Light scattering imaging model for total internal reflection microscopy

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This talk outlines the numerical model for modelling of light scattering in Total Internal Reflection Microscopy (TIRM). This model focuses on how light scatters from an axisymmetric particle with any orientation within a layered medium [1]. In TIRM the incident light strikes the substrate at the angle larger than a critical angle and produces the evanescent wave. The scattered by a particle evanescent wave is then captured as an image [2]. To solve the scattering challenge, we employ the T-matrix method alongside the rotation addition theorem for spherical vector wave functions. The imaging of the scattered field is achieved through the Debye diffraction integral. Through numerical simulations, we identify two distinct operational modes for TIRM: the first (see Figure 1a), at an incident angle below the critical angle for total internal reflection, allows for the assessment of the particle's size and orientation; the second (see Figure 1b), at an incident angle exceeding the critical angle, is optimal for gauging the distance between the particle and the surface.

We present an analysis of the computational resources required to simulate TIRM images for particles varying in size. Additionally, we discuss the potential for creating a database of TIRM images to facilitate morphology analysis.

The original TIRM code described in [1] was parallelized that allowed us to perform a set of simulations simontaniously. We used this feature to assess the impact of uncertainties in layer thicknesses.

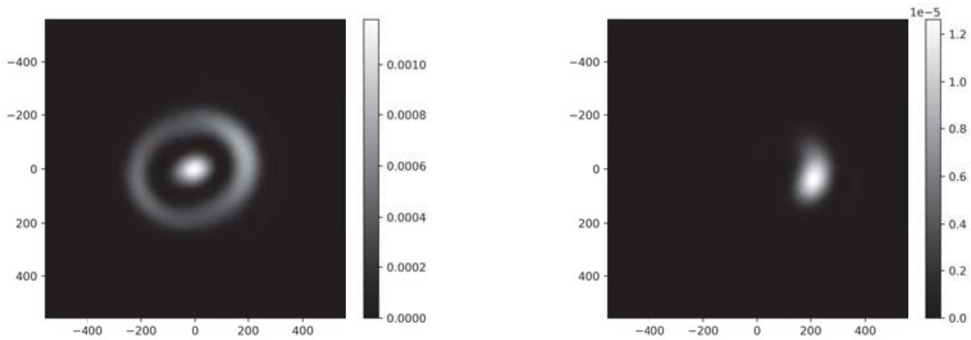
In our investigation, the model addresses the immersion layer with thickness d_{cell} and the subjacent glass slide with thickness d_{glass} coherently, implying that these elements are considered in terms of their field amplitudes. This methodology is necessitated by the imperative to precisely compute the image of the scattered field, for which the Debye diffraction integral, focusing on field amplitudes, is utilized. For coherent simulations to be deemed accurate, it is essential that the thicknesses d_{cell} and d_{glass} are determined with an accuracy that is on the order of the wavelength scale [3]. We assume that the tolerances for thickness are around 10 μm and evaluate the impact of such uncertainties in layer thickness on the detector signal. Our approach encompasses:

1. Considering d_{cell} and d_{glass} as independent random variables, each adhering to a uniform distribution,

2. Generating N_d sample pairs $d_k = (d_{\text{cell}k}, d_{\text{glass}k})$, for $k = 1, \ldots, N_d$, within the specified ranges that encapsulate their mean values, denoting mean by $\overline{d}$, tolerance by δ, and standard deviation by $\sigma = \delta/\sqrt{3}$,

3. Calculating the average of a specified energetic scattering parameter f—this could encapsulate the differential scattering cross section, the detector's integral response, or the focus intensity in image space—across these thickness samples d_k, thereby, determining $\overline{f(d)} = (1/N_d)\sum_k f(d_k)$.

Particularly, the objective is to compare $\overline{f(d)}$ with $f(\overline{d})$. In Fig. 2, the differential scattering cross sections $\overline{\sigma_{\text{X}}(d)}$ and $\sigma_{\text{X}}(\overline{d})$, where $\text{X} = \perp, \parallel$, are illustrated. In this simulation scenario, we set $N_d = 1000$, with $\overline{d}_{\text{cell}} = 2.0 \times 10^3\ \mu m$ and $\overline{d}_{\text{glass}} = 1.0 \times 10^3\ \mu m$ as the mean thicknesses, and $\delta_{\text{cell}} = \delta_{\text{glass}} = 10\,\mu m$ as the tolerances. Utilizing a Python script, which acts as a wrapper for the original Fortran model, facilitated automation in handling output files from distinct runs and generating input files for each simulation. Leveraging the parallelization capabilities of Python's joblib library, tasks were distributed across 12 servers, each outfitted with 80 cores, allowing for the simultaneous execution of approximately 960 cases. However, constraints on shared RAM limited concurrent processing to about 300 cases. The completion of the full suite of 1,000 simulations was achieved in 40 minutes. The results elucidated that $\overline{\sigma_{\mathrm{X}}(d)}$ approximates a smoothed version of $\sigma_{\mathrm{X}}(\overline{d})$, with the angular scattering profiles scrutinized by the detector closely aligning. Consequently, the integral responses of the detector are nearly identical, with $\overline{P(d)} = 22.210$ and $P(\overline{d}) = 22.227$, highlighting the model's resilience to variations in layer thickness.



a) b)

Figure 1: Simulated images of a particle with the long axis of 1.78 micron and short axis of 1.05 micron, the Euler angles of particle orientation are 160 and 30 degrees. The simulations are conducted under two conditions: a) with an angle of incidence at 0 degrees, and b) with an angle of incidence at 68.5 degrees.

References

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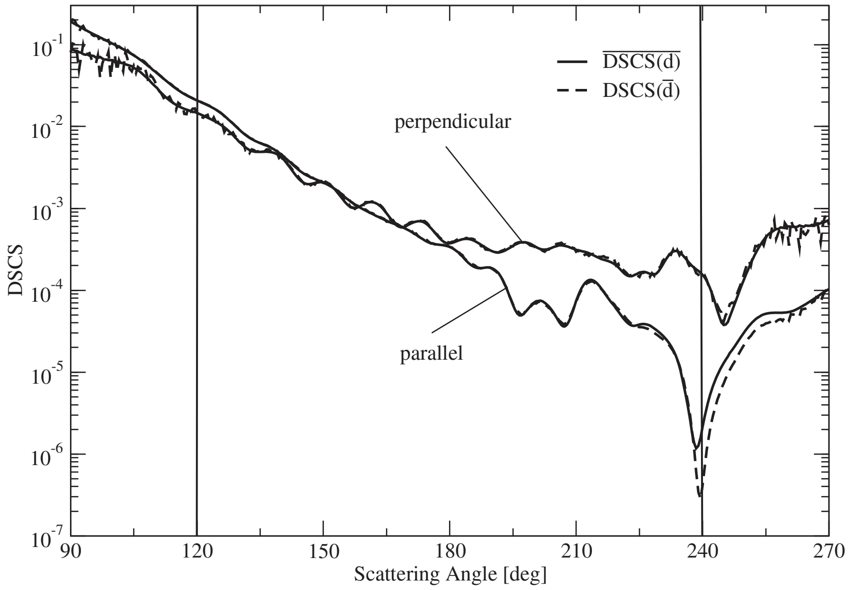

Figure 2: Example of differential scattering cross sections $\overline{\sigma_{\mathrm{X}}(d)}$ (denoted by $\overline{\mathrm{DSCS}(d)}$) and $\sigma_{\mathrm{X}}(\overline{d})$ (denoted by $\mathrm{DSCS}(\overline{d})$) for parallel and perpendicular polarizations. The vertical lines at 120° and 240° define the angular scattering domain analyzed by the detector.

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