Machine-learning assisted nm-scale thin film prediction with Hyperspectral imaging system

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***Abstract*—Hyperspectral imaging (HSI) provides a powerful non-destructive approach for nanoscale layer characterization by simultaneously capturing spectral and spatial information. In this study, we propose an HSI-based framework for resolving layer thickness down to the nanometer scale, particularly in inkjet-printed nanomaterial films such as ZnO and quantum-dot (QD) layers used in QD-LED devices. Conventional optical models based on bulk refractive indices (n, k) fail for nanoparticle systems due to quantum confinement and altered electronic states. To address this, we integrate mutual information (MI) analysis with machine learning, employing a denoising autoencoder (DAE) for dimensionality reduction and robustness against spectral noise. The Kraskov–Stögbauer–Grassberger (KSG) estimator quantifies the spectral–thickness relationship, revealing that sufficient information for nanometer-scale estimation exists even under realistic noise and partial spectrum conditions. Experimental validation using AFM and ellipsometry confirms the accuracy of the proposed HSI approach. This framework establishes a pathway for high-throughput, non-contact, and spatially resolved film thickness mapping, enabling in situ process monitoring and optimization in advanced display manufacturing.**

Keywords—Hyper spectral imaging, Inkjet fabrication, quantum dot LED

I. Introduction (*Heading 1*)

Hyperspectral imaging (HSI) has emerged as a powerful tool for material characterization, offering a unique combination of spectral and spatial resolution that enables the non-destructive probing of subsurface features with nanometer-level sensitivity. Unlike conventional imaging techniques, which typically acquire intensity values at discrete wavelengths or broad spectral bands, HSI captures a continuous spectrum at each pixel. This capability facilitates precise identification of material properties such as thickness, composition, and structural uniformity across complex surfaces [1]-[5].

Recent advances in optical instrumentation and computational imaging have propelled HSI into microscale applications, including semiconductor inspection, biomedical diagnostics, and advanced display manufacturing. At its core, HSI measures wavelength-dependent reflectance, transmittance, and absorbance across ultraviolet to infrared regions—enabling inference of physical parameters such as film thickness via optical interference effects. When light is incident on thin films, constructive and destructive interference modulates the reflected spectrum, producing characteristic spectral fringes from which thickness information can be inferred.

This principle holds particular promise for inkjet-printed optoelectronic devices—notably, soluble OLEDs and QD-LEDs—where achieving uniform thin films is inherently more challenging than with conventional vacuum deposition methods [6]. Nanometer-scale thickness control is critical for color fidelity, charge transport, and device efficiency. However, traditional techniques such as atomic force microscopy (AFM) and spectroscopic ellipsometry, while precise, are often limited by low throughput, destructive contact modes, or small area coverage.

In this context, HSI offers a compelling alternative: a high-throughput, non-contact, and spatially resolved measurement platform capable of monitoring nanoscale variations across entire panels. For display manufacturing, where sub-nanometer tolerances govern visual performance, the ability of HSI to map film uniformity in situ can fundamentally change process diagnostics and yield optimization.

Nonetheless, deploying HSI for nanometer-scale thickness estimation is non-trivial. Practical implementation is challenged by high-dimensional spectral noise, limited wavelength ranges imposed by specific optical setups, and the spectral overlap inherent in multilayer structures. Moreover, the stochastic nature of inkjet-deposited films introduces heterogeneity that conventional models struggle to resolve. Key questions remain unanswered: Does the reflection spectrum contain sufficient information to extract thickness under realistic noise conditions? Can individual layers be resolved in complex stacks using only partial spectra.

In this study, we present a HSI framework optimized for nanometer-resolution thickness estimation in inkjet-printed thin films. Our approach integrates mutual information analysis to assess the information content of spectral data, a denoising autoencoder for dimensionality reduction, and validation against AFM and spectroscopic ellipsometry. By combining physical modeling with machine learning-based spectral interpretation, we demonstrate that HSI can deliver accurate and reliable thickness mapping of non-uniform, multilayered nanofilms under practical measurement constraints.

II. Experimental Setup

A custom-built line-scan hyperspectral imaging (HSI) system was employed to acquire reflection spectra with sub-nanometer precision. The optical setup is schematically illustrated in **Figure 1a**. A broadband light source (Deuterium–Tungsten lamp) was used to provide uniform illumination across the ultraviolet–visible range (200–1000 nm). The reflected light was collected through an achromatic UV-transmissive objective lens (LMU-20X-UVB, Thorlabs) and directed into a spectrometer (Kymera 193i, ANDOR) coupled to a high-sensitivity CCD camera (iKON-M 934, ANDOR). All mirrors and optical components were UV-enhanced to ensure sufficient detection efficiency in the short-wavelength region.

The HSI system operates in a **line-scan mode**, where the built-in slit of the spectrometer defines the field of view along the x-axis. By translating the sample along the orthogonal direction using a computer-controlled XY motorized stage, two-dimensional hyperspectral images were reconstructed from sequentially captured spectral lines. The system was controlled through a custom LabVIEW-based software interface, enabling synchronized control of stage movement, camera exposure, slit width, and optical alignment. The integration time for each line scan was 0.1 s, optimized to balance signal-to-noise ratio and acquisition speed.

To validate the proposed analysis framework, inkjet-printed **ZnO nanoparticle** and **InP quantum dot (QD)** thin films were prepared as model samples. Transmission electron microscopy (TEM) images and refractive index profiles of the nanoparticles were taken, confirming particle sizes of 2–3 nm and reduced optical constants compared to their bulk forms. The air gaps between nanoparticles contribute to a lower effective refractive index ($n < 1.6$), further supporting the need for data-driven spectral interpretation.

III. Results

Prior to conducting experiments, the mutual information (MI) between reflection spectra and layer thickness was computed using the Kraskov–Stögbauer–Grassberger (KSG) estimator. Unlike traditional histogram-based MI estimators, which are highly sensitive to binning parameters and data dimensionality, the KSG estimator is non-parametric and robust against high-dimensional noise and entropy overestimation. Simulation targets included both single-layer and double-layer thin films to analyze their spectral–thickness relationships.

In this study, we aimed to estimate layer thickness using single-shot hyperspectral imaging (HSI). The model system consisted of ZnO nanoparticles with diameters of 2–3 nm. While analytical approaches can be directly applied to bulk materials with known optical constants (n and k), such constants become unreliable in nanoparticle systems due to quantum confinement effects and modified electronic density of states. Consequently, data-driven machine learning approaches offer a more practical and accurate alternative.

For QD-LED devices, two layers are generally sufficient to represent the essential structure: an emissive quantum dot (QD) layer and a ZnO-based electron transport layer (ETL). The hole injection and transport layers are typically fabricated by vacuum deposition, resulting in uniform thickness. However, solution-processed nanoparticle layers formed by inkjet printing exhibit strong thickness non-uniformity due to capillary and Marangoni effects. Although multi-solvent inks can partially suppress the coffee-ring effect, achieving complete uniformity remains difficult. Thus, a rapid, in-situ layer thickness monitoring system is urgently needed for inkjet-assisted pixelation. Current techniques such as ellipsometry offer sub-nanometer resolution but are limited by low spatial coverage and incompatibility with pixelated geometries due to sidewall obstruction.

To address these limitations, we employed a mutual information–based framework integrated with machine learning. The effectiveness of conventional reflection analysis is significantly reduced in nanomaterials because their optical constants deviate from those of their bulk counterparts. For instance, in QD-LEDs consisting of QD and ZnO nanoparticle layers, both materials exhibit altered refractive indices, rendering traditional optical models inadequate. To overcome this issue, we adopted a data-driven approach for thickness estimation using machine learning.

For simulation, we assumed constant refractive indices of $n = 2.0$ and $n = 1.6$ for the QD and ZnO layers, respectively, across the spectral range. Synthetic reflectance spectra were generated for 16 distinct ZnO thicknesses and 16 combinations of QD/ZnO double layers. The analysis wavelength range spanned from 200 to 1000 nm, producing an 800-dimensional spectral input vector. Notably, thinner ZnO layers exhibited resonance peaks shifted toward shorter wavelengths, emphasizing the importance of the UV range for sub-100 nm film analysis.

To calculate MI, three key preprocessing strategies were applied:
(1) **Dimensionality reduction**—the 800-dimensional input spectra were compressed into a 10-dimensional latent space using a denoising autoencoder (DAE), which retained essential features while minimizing redundancy and noise sensitivity.
(2) **Denoising training**—the autoencoder was trained to reconstruct clean spectra from noisy inputs, improving robustness against measurement noise.
(3) **Spectral masking**—binary masks were used to zero out specific wavelength regions, mimicking limited spectral acquisition setups and enabling evaluation of model performance under partial spectral availability.

Overall, this MI-guided, machine-learning-assisted hyperspectral approach effectively quantified the thickness-related information contained within reflectance spectra. It demonstrated the feasibility of applying HSI for nanoscale thickness estimation in multilayer nanostructures where conventional optical analysis is limited.

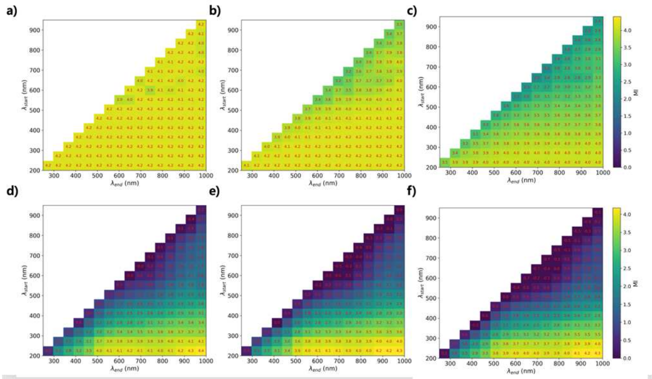

Fig. 1. Mutual information analysis of calculated reflection spectra for QD and QD/ZnO multilayers under varying noise conditions. (a–c) Mutual information maps for QD single-layer spectra under noise levels of 0% (a), 1% (b), and 3% (c). (d–f) Mutual information maps for QD/ZnO double-layer spectra under noise levels of 0% (d), 1% (e), and 3% (f). Color indicates the amount of mutual information between reflection spectra and corresponding layer thickness across spectral regions.

IV. Conclusion

In this study, we demonstrated a hyperspectral imaging (HSI)–based framework for nanometer-scale thickness analysis in multilayered nanoparticle films. By integrating mutual information (MI) theory with a denoising autoencoder (DAE) and the Kraskov–Stögbauer–Grassberger (KSG) estimator, we quantitatively evaluated the information content of reflection spectra with respect to layer thickness. The proposed approach overcomes the limitations of conventional rule-based optical modeling, which fails in nanomaterial systems where refractive indices deviate from bulk properties due to quantum confinement effects.

Simulation results revealed that reflection spectra retain sufficient thickness-dependent information even under realistic noise and limited wavelength conditions. The MI analysis identified wavelength regions most sensitive to thickness variations, providing valuable insight into spectral feature selection for data-driven models. Moreover, the DAE-based dimensionality reduction preserved essential spectral information while mitigating noise effects, ensuring robust prediction performance.

The developed HSI system—equipped with UV–Vis optics and line-scan acquisition—demonstrated its capability for high-throughput, non-contact, and spatially resolved thickness mapping of inkjet-printed ZnO and QD nanoparticle films. This framework can serve as a foundation for in situ process monitoring and uniformity control in advanced display manufacturing, where sub-nanometer precision is critical for device performance. Future work will extend this approach to complex multilayer structures and real-time optical feedback for closed-loop printing control.

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