TM Wave Propagation in Optical Nanostructures with a Third-Order Nonlinear Response: Modeling and Validation with COMSOL

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Introduction

An enhanced method [1] is used for analysis of third-order nonlinearities in optical nanostructures with scalar TM (H-field) frequency domain formulation. After embedding it in COMSOL Multiphysics it is shown to produce fast and accurate results without superfluous vector E-field formalism. A standard TM representation based on cubic non-linear susceptibility $\chi^{(3)}$ results in an intractable implicit equation, but our technique alleviates this problem. In addition to a universal approach, simpler, more efficient solutions are proposed for media with $\chi^{(3)}$ having solely either the real part (lossless Kerr-type medium) or the imaginary part (non-linear absorbing medium). Combining these solutions in 2D TM regime with COMSOL RF module, we show fast and reliable simulation examples successfully validated with several alternative approaches.

First, the resulting implicit equation for the dielectric function is solved in terms of the H-field. Although a general solution can be readily obtained, it required a detailed *ad hoc* analysis depending on the linear loss (or gain) and a specific type of nonlinear effect, and goes beyond the scope of this study. Our application-specific assumptions allow for solving the problem with the Chebyshev (trigonometric) approach [2].

Use of COMSOL Multiphysics

The simulation results, performed using COMSOL Multiphysics with a scalar H-field formulation, were validated in two stages.

1D Case Validation. First, we considered a TM wave normally incident on a uniform nonlinear film. The solution obtained with the 2D scalar formulation was found to be in complete agreement with the solution obtained for a TE analog, and match well the solution based on a standard nonlinear ODE technique [3].
2D Case Validation. The solution for a representative set of 2D nanostructures was tested versus 3D full-wave simulations obtained from a much more complex vectorial FE model with the nonlinearity defined directly through E-field for the identical nanostructures. Compared with the 3D formulation, the 2D H-field formulation showed a substantially faster performance converging over a broader range of nonlinearities.

Conclusion

In summary, we present an instrumental approach to FE modeling of third-order nonlinear interactions in 2D optical nanostructures. The method blends naturally with the RF module of COMSOL Multiphysics and eliminates the need for complex and time-consuming 3D full-wave simulations in many cases of practical interest such as TM wave interaction with single-periodic plasmonic metamaterials with a third-order non-linear response. Moreover, the proposed method has a wider application that goes beyond optical nonlinear metamaterials and photonics, or even beyond nonlinear optics and substantially extends the capabilities of COMSOL for computationally demanding multiphysics modeling.

Reference

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3. H. V. Baghdasaryan and T. M. Knyazyan, "Problem of plane EM wave self-action in multilayer structure: An exact solution," *Optical and Quantum Electronics* **31**, 1059-1072 (1999).