Ellipsometric Analysis of Cr_2O_3 Thin Films on Sapphire for Advanced Mirror Applications

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Abstract

This application note presents an ellipsometric analysis of approximately 110 nm thick Cr_2O_3 films epitaxially grown on sapphire substrates. The Cr_2O_3 films exhibit epitaxial crystalline growth along the c-axis, adopting the corundum structure characteristic of both the film and the substrate.

Using the **HORIBA UVISEL Plus** spectroscopic ellipsometer, we determined the film thickness and extracted optical constants across the ultraviolet to near-infrared spectral range.

The inherent birefringence from the sapphire substrate was carefully considered in the modeling, providing detailed insights into their anisotropic optical properties. These findings contribute to optimizing Cr_2O_3 coatings for high-precision crystalline mirrors in gravitational wave detectors, where material quality and optical performance are critical.

Background and Challenges

Chromium oxide (Cr_2O_3) thin films are known for their excellent chemical stability, optical transparency, and mechanical strength, making them attractive for advanced optical coatings. When combined with sapphire substrates, these films offer enhanced durability and superior optical quality, which are essential in demanding applications.

In particular, Cr_2O_3 coatings are of great interest for high-precision crystalline mirrors used in gravitational wave detectors. These mirrors require coatings with exceptional optical performance and long-term stability to achieve the sensitivity needed for detecting faint gravitational signals.

While previous studies [1,2] have reported optical properties of Cr_2O_3 films on different substrates, detailed ellipsometric analysis on epitaxial Cr_2O_3 grown on sapphire remain limited. Understanding the optical properties and film quality in this specific configuration is crucial for advancing next-generation mirror designs.

Experimental Procedure

A Cr_2O_3 thin film with an approximate thickness of 110 nm was epitaxially grown on a sapphire substrate with a thickness of 430 µm. The sapphire substrate surface corresponds to the c-plane orientation, which supports the epitaxial growth of Cr_2O_3 with the corundum crystal structure.

The optical characterization was performed using a HORIBA UVISEL Plus spectroscopic ellipsometer (Figure 1). The system is equipped with a 150 W xenon lamp as the light source and an automatic goniometer for precise angle control.

The DeltaPsi2 software provided robust multilayer fitting capabilities, essential for handling complex anisotropic models.

Figure 1: UVISEL Plus spectroscopic ellipsometer equipped with advanced phase modulation and double monochromator system (source: HORIBA)

Spectroscopic ellipsometry measurements were conducted in the spectral range from 0.6 to 6.5 eV (190-2100 nm), with a fixed angle of incidence of 70°, chosen to maximize sensitivity to the film properties. A spot size of approximately 1 mm was used for point measurements. To assess thickness homogeneity, mapping measurements were performed on a 9-point grid distributed across the sample surface.

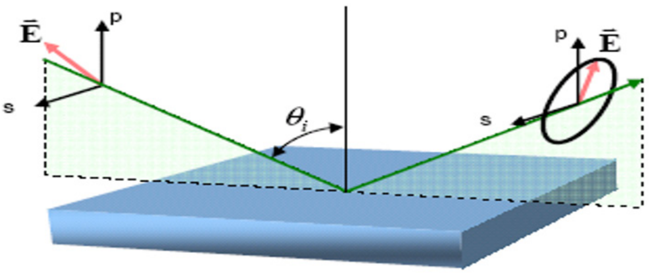
The ellipsometric parameters Is and Ic were acquired, where

$$\mathrm{Is} = \sin(2\Psi) \times \sin(\Delta)$$

and

$$\mathrm{Ic} = \sin(2\Psi) \times \cos(\Delta)$$

Here, Ψ and Δ represent the amplitude ratio and phase difference of the reflected light along the two-polarization axis , parallel (P) and perpendicular (S) to the incident plane.



Ellipsometry Measurements: Experimental Is & Ic Data

The acquired ellipsometric data (Figure 2) were collected over the full spectral range using the HORIBA UVISEL Plus system. In this figure, the experimental curves for Is (blue) and Ic (red) illustrate the raw optical response of the Cr_2O_3 thin film on sapphire before any modeling or fitting is applied.

These precise measurements provide the essential foundation for further optical analysis, enabling accurate extraction of film thickness, refractive index, and extinction coefficient in subsequent modeling steps. The high sensitivity and wide spectral coverage of the UVISEL Plus system ensure reliable and detailed characterization even for complex thin film structures.

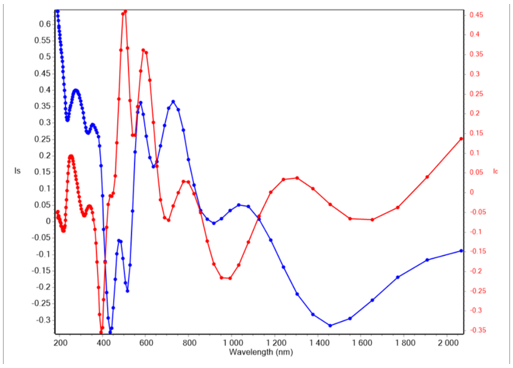


Figure 2: Ellipsometry Measurements: Experimental Is & Ic Data

Optical Modeling Approach and Multilayer Structure

The ellipsometric model was developed to represent the multilayer structure of the sample, consisting of an ~110 nm Cr_2O_3 thin film epitaxially grown on a 430 µm-thick sapphire (Al_2O_3) substrate.

The structure includes three main components: the sapphire substrate, the Cr_2O_3 layer, and a surface roughness layer on top (Figure 3). This roughness layer, modeled using the Effective Medium Approximation (EMA) with a 50% Cr_2O_3 and 50% void composition, compensates for interface imperfections and enhances the accuracy of the fit.

Backside reflections from the transparent sapphire substrate were also incorporated, as they can significantly affect the measured ellipsometric signal.

A single Tauc–Lorentz dispersion model was used to describe the optical response of Cr_2O_3, with its dielectric function parameterized to capture both absorption and refractive behavior across the spectral range. Refractive index data from the DeltaPsi2 materials library served as initial input values.

Finally, the model parameters - film thickness, refractive index, and extinction coefficient - were optimized to match the experimental Is and Ic spectra, enabling precise extraction of optical constants.

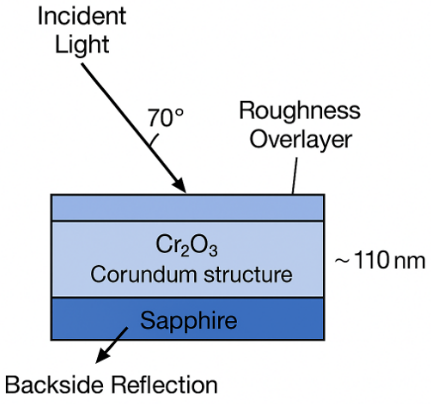


Figure 3: Schematic Model of the Cr_2O_3 Layer on Sapphire Substrate

Ellipsometry Results: Model Fit, Optical Constants, and Film Thickness

Figure 4 shows the fitting results for the Cr_2O_3 layer on sapphire. In this figure, the solid lines represent the theoretical model fit, while the dots correspond to the experimental data for Is (blue) and Ic (red), as a function of photon energy (0.6–4 eV). A Tauc–Lorentz dispersion function was used to describe the optical properties of the chromium oxide layer. Good agreement between model and experiment confirms the robustness of the fitting approach.

This fitting enables a reliable determination of the film's thickness and optical constants, which are essential for optimizing advanced optical coatings.

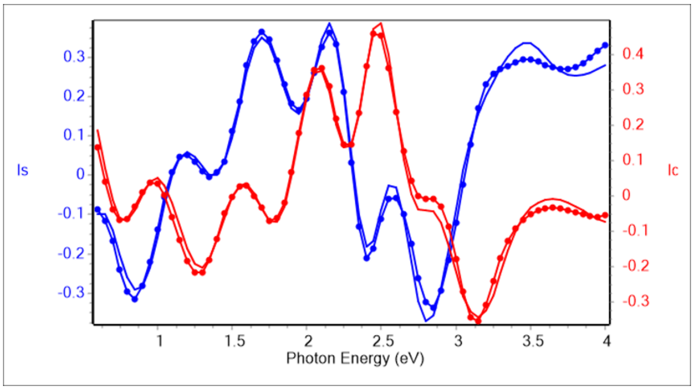


Figure 4: Comparison between experimental ellipsometric data (Is & Ic) and model fit for Cr_2O_3 layer on sapphire.

From the fitting results, the film roughness was estimated at approximately 3.23 nm, and the Cr_2O_3 layer thickness was around 109.3 nm, confirming good uniformity and coverage. The optical band gap (Eg) was found to be 2.85 eV, indicating semiconducting behavior.

As shown in Figure 5, the refractive index (n) increases from 2.4 to 3.0 in the 0.6–4 eV range, while the extinction coefficient (k) remains close to zero at lower energies and rises above 3 eV, reflecting low absorption in the visible region and higher absorption at higher photon energies. At 632.8 nm (1,96 ev), n is 2.462 and k is zero, confirming high transparency at this wavelength.

These results underline the high optical quality of the film and demonstrate the reliability of the applied model.

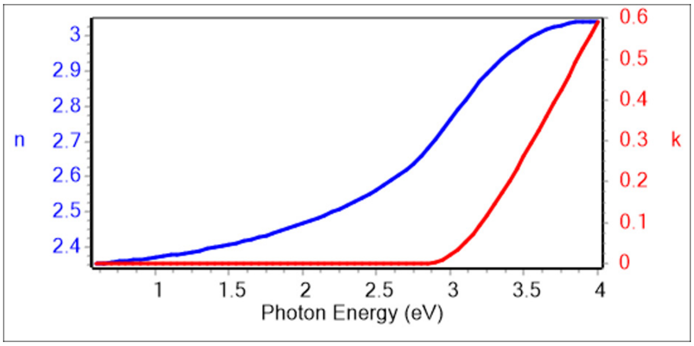


Figure 5: Dispersion of refractive index (n) and extinction coefficient (k)

Thickness and Optical Uniformity Mapping with UVISEL Plus

To assess film uniformity across a larger area, a mapping measurement was performed using a 9-point perpendicular grid (separated by 8 mm in X and Y) in the spectral range of 0.6–4 eV, as shown in Figure 6. Thanks to the integrated motorized XY stage of the HORIBA UVISEL Plus system, high-precision, fully automated point-to-point mapping was achieved with excellent reproducibility.

The average film thickness was approximately 105.3 nm, with values ranging from 101.7 nm at the edges to 109.3 nm at the center. This thickness distribution is clearly visualized in the 2D wafer plot (Fig. 6).

The optical band gap (Eg) was also highly consistent across the wafer, with an average of 2.85 eV and minimal variation (~0.003 eV). These results highlight the high quality and reproducibility of the deposition process, and they showcase the advanced mapping and analysis capabilities of the HORIBA UVISEL Plus system for detailed thin film characterization.

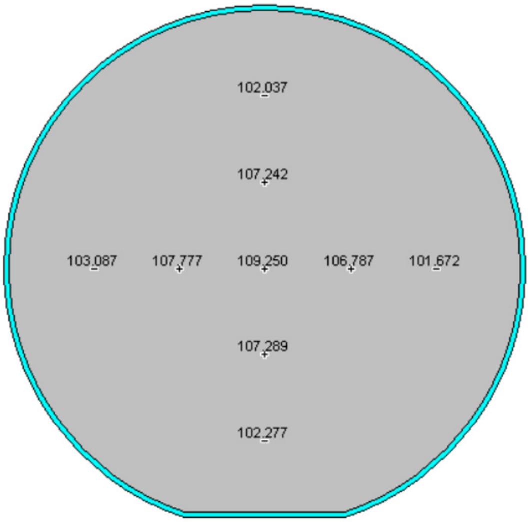


Figure 6: 2D Wafer Plot: 9-Point Thickness Uniformity Mapping

Conclusion

This study demonstrates the capability of the HORIBA UVISEL Plus ellipsometry to deliver precise, reliable characterization of epitaxial Cr_2O_3 thin films on sapphire. By combining advanced multilayer modeling — including birefringence effects and a dedicated roughness layer — with a wide spectral measurement range, we achieved accurate determination of film thickness, roughness, and optical constants.

The spatial resolution enabled by the motorized XY stage revealed thickness variations across the wafer, confirming uniformity and reproducibility of the deposition process. The extracted optical band gap (2.85 eV) and dispersion of n and k further validate the film's suitability for high-performance optical applications.

Together, these results highlight how the UVISEL Plus system transforms thin film ellipsometry into a powerful, application-driven tool for optical coating, providing both scientific insight and practical advantages for demanding coating developments.

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KU LEUVEN

References

1. Segay, M., et al. (2023). Optical response of green synthesized thin Cr_2O_3 films prepared via drop and spin coatings. Materials Today: Proceedings, 2023. https://doi.org/10.1016/j.matpr.2023.06.225
2. Salari Mehr, M., et al. (2023). Mechanical and Optical Properties of Cr_2O_3 Thin Films Grown by Atomic Layer Deposition Method Using $Cr(thd)_3$ and Ozone. Nanomaterials, 13(19), 2702. https://doi.org/10.3390/nano13192702

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