

## TOPOLOGY OPTIMIZATION FOR THE MICROSTRUCTURE DESIGN OF PLASMONIC COMPOSITES

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### Abstract

Composites with plasmonic inclusions, such as silver-dielectric composites, exhibit extreme properties that can dramatically enhance the capability and performance of optical devices, such as a superlens [1] and optical nanocircuits [2]. For the design of such plasmonic composites, Wallén et al. [3,4] numerically investigated periodic silver-dielectric composites that demonstrate an effective permittivity of  $-1$ , for the design of a near-field superlens and composites that have extreme anisotropy. However, their designs were limited to simple inclusions, such as those with a low volume fraction circular shape, since their design method was based on mixing formulas, such as the Maxwell-Garnett mixing formula and the Rayleigh formula. To exploit the desirable properties of such composite materials to the full, a systematic design approach, such as the inverse homogenization method [5], is most efficient for designing the microstructure that forms the composite material. Inverse homogenization has been applied to many material property design problems, such as the design of materials with a negative thermal expansion coefficient, a negative Poisson's ratio, or desirable values of Young's modulus, magnetic permeability, or dielectric permittivity. In this study, a gradient-based topology optimization method is presented for the microstructure design of plasmonic two-phase composites that provide desired values of effective permittivity, including negative values.

Composite materials can be usually modeled as materials consisting of a periodic array of unit cells, and the effective properties of the overall structure can be computed using mixing formulas or homogenization methods. In this study, we use an energy-based homogenization method [6] that computes the effective properties based on the results of finite element analysis and can handle complicated inclusions in addition to the simple inclusions that classical mixing formulas can work with. The optimization problem is formulated as a problem to minimize the square of the difference between the effective permittivity and a prescribed value, or to minimize or maximize the effective permittivity when the design goal is to obtain extreme values. The optimization algorithm uses the adjoint variable method (AVM) for the sensitivity analysis and the finite element method (FEM) for solving the equilibrium and adjoint equations, respectively. A PDF-based filter and Heaviside function are used to obtain clear optimized configurations and the method of moving asymptotes (MMA) is used for updating design variables. In plasmonic materials, due to surface plasmon resonance, the electric field is markedly enhanced at the interface between the plasmonic and dielectric material, namely the structural interfaces between the negative and positive permittivity materials. To appropriately capture this phenomenon, it is important to express these interfaces exactly, so the finite element mesh is regenerated at every iteration during the optimization process here, so that the mesh accurately fits the zero iso-surface of the electric permittivity. Several design problems show that appropriate unit cell configurations that exhibit the prescribed electric permittivity can be obtained for isotropic and anisotropic design problems. The permittivity values obtained by the optimization are compared with theoretical bounds, such as Weiner's arithmetic means, harmonic means, and the Hashin-Strikman bound, and the results show that the values obtained by the proposed optimization method are in good agreement with these theoretical bounds. Finally, the near-field superlens design problem is presented to confirm the utility of the presented method.

### Reference

1. W. Cai, D. A. Genov, V. M. Shalaev, Superlens based on metal-dielectric composites, *Physical Review B*, Vol.72, (2005), 193101.
2. N. Engheta, Circuits with light at nanoscales: Optical nanocircuits inspired by metamaterials, *Science*, Vol.317, (2007), pp.1698-1702.
3. H. Wallén, H. Kettunen, A. Sihvola, Mixing formulas and plasmonic composites, *Metamaterials and Plasmonics: Fundamentals, Modelling, Applications*, NATO Science for Peace and Security Series B: Physics and Biophysics, Vol.10, No.4, (2009), pp.91-102.
4. H. Wallén, H. Kettunen, A. Sihvola, Composite near-field superlens design using mixing formulas and simulations, *Metamaterials*, Vol.3, No.3-4, (2009), pp.129-139.
5. O. Sigmund, Materials with prescribed constitutive parameters: an inverse homogenization problem, *International Journal of Solids and Structures*, Vol.31, No.17, (1994), pp.2313-2329.
6. Z. Hashin, Analysis of composite materials - a survey, *Journal of Applied Mechanics*, Vol.50, No.3, (1983), pp.481-505.