All-dielectric metasurface filters for mid-infrared range

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Abstract. In the present work, a metasurface composed of PbTe spherical particles and located on Ge substrate is considered. We show that it acts in two anti-reflective regimes: depending on geometrical parameters of the structure, it can be a narrow or a wide-range filter. The reason is that the incident radiation excites different dipole resonances of the metasurface. For high-index dielectric materials, we obtain conditions for the validity and accuracy of the dipole approximation and the locations of dipole magnetic and electric resonances.

1. Introduction

In thermal imagers, germanium (Ge) lenses are commonly used. In the actual range from 8 to 12 μm (long-wavelength mid-infrared range), this material is attractive due to its extremely low absorption and high index $n_{\text{substr}} \approx 4.0$. This results in a great reflection from the lens. To reduce the reflection, single-layer coatings are commonly applied. The latter is a thin film, for which the optimum refractive index equals to 2. However, such a material does not exist in nature. In practice, zinc selenide (ZnSe, $n \approx 2.4$) or commercial material Irtran-2 ($n \approx 2.2$) are used. Unfortunately, they do not provide complete suppression of the reflection from the structure at any wavelength from the considered range.

An alternative approach is to apply a coating based on the metasurface [1]. This tendency seems to be promising, because with the help of the metamaterial paradigm it is possible to obtain practically any effective refractive index of the coating. In this paper we consider an anti-reflective metasurface coating composed of lead telluride (PbTe, $n \approx 5.6$) spherical particles for the air-germanium interface. Optimization of the geometric parameters of the structure was carried out and zero reflection was obtained at the wavelength $\lambda_0 = 10$ μm.

2. Structure optimization

We start with a specification of the structure under study. A semi-infinite Ge substrate is illuminated by normally incident plane wave. On the substrate there is a square array with periodicity $p$ of spherical dielectric scatterers with radius $r$. For the metaatoms PbTe material was chosen. It has one of the highest refractive indexes and also zero losses, therefore, it provides a significant field enhancement at the resonant wavelengths [2].

Our goal is to determine optimal geometrical parameters providing minimal reflection $R_s$ from the whole structure (the metasurface and the substrate). Additional restrictions on the parameters are
proposed in [3], [4]. They are associated with the fabrication process \((r \geq 50 \text{ nm}, p \geq 4r)\) and the applicability of the model (see the next paragraph).

The solution of the problem is reduced to multiple solutions of the direct problem [5], i.e., calculations of the characteristics of substrated metasurface. From one computation to another one, optimization parameters are directionally modified. It is advisable to use analytical models. Most of the modern models of metasurfaces are derived in the dipole approximation. Thereby, the question of its validity and accuracy arises.

2.1. Dipole response of spherical particles

Within the dipole approximation, each metaatom is replaced by a pair of electric and magnetic dipoles. In the present work, we verify the replacement basing on the dipole approximation (DA) validity criterion [6] (Figure 1). We show that for a high-index dielectric sphere, the dependence \(\lambda/r_{\text{max}}(n)\) is linear in the mid-infrared range (Figure 2). Here, \(r_{\text{max}}\) is the maximal radius. We have also obtained the relations describing the positions of the electric (EDR) and magnetic (MDR) dipole resonances. They agree with experimental data [7]. Note that lines of MDR and EDR are located above black one (validity of the DA), that is, they satisfy the criterion.

\[ \frac{\lambda}{r_{\text{max}}} = 1.98n + 0.37, \quad \text{EDR} \quad \left( \frac{\lambda}{r_{\text{max}}} = 1.32n + 0.87 \right) \]  

\[ \frac{\lambda}{r_{\text{max}}} = 1.35n + 0.55, \quad \text{validity of the DA} \]

\[ \lambda, \mu m \]

\[ \lambda/r_{\text{max}} \]

\[ r_{\text{max}} \]

\[ n \]

\[ m \]

\[ \text{MDR} \]

\[ \text{EDR} \]

\[ \text{validity of the DA} \]

**Figure 1.** The validity of the dipole approximation for a PbTe spherical particle. When the criterion is fulfilled the colour is white.

**Figure 2.** Line approximations of MDR \((\lambda/r_{\text{max}} = 1.98n + 0.37)\), EDR \((\lambda/r_{\text{max}} = 1.32n + 0.87)\) and the equation of the DA validity \((\lambda/r_{\text{max}} = 1.35n + 0.55)\).

2.2. Results

The properties of the whole considered structure can be well described using the uncoupled-element model [8]. The Fresnel coefficients of the metasurface are calculated within the validity domain of the dipole approximation using the model of interacting induced dipoles [9].

The results of the optimization are depicted in Figure 3. The domain of the arguments is above the dashed line (technological constraint \(p \geq 4r\)). The markers show the positions of the obtained minima. Total reflectance compensation occurs when the magnitudes are matched and the phases of the electric and magnetic dipole moments differ by \(\pi\). Figures 4-6 show the reflection spectra. The coloured lines correspond to the ranges in which the dipole approximation criterion is satisfied.

From the plots, one can see that the reflection minima can be caused by different reasons. 1) Tightly located non-resonant particles (Figure 4, magenta colour). 2) Interference between the substrate and the metafilm, the particle size is chosen to provide the first magnetic dipole resonance (Figure 5, blue colour). 3) Minimum occurring due to the magneto-electric interaction (Figure 6, red colour). Note that the latter case corresponds to the reflection compensation in the broad range. The width of the range with small reflection is determined by the positions of the dipole resonances.
For the sake of comparison, the reflection spectrum of a thin film made of Irtran-2 and placed on the same substrate is depicted (Figure 6, yellow colour). It is easy to see that using of this one-layer coating does not allow to achieve zero reflectance at 10 μm. However, it provides small reflectance in the entire range from 8 to 12 μm. On the other hand, the metasurface coating acts as a perfect high-quality filter (see blue curve) or a quite good broad filter (see red curve).

**Figure 3.** Reflectance $|R_d(p,r)|^2$ and results of the minimization of substrated metasurface at $\lambda_0 = 10 \, \mu m$.

**Figure 4.** The reflection spectrum for the obtained optimal $p$ and $r$ at non-resonant case (magenta line). Other curves are indicated on the legend.

**Figure 5.** The reflection spectra for the obtained optimal $p$ and $r$ at MDR (blue line). Other curves are indicated on the legend (Figure 4).

**Figure 6.** The reflection spectra for the obtained optimal $p$ and $r$ between EDR and MDR (red line). Yellow line corresponds to thin film coating. Other curves are indicated on the legend (Figure 4).
3. Conclusion
We consider the optimization of metasurface composed of PbTe spherical particles located on Ge substrate. The constrains on its geometric parameters are found. We show that such structure can be a perfect narrow or a good wide-range filter.

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