Optimization of an Isotropic Metasurface on a Substrate

Zhanna O. Dombrovskaya[1] , Alexander N. Bogolyubov[2]

M.V. Lomonosov Moscow State University, Russia

E-mail: [1]dombrovskaya@physics.msu.ru; [2]bogan7@yandex.ru

Abstract Basing on the idea of regularization, we propose an actual well-posed formulation of the problem for accurate optimization of all-dielectric isotropic substrated metasurface parameters at normal incidence. The limitations caused by the specifics of the technological process and the applicability of the physical model are taken into account. The behavior of the constructed functional is discussed.

Introduction

In this paper, we consider an isotropic metafilm with period p $(2a < p \ll \lambda_0)$, composed of spherical dielectric scatterers with radius a and permittivity $\tilde{\varepsilon} = \varepsilon' + i\varepsilon''$ located at "air-dielectric" interface (permittivity ε). Such structures are widely used as light-trapping covers, in the Raman spectroscopy and other applications. Depending on the particular task, the metasurface is required to provide maximum or minimum values of the reflection, transmission or absorption coefficients. Our goal is to design the parameters p, a and $\tilde{\varepsilon}$ providing a priori given dependencies $|r(\lambda,\varepsilon)|^2$ and $|t(\lambda,\varepsilon)|^2$. This problem is ill-posed [1].

Direct and inverse problem

In contrast to three-dimensional metamaterial, metafilm is described by electric χ_{es} and magnetic χ_{ms} surface susceptibilities [2] and not by means of bulk material parameters of homogeneous layer [3]. In the case of normal incidence, the structure under consideration is characterized by the following reflection R and transmission T coefficients (temporal dependence $e^{-i\omega t}$) [4]:

$$R(\lambda,p,a,\tilde{\varepsilon},\varepsilon) = \frac{(1+e)\left(1-\sqrt{\varepsilon}m\right)-\left(\sqrt{\varepsilon}-e\right)(1+m)}{(1-e)\left(1-\sqrt{\varepsilon}m\right)+(\varepsilon-e)(1-m)}, \quad T(\lambda,p,a,\tilde{\varepsilon},\varepsilon) = \frac{(1+e)(1+m)+(1-e)(1+m)}{(1-e)\left(1-\sqrt{\varepsilon}m\right)+(\varepsilon-e)(1-m)}, \tag{174}$$

where $e = ik\chi_{es}/2$, $m = -ik\chi_{es}/2$; $k = 2\pi/\lambda$ is the wave number.
We introduce a vector $\mathbf{x} = \{p, a, \varepsilon', \varepsilon''\}$, describing the optimization parameters of the metafilm. Let $f(\lambda,\varepsilon) = |r(\lambda,\varepsilon)|^2$ be the reflectivity of the metasurface given on the interval $[\lambda_1,\lambda_2]$ for some dielectric substrate. In general, it is a given function from L_2 space, but commonly in applications it is often required to achieve maximum $f(\lambda,\varepsilon) \equiv 1$ (a perfect mirror) or minimum $f(\lambda,\varepsilon) \equiv 0$ (an anti-reflective coating) reflection. Let E_4 be a 4-dimensional vector space, C_4 is a closed convex set

$$C_4 = \left\{\mathbf{x} \in E_4 : \quad p > 2a, \quad a > 0, \quad \varepsilon'_{min} \le \varepsilon' \le \varepsilon'_{max}, \quad \varepsilon'' \ge 0\right\}. \tag{175}$$

The problem is to approximate the substrated metasurface reflectivity $R(\lambda,p,a,\tilde{\varepsilon},\varepsilon)$ provided by nonlinear operator $A(\mathbf{x},\lambda,\varepsilon) = |R(\lambda,p,a,\tilde{\varepsilon},\varepsilon)|^2$, which is described by $\mathbf{x}$-vector at C_4, to the required $f(\lambda,\varepsilon)$ within some accuracy δ,

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taking into account additional restrictions on the synthesized structure. Such a restriction may consist in obtaining the largest possible size of meta-atoms since this significantly simplifies the fabrication of identical samples. We emphasize that formulas (174) are valid only in the case of a dipole approximation. The replacement of sphere by the pair of electric and magnetic dipoles is valid for samples with $a \le \lambda_0/s$, where s is constant (i.e., for silica glass $s = 6$, see [5]), λ_0 is the wavelength of the incident monochromatic wave.
Then the inverse problem can be formulated as follows. It is required to determine the vector $\mathbf{x}$, which minimizes the functional

$$F^\beta[\mathbf{x}] = \| A(\mathbf{x},\lambda,\varepsilon) - f(\lambda,\varepsilon)\|^2_{L_2} + \beta|a - \lambda_0/s| = \min, \quad \mathbf{x} \in C_4, \tag{176}$$

where $\beta > 0$ is the regularization parameter [1], which should be chosen according to δ. From (176) we can find $\mathbf{x}$ for different values of β. Note that the operator $A(\mathbf{x},\lambda,\varepsilon)$ and the input data $f(\lambda,\varepsilon)$ are supposed to be given exactly, so the statement (176) does not take their errors into account. However, it is suitable for optimizing the geometric and material parameters of the metasurface in order to achieve the desired properties.
For isotropic substrated metafilm, operator $A(\mathbf{x},\lambda,\varepsilon)$ is given by the analytical formula from (174), therefore, for the minimization of the functional (176), we can imply numerical methods requiring its derivatives. Preliminary analysis showed that $F^\beta[\mathbf{x}]$ has a large number of local minimums. In order to find all of them, it is recommended to choose $\sim 10^4$ pseudorandom points from C_4 as initial estimates. From these minimums we choose the best one which meets additional physical and technical requirements: dielectric permittivity $\tilde{\varepsilon}$ should correspond to chemically inert substance in a solid state, meta-atoms should not be fragile, the metafilm should possess good adhesive properties in relation to the substrate, etc. The obtained minimum is not necessarily global.

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