Nonlocal effective medium (NLEM) for quantitative modelling of nanoroughness in spectroscopic reflectance

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Spectroscopic reflectance is a versatile optical tool for the characterization of transparent and semi-transparent thin films in terms of thickness and refractive index. The Fresnel equations are used to interpret the measurements, but their accuracy is limited when surface roughness is present. Nano-roughness can be modelled through a discretized multi-slice and effective medium approach, but up to date this offered mostly qualitative and not quantitative accuracy. Here we introduce an adaptive and nonlocal effective medium approach, which considers relative size and environment of each discretized slice. We develop our model using finite-difference time-domain simulation results and demonstrate its ability to predict nano-roughness size and shape with relative errors < 3% in a variety of test systems. The accuracy of the model is directly compared with the prediction capabilities of the Bruggeman and Maxwell-Garnett models, highlighting its superiority. Our model is fully parametrized and ready to use for exploring the effects of roughness on the reflectance without the need for costly 3D simulations, and to be integrated in the Fresnel simulator of spectroscopic reflectance tools.