Optical Properties of Hyperbolic Metamaterials Using Density Functional Theory

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Hyperbolic metamaterials are characterized by a negative permittivity in one or two spatial dimensions. One way to achieve this is by forming a periodic array of alternating metal and dielectric layers.[1] In the frequency range where the permittivity components parallel and perpendicular to the layers have opposite signs, the isofrequency surface for the extraordinary polarization is hyperboloidal. In the limit of infinitesimal layer thickness, the effective medium theory (EMT), a phenomenological one, predicts the frequency dependence of the dielectric function of the multilayer system in terms of the corresponding functions for the bulk metal and dielectric.

To test the validity of the relations predicted by EMT, we carried out first-principles calculations, using density functional theory, on bulk BaZrO3, a dielectric, and bulk TiN, a metal, along with a system consisting of a periodic stack of alternating layers of BaZrO3 and TiN. The thickness of the dielectric and metal layers is only a few nanometers, far below the wavelength of light in the visible and near-ultraviolet range. BaZrO3 is a perovskite with a lattice constant of 0.419 nm, while TiN is face centered cubic with a lattice constant of 0.423 nm, indicating excellent lattice matching between the two structures. Electronic structure and optical properties calculations are carried out using the all-electron, full potential, linear augmented plane wave method as implemented in the WIEN2k code.[2] For bulk BaZrO3 and TiN, the dielectric function is isotropic, whereas for the stack of alternating BaZrO3 and TiN layers, it is anisotropic.

Our calculations of the permittivity components, parallel and perpendicular to the layers, show that a range of frequencies exists for which these two components have opposite signs, indicating that within this range, the multilayer system acts as a hyperbolic material. We compared our calculated frequency dependence of the permittivity components with those predicted by the effective medium theory. Although qualitative agreement is found between the results of density functional calculations and the predictions of the effective medium theory, some significant quantitative deviations are found. In future work, we will consider different dielectrics and metals that would reduce absorption losses and display hyperbolic behavior in different frequency ranges.

References:

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