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Ptychographic imaging ellipsometry using visible and extreme ultraviolet light

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Abstract: We show how to utilize ptychographic measurements in reflection, to obtain maps of height and complex refractive indices, using visible and extreme ultraviolet light sources. This technique enables flexible, high-resolution imaging of multi-element microstructures. © 2025 The Author(s)

Main Text

Measuring optical properties of specimen is essential in many branches of science and industry. As such, the complex refractive index manifests as one of the key properties which can be used to infer material specific composition and physical structure of the specimen. The complex refractive index defines how light propagates in the specimen. From there, other characteristics like amplitude changes and phase shifts at interfaces can be derived.

Ellipsometry has been established to be the standard measuring technique to retrieve complex refractive indices [1, p. 62]. In this technique, the reflected light from a specimen is captured, using different states of the input beam. By changing the polarization, wavelength and/or angle of incidence of the illumination, relative amplitude change and phase shifts upon reflection are measured. This approach works well for bulk materials and uniform specimen. However, with the advent of fabricated nanostructures and metamaterials that have spatially varying refractive index, a new measuring technique is required. Although combining imaging with ellipsometry is possible [2–5], setups become complex due to optical aberrations and the highly oblique incidence angles involved. Measuring spatially varying refractive indices is therefore challenging.

In this work, we propose a new approach to retrieve a map of complex refractive indices. At the core of our work, we use ptychography [6,7], which is a lensless imaging technique that uses an iterative algorithm to computationally reconstruct the specimen. Similar to ellipsometry, we perform ptychography in reflection using different polarization states and multiple angle of incidences of the illumination, as depicted in Fig. 1a). Building upon these reconstructions, we developed another algorithm that retrieves complex refractive indices.

In ptychography, a series of diffraction patterns is captured while scanning with a coherent illumination beam over a specimen. Because only intensities of the diffraction patterns are acquired, all phase information of the electric field is lost. Ptychography solves this problem by ensuring redundancy in the diffraction patterns, by having overlap when illuminating the sample such that similar features are illuminated at adjacent scanning positions. We use an iterative algorithm based on automatic differentiation (AD) [8], that models the interaction of the illumination field with the sample. A simplified forward loss function at scanning position k can be defined as

$$L_k(P,O) = \sum_{\mathbf{x}} \left| \mathscr{P}_{\lambda,\theta} \left[P_S(\mathbf{x}) \cdot O_S(\mathbf{x}-\mathbf{y}_k) \right] - \sqrt{I_k} \right|^2 , \tag{1}$$

where P and O are optimizable variables describing the illuminating probe and sample object respectively with linear polarization state S. A differentiable propagator $\mathscr{P}_{\lambda,\theta}$ forwards the exit surface wave $(P \cdot O)$ to the detector plane, where the amplitude is compared with the measured intensity I_k. Hereby the propagator has to account for the oblique angle of incidence θ and wavelength λ, with which the sample is being illuminated. Since the measurement is performed in reflection geometry, the reconstructed complex object O can be interpreted physically as relative reflectivities in the sample. As such, O encodes amplitude and phase changes that occur because of changes of the refractive index profiles from the retrieved complex reflectivity maps. An additional phase change is caused by a height variation between two spatially separated features on the sample.

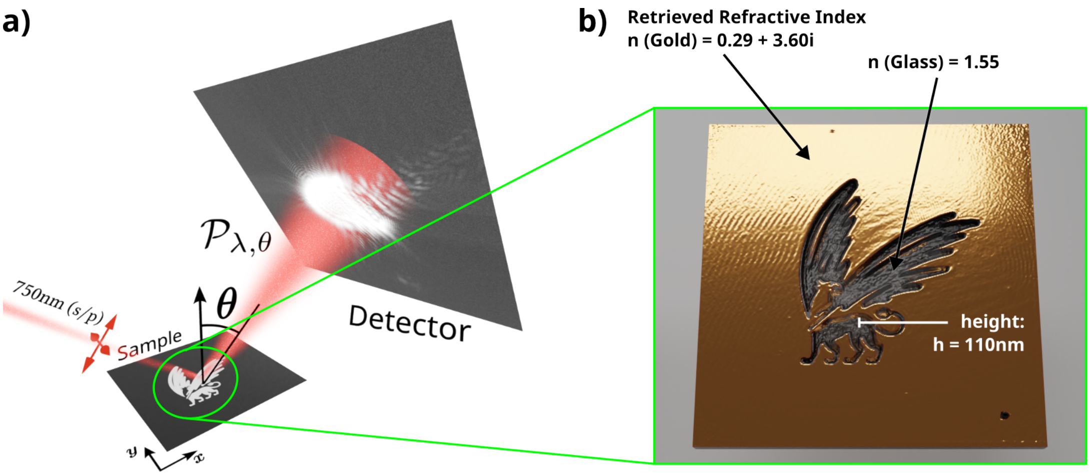

Fig. 1: a) Illustration of the experimental setup. Here a coherent light source of $\lambda = 750\,\text{nm}$ with s-/p-polarization was used. Reflection from the sample results in a diffraction pattern that is captured by the detector. b) False color 3D render of the retrieved map of refractive indices of the specimen. Side length of the square sample is 1 mm.

These amplitude and phase changes can be calculated from the Fresnel equations, provided that refractive indices and heights are known. However, it is not possible to invert these equations to obtain an analytical expression for the refractive indices. Therefore, we introduce a new differentiable loss function that compares the measured amplitude and phase changes with the theoretically estimated ones. After minimizing the loss function via automatic differentiation, we retrieve a full map of complex refractive indices plus a height map. While a measurement at a single angle in principle provides sufficient information, we overdetermine the loss function by repeating the measurement at multiple angles and polarization states, which allow more robust and precise retrieval of refractive indices. By doing Monte Carlo simulations drawing from a normal distribution around the measured reflectivities, we can assess the measurement uncertainty.

Ptychographic ellipsometry comes with advantages over conventional imaging ellipsometry. Firstly, as ptychography is a lensless imaging technique, it does not introduce aberrations caused by optical components. The absence of lenses allows imaging at oblique incidences with in principle diffraction-limited resolution. Furthermore, not relying on optical components enables ptychographic ellipsometry to work with a wide range of coherent light sources. Thus, shorter wavelengths can be used to enhance the resolution of the retrieved refractive index maps. It also allows characterizing dispersion of the sample.

In this work, we validate our implementation of the AD-based retrieval of complex refractive indices and height maps, by applying it on experimental datasets. For that, we retrieve refractive indices of a two-layer fabricated sample containing microstructures, using visible light sources ($\lambda = 750\,\text{nm}$). The retrieved map of refractive indices is visualized in Fig. 1b). Finally, we show our progress on applying this measuring technique using extreme ultraviolet (EUV) ($\lambda = 38\,\text{nm}$) from a high-harmonic generation (HHG) source. Using EUV light sources, we push spatial resolution and accuracy in height retrieval.

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