis of the pseudo-dielectric function allowed for the simultaneous evaluation of the real ($\varepsilon_1$) and imaginary ($\varepsilon_2$) components, providing insight into the optical behavior of the system. The calculated spectra of the pseudo-dielectric functions are presented in Fig. 4.

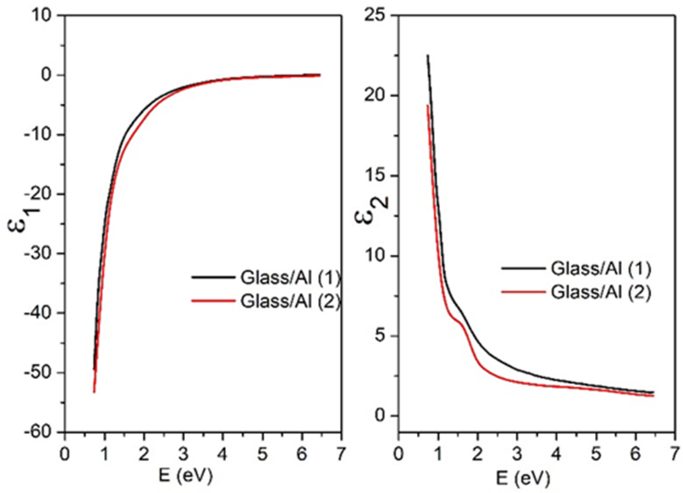


**Figure 4.** Real ($\varepsilon_1$) and imaginary ($\varepsilon_2$) parts of the pseudo-dielectric function of Al thin films with different structural parameters

The obtained spectral dependences of $\varepsilon_1$ and $\varepsilon_2$ indicate that the films' optical response is influenced by both intrinsic material properties and surface-related effects. Variations in these functions reflect differences in light interaction within the multilayer system, including contributions from interfaces and surface morphology.

The optical constants, namely the refractive index (n) and extinction coefficient (k), were extracted from the dielectric function and are shown in Fig. 5.

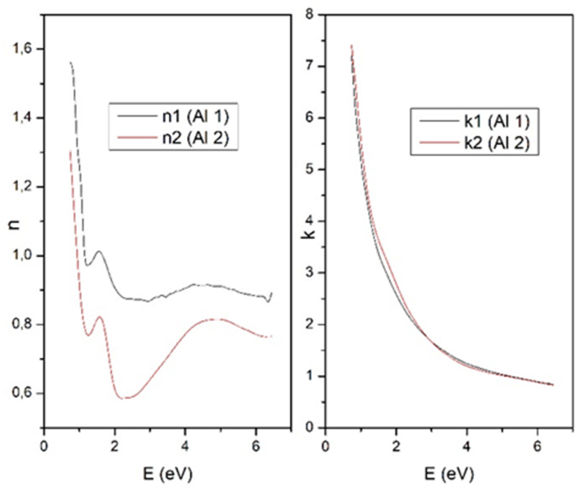


**Figure 5.** Refractive index (n) and extinction coefficient (k) of Al thin films as a function of photon energy

As shown in Fig. 5, the optical constants are strongly affected by surface and interfacial properties. The refractive index is sensitive to structural inhomogeneities and surface morphology, which alter the effective optical medium. At the same time, the extinction coefficient reflects absorption processes and light interactions within the metallic layer. At lower photon energies, the extinction coefficient is relatively high, indicating stronger absorption in the metallic Al films. As photon energy increases, the extinction coefficient gradually decreases across the investigated spectral range, indicating reduced absorption losses. These trends are consistent with the optical behavior observed for metallic thin films. In addition, the presence of a surface oxide layer and surface roughness modifies the optical path and boundary conditions, which in turn affects the extracted values of n and k. Therefore, accurate determination of optical constants requires careful consideration of both surface and interface effects within the multilayer structure. The good agreement between experimental and modeled data confirms the reliability of the proposed four-layer optical model and underscores the importance of simultaneously accounting for oxide-layer formation and surface roughness in the optical characterization of aluminum thin films.

The observed spectral behavior of the optical constants is mainly governed by the free-electron response of aluminum and by the influence of the oxide layer and surface morphology. The obtained optical constants are in reasonable agreement with the well-established optical data reported for aluminum by Palik [25], Rakic et al. [26], and Aspnes[24]. Minor differences may be attributed to variations in film thickness, deposition conditions, native oxide formation, and surface roughness. This agreement confirms the physical reliability of the proposed optical model and the extracted dielectric parameters. Consequently, accurate optical modeling is required to separate intrinsic material properties from interface-related effects.

***4.3 Surface and Oxide Effects***. The surface morphology and the presence of a native oxide layer ($Al_2O_3$) play a crucial role in determining the optical behavior of aluminum thin films. Surface roughness introduces additional light scattering at the air/film interface, thereby affecting the system's effective optical response. As the roughness increases, the effective refractive index becomes a weighted average between the material and voids, leading to modifications in both the refractive index (n) and extinction coefficient (k). The surface roughness was described using the Effective Medium Approximation (EMA), where the roughness layer was modeled as a mixture of $Al_2O_3$ and voids. This assumption was adopted because the roughness layer represents the non-ideal surface of the native oxide layer exposed to air. Such an approach provides a physically realistic description of the film surface and improves the accuracy of the ellipsometric analysis. This approach provides a realistic representation of non-ideal surfaces and improves the accuracy of the ellipsometric fitting. In addition to roughness effects, the formation of a native aluminum oxide ($Al_2O_3$) layer significantly influences the optical response. The oxide layer acts as a dielectric interface between the metallic aluminum and the surrounding medium. Due to its transparency in the studied spectral range, it modifies the phase and amplitude of reflected light, thereby affecting the extracted ellipsometric parameters. Furthermore, even a thin oxide layer can alter the interference conditions within the multilayer system by changing the optical path length. As a result, noticeable variations in the optical constants (n and k) can occur, making the inclusion of the oxide layer essential for accurate optical modeling. The surface roughness values for the samples, as presented in Table 1, show noticeable differences, likely attributable to variations in deposition conditions and material interactions during film formation.

**Table 1.** Structural parameters of Al thin films

| Samples | Roughness (nm) | $Al_2O_3$ (nm) | Al (nm) |
|---|---|---|---|
| Al 1 | 11.04 ± 0.2 | 13.33 ± 0.5 | 100 |
| Al 2 | 6.55 ± 0.4 | 13.09 ± 0.7 | 80 |

Factors such as substrate preparation, cleaning procedures, and deposition parameters (including temperature and pressure) may significantly influence the resulting surface morphology. In particular, interfacial processes occurring between the aluminum layer and the oxide phase ($Al_2O_3$) can affect the nucleation and growth mechanisms, leading to differences in surface uniformity. On the other hand, the thickness of the $Al_2O_3$ layer remains nearly constant for both samples, indicating a relatively stable oxidation process. Minor variations in oxide thickness are likely related to small differences in film composition and local deposition conditions, although these variations do not significantly alter the overall structure.

Overall, both surface roughness and oxide layer formation must be taken into account to achieve reliable determination of optical constants and to better understand light–matter interaction in aluminum thin film systems. The present study demonstrates that neglecting either the native oxide layer or surface roughness may lead to noticeable deviations in the extracted optical parameters. Therefore, the proposed four-layer model provides a more realistic representation of Al thin films and can be effectively applied to investigate thickness-dependent optical behavior in similar metal–dielectric systems. Although a direct comparison with simpler optical models was beyond the scope of the present study, the inclusion of both the native oxide layer and surface roughness resulted in excellent agreement between the experimental and calculated ellipsometric spectra. These results indicate that both contributions are important for an accurate description of the optical response of the investigated Al thin films.

## CONCLUSIONS

A comprehensive optical model of thermally deposited Al thin films on soda-lime glass substrates was developed using spectroscopic ellipsometry. By simultaneously considering the metallic Al layer, the native $Al_2O_3$ oxide layer, and surface roughness, the proposed four-layer model accurately described the experimental data and enabled reliable determination of optical constants and structural parameters. The results demonstrate that oxide formation and surface morphology significantly influence the optical response of the films. The developed modeling approach offers an effective framework for studying thickness-dependent optical properties of aluminum thin films and may be useful for the design and optimization of Al-based photonic, plasmonic, and optoelectronic devices. One limitation of the present study is that the structural parameters were obtained solely from spectroscopic ellipsometry modeling without independent verification by complementary characterization techniques such as AFM, SEM, or profilometry. Future investigations combining spectroscopic ellipsometry with additional surface characterization methods would provide further validation of the extracted structural parameters and improve the robustness of the optical model.

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## МОДЕЛЮВАННЯ ОПТИЧНИХ ТА ПОВЕРХНЕВИХ ВЛАСТИВОСТЕЙ ТОНКИХ АЛЮМІНІЄВИХ ПЛІВОК ЗА ДОПОМОГОЮ СПЕКТРОСКОПІЧНОЇ ЕЛІПСОМЕТРІЇ

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У цьому дослідженні тонкі плівки алюмінію (Al), нанесені на підкладки з натрієво-кальційного скла, досліджувалися за допомогою спектроскопічної еліпсометрії з акцентом на оптичне моделювання та характеристики поверхні. Плівки були виготовлені методом термічного осадження в контрольованих умовах вакууму. Для точного узгодження з експериментальними еліпсометричними даними було розроблено багатошарову оптичну модель, що включає Al, природний оксид ($Al_2O_3$) та шари шорсткості поверхні. Аналіз проводився в діапазоні енергії фотонів 0,5–6 еВ під різними кутами падіння. Для представлення діелектричної реакції оксидного та металевого шарів відповідно були застосовані моделі дисперсії Коші та Лоренца. Шорсткість поверхні моделювалася за допомогою наближення ефективного середовища. Отримані результати демонструють, що морфологія поверхні та формування оксидного шару відіграють значну роль у визначенні оптичної поведінки тонких плівок Al. Було виявлено, що варіації шорсткості поверхні та властивостей інтерфейсу впливають на показник заломлення та коефіцієнт згасання. Розроблена оптична модель показала хорошу відповідність експериментальним даним, що підтверджує її надійність для опису складних тонкоплівкових систем. Ці результати підкреслюють важливість точного оптичного моделювання для проєктування та оптимізації тонкоплівкових матеріалів в інженерних і оптоелектронних застосуваннях.

**Ключові слова:** *спектроскопічна еліпсометрія; оптична модель; діелектричні константи; тонкі шари*