

## A software for simulation and inverse design of nanophotonic metamaterials based on periodic metasurfaces

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A metamaterial (MM) embeds a metasurface (MS). An important type of MS is a periodic-pattern one which is in fact optically thin 1D or 2D grating. Fourier-Floquet modal method for simulation of gratings, was first developed for volume gratings. Extended to surface-relief ones in 1980's, it was dubbed rigorous coupled-wave analysis (RCWA). Despite the RCWA versatility, strong evidence of its overall numerical instability, and lacking convergence was reported in 1990's. Since then, RCWA has been recasting to overcome those problems. Our RCWA recast includes: (i) original in-layer S-matrix algorithm; (ii) Fourier-factorization recast due to line- and zigzag-inverse Laurent rule  $s$ ; (iii) normal-vector method. While (i) provides numerical stability, (ii)-(iii) improve convergence. This implementation was coded with MATLAB and integrated in a constantly updated toolbox GRATOR.

MATLAB's crucial facilities comprise state-of-art linear algebra and optimization packages; its codes are highly programming efficient, and graphics includes a graphical user interface (GUI) builder.

Figure below shows the GRATOR's architecture, open for a custom user, in which 1D-G and 2D-G sub-blocs run independent codes for simulation 1D and 2D gratings. The objective functions for the inverse designs can be, depending on an application, electromagnetic (EM) fields derived quantities.

As an example, we will present the design of a perfect photo-absorption MM. It embeds a  $\text{SiO}_2$  bilayer microcavity enclosing an ultrathin, 25nm thick, Si layer, and front  $\text{Si}_3\text{N}_4$ -air and back  $\text{Si}_3\text{N}_4$ - $\text{SiO}_2$  grating on  $\text{Si}_3\text{N}_4$  layer MSs wrapping. We require this MM to absorb at the wavelength  $\lambda_0 = 0.8\mu\text{m}$  all p-polarized light input from backside at normal and obtain its structural dimensions by the design. The simulated MM's absorption band is ultranarrow with quality factor  $Q \approx 5,926$ . We visualized and analyzed the EM fields  $\mathbf{E}$ ,  $\mathbf{H}$  and Poynting vector  $\mathbf{S}$  at  $\lambda_0$ . This example demonstrates the tight confinement of the  $\mathbf{E}$ ,  $\mathbf{H}$  and singular EM power density  $\mathbf{S}$  flows bearing most topological-photonics peculiarities.