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On the modeling of ellipsometry data at large angles of incidence using finite-difference time-domain method

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Abstract
The development of efficient finite-difference time-domain (FDTD) modeling of spectroscopic ellipsometry (SE) data can provide a versatile scheme for advanced quantitative optical characterization of samples of interest in nano-optics and plasmonics. The FDTD method offers attractive advantages due to its simplicity, generality, and natural adaptability to 3D or non-periodic structures as well as complex, for example non-linear, effects. However, FDTD modeling of SE data is challenging due to difficulties when large oblique angles of incidence (AoI), which provide increased SE sensitivity, are used. Recently, we proposed a solution to improve the accuracy of FDTD modeling of SE data at large (> 50°) AoI which was shown to work well in single wavelength calculations. Here, we demonstrate an implementation of this solution in the spectral range from 200 nm to 1400 nm found in modern UV-Vis-NIR SE instruments. The proposed correction is quantified by an spectrally averaged unbiased χ^2 error estimator between the FDTD method simulations and the theoretical SE calculations using standard Fresnel's coefficients and matrix transfer algorithm. Using prototypical Au substrates it is shown that the remaining FDTD modeling errors at 70° AoI are equivalent to an uncertainty in the sample's surface roughness of ~0.4 nm which is comparable to the FDTD model's *z*-direction resolution used in this work. These results confirm the power of FDTD method as a reliable technique to model SE data and the potential use of the FDTD-SE approach as a powerful technique for quantitative optical characterization of complex samples.