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Validity of effective medium theory in multilayered hyperbolic materials

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ABSTRACT

Metal-dielectric multilayers can be designed to exhibit remarkable optical properties, including negative refraction for subwavelength superlensing. In this study, the applicability of the medium-homogenized effective medium theory (EMT) in place of multilayered thin-film optics is examined. Three metal-dielectric material and thin film thickness combinations that give rise to hyperbolic dispersion in different spectral regions are considered. In addition to investigating the radiative properties, the energy streamline method is used to determine the refraction angle and lateral displacement of rays. The electromagnetic fields inside the films are depicted to illustrate the coherent effect or the lack thereof. The radiative penetration depth is profiled to understand the effectiveness and limits of such multilayers in optical manipulation. The conditions and mechanism for the breakdown of EMT are elucidated in this case study.

1. Introduction

One-dimensional periodically stratified media, or multilayers, are often used for antireflection and wavelength-selective thermal radiation applications [1,2]. Recently, negative refraction has been demonstrated using carefully designed metal-dielectric or semiconductor multilayers due to their effective anisotropic permittivities [3–5]. It is easier to construct nonmagnetic hyperbolic metamaterials of single negative electrical permittivity, as the free electron motion is confined in one spatial direction [5]. This anisotropy of the combined homogeneous material slab is accomplished by patterning or depositing isotropic constituent layers in alternating fashion. Hyperbolic metamaterials are developed and refined to achieve sub-diffraction imaging through subwavelength nanostructures or nanofilms [6–8]. Other thermal engineering applications of hyperbolic multilayers are coherent radiative emission, electromagnetic waveguiding, and near-field thermophotovoltaic or thermal rectification [9–14].

In this study, the energy streamlines and radiative properties are closely inspected for various experimentally achieved multilayers to reevaluate and validate existing modeling assumptions. A metal-dielectric multilayer in the visible wavelengths and two semiconductor multilayers in the infrared are considered. Semiconductor multilayers consist of alternating undoped and metal-alloy layers, the latter of which the doping concentration can be tuned for desirable spectral response. The radiative behaviors are studied using the transfer matrix method (TMM) and effective medium theory (EMT). TMM is formulated using a system of linear equations for each constituent layer, with given isotropic permittivity (dielectric function) and thickness. On the other hand, EMT treats the stratified layered structure as a homogeneous medium with an effective permittivity tensor. This requires that the thicknesses of the constituent layers be much smaller than the wavelength of consideration. This work examines the radiative properties, energy streamlines, and electromagnetic fields of varying multilayer configurations and their spectral ranges. The outcomes should uncover conditions when EMT is not suitable for estimating multilayer properties, and describe the mechanisms or quantitative criteria for the breakdown of EMT in specific applications.

2. Methods

Fig. 1 illustrates the multilayers containing alternating dielectric (d) and metal (m) media. The period Λ is the sum of one of dielectric (d_d) and metal (d_m) layers' thicknesses. The incidence angle from vacuum of unity permittivity is denoted as θ_i. After N multilayer periods, the medium of outgoing rays is also a vacuum. The transfer matrix method (TMM) has been used to determine the radiative properties and spatially-varying Poynting vector in layered thin films [1,2]. In the present study, only transverse magnetic (TM) waves that may support negative refraction are considered. The Fresnel coefficients for a uniaxial medium can be obtained from Ref. [15] to modify the TMM so that each layer can be a uniaxial medium. The consecutive products of the matrix set determine the field amplitudes inside each layer by applying boundary conditions. Analytical expressions for the field amplitudes with 3 layers, the center containing a thin film, can be found in Refs. [16,17].

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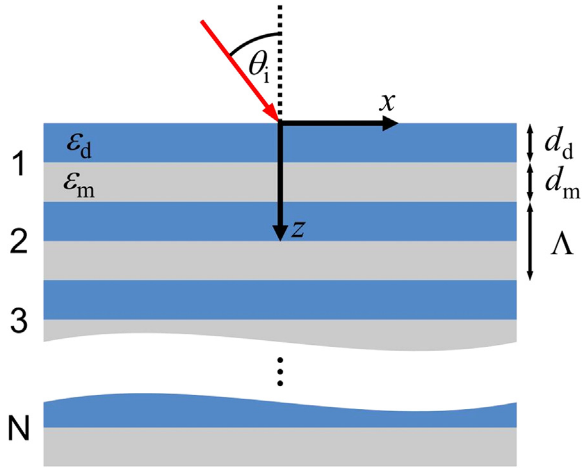

Fig. 1. Illustration of a periodic metal-dielectric multilayer. The incident and outgoing media are vacuum.

The known electric and magnetic fields are determined by applying Maxwell's equations to obtain the time-averaged Poynting vector, whose components are determined by

$$S_x = 0.5\mathrm{Re}\left(E_z \times H_y^*\right) \tag{1}$$

and

$$S_z = 0.5\mathrm{Re}\left(E_x \times H_y^*\right) \tag{2}$$

where the * signifies the Hermitian complex transform of the function. The Poynting vector is only a function of z, since the x and temporal terms are cancelled. A simple spatial extrapolation method of the Poynting vector maps the energy streamlines (ESL) [16]. The planes perpendicular to the energy streamlines represent the domain of phase fronts. The radiative properties, reflectance and transmittance, are determined by the ratios of field amplitudes.

A way to homogenize a medium into a single slab is to use EMT. For periodic multilayered structures, Rytov [18] developed analytical formulation to approximate the stratified medium with a uniaxial dielectric tensor under the condition when the wavelength of the incidence electromagnetic radiation is much longer than the unit cell, in this case defined as either d_d or d_m. The above expressions are suitable for anisotropic metal and dielectric layers as well, forming a class of hyperbolic metamaterials [19–21]. The applicability of EMT for near-field thermal radiation was discussed by Liu et al. [14]. The anisotropic permittivity of the multilayer is given in the ordinary direction (perpendicular to the optical axis along z) and extraordinary direction (parallel to optical axis), viz. [13,20],

$$\varepsilon_{\mathrm{O}} = f\varepsilon_{\mathrm{m,O}} + \left(1-f\right)\varepsilon_{\mathrm{d,O}} \tag{3}$$

and

$$\varepsilon_{\mathrm{E}} = \frac{\varepsilon_{\mathrm{m,E}}\varepsilon_{\mathrm{d,E}}}{f\varepsilon_{\mathrm{d,E}} + \left(1-f\right)\varepsilon_{\mathrm{m,E}}} \tag{4}$$

Here, the filling ratio is the quotient of the slab thickness of metal to period size ($f = d_{\mathrm{m}}/\Lambda$). Typically, the filling ratio is bounded between 0.2 and 0.8, else the radiative properties between TMM and EMT have found to diverge [20]. Since EMT is only a function of the relative constituent layer thicknesses, the period can be successively varied in the calculation to examine the validity of EMT by comparing with the calculations based on TMM.

Since metals usually possess negative permittivity, the overall permittivity of the multilayer given by Eqs. (3) and (4) may also be negative. The two equations allow two types of electrically hyperbolic dispersions: Type I and Type II. Type I is defined by $\varepsilon_{\mathrm{O}}' > 0$ and $\varepsilon_{\mathrm{E}}' < 0$ [5,19,20]. Type II is defined by $\varepsilon_{\mathrm{O}}' < 0$ and $\varepsilon_{\mathrm{E}}' > 0$. Only the anomalous dispersion in Type I hyperbolic metamaterials enable negative angle refraction of propagating waves (solely real wavevectors) inside the homogenized medium [21–23].

3. Results and Discussion

Alternating metal and dielectric layers have achieved left-handed response in visible wavelengths, which benefits toward optical waveguiding and subdiffraction imaging [5,8,11]. These simply-constructed thin films typically contain evaporated nanometers-thick metal layers over large surface areas, consisting of elements such as gold or silver [24,25]. The dielectric layers within the course of wavelengths of interest are resonance-free, thus good impedance matching with air and relatively low radiative attenuation [11]. On the other hand, instead of metal layers, which may contain enormous loss due to electron carrier absorption, semiconductor layers may be substituted in. Semiconductors are simple to deposit, and once formed, can have adjustable electron density or doping concentrations to give more or less metallic behavior [26,27]. Examples of dopable semiconductor materials are metal nitrides, silicon, germanium, indium, and many others [28,29].

3.1. *Choice of materials*

To elucidate the differences of multilayer compositions toward the radiative properties, three multilayers with known material properties are compared. Three metal- or semiconductor-dielectric multilayers are presented, with their dielectric function and Drude model parameters listed in Table 1. The first material system is a hyperbolic multilayer containing silver (Ag) and rutile (TiO_2), which was reported in Ref. [25] to demonstrate negative refraction in the UV to visible wavelengths. The fabricated structure consisted of three MDMDM units, with each layer having approximately $d_{\mathrm{d,m}} = 30$ nm in thickness. In the simplifying case presented here, the alternating unit is just DM. Equivalently, $N = 8$ according to the multilayer geometry shown in Fig. 1. Semiconductor-dielectric layers were employed in Ref. [26] in which the former material is achieved by doping zinc oxide with aluminum (AZO-ZnO). The fabricated thin film was reported to have 16 alternating layers ($N = 8$), each 60 nm thick. In this particular study, the doping concentration of the AZO layers is chosen to be 4.3×10^{20} cm^{-3}. The semiconductor substitute for metal offers tunability by means of doping, and has less loss while offering negative permittivity. Furthermore, fabrication of doped semiconductors is more integrated, and does not require very thin layer deposition. For this configuration, the semi-continuous boundary between layers is delineated and controlled by the diffusion process of dopants. Another type of semiconductor-dielectric multilayers was proposed in Ref. [27], which consist of aluminum or gallium-doped indium arsenide ($Al_{0.48}In_{0.52}As$-$In_{0.53}Ga_{0.47}As$). The

Table 1
Dielectric function and Drude model parameters of hyperbolic multilayers.

	ε_d	ε_∞	ω_{p} (rad/s)	γ (rad/s)
Ag-TiO_2 [25]	⊥6.3 − 9.1; ∥7.8 − 11.5	1.0	1.39×10^{16}	2.73×10^{13}
AlZnO-ZnO [26]	4.0	4.0	1.04×10^{15}	1.85×10^{14}
AlInAs-InGaAs [27]	10.23	12.15	2.14×10^{14}	1.00×10^{13}