Metallic photonic crystals at optical wavelengths

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We theoretically study three-dimensional metallic photonic-band-gap (PBG) materials at near-infrared and optical wavelengths. Our main objective is to find the importance of absorption in the metal and the suitability of observing photonic band gaps in this structure. For that reason, we study simple cubic structures and the metallic scatterers are either cubes or interconnected metallic rods. Several different metals have been studied (aluminum, gold, copper, and silver). Copper gives the smallest absorption and aluminum is more absorptive. The isolated metallic cubes are less lossy than the connected rod structures. The calculations suggest that isolated copper scatterers are very attractive candidates for the fabrication of photonic crystals at the optical wavelengths.

There has been growing interest in the development of easily fabricated photonic-band-gap (PBG) materials operating at the optical frequencies; these are periodic dielectric materials exhibiting frequency regions where electromagnetic (EM) waves cannot propagate. The reason for the interest in PBG materials arises from the possible applications of those materials in several scientific and technical areas such as filters, waveguides, optical switches, cavities, design of more efficient lasers, etc. Most of the research effort has been concentrated on the development of two-dimensional and three-dimensional PBG materials consisting of positive and frequency-independent dielectrics because, in that case, one can neglect the possible problems related to the absorption.

There are several studies of metallic photonic crystals which are mostly concentrated at microwave, millimeterwave, and far-infrared frequencies.²⁻⁹ In those frequencies, metals act like nearly perfect reflectors with no significant absorption problems. There are certain advantages to introducing metals to photonic crystals. These include reduced size and weight, easier fabrication methods, and lower costs. A recent theoretical study suggested that a face-centeredcubic lattice of metallic scatterers can have a complete photonic band gap. 10 However, the absorption of metal was completely ignored in this study. Here, we use the transfermatrix method to study the effect of absorption of metal at the near-infrared and optical frequencies. In particular, we study a simple-cubic structure of metallic cubes or interconnected metallic rods. Aluminum, copper, gold, and silver have been used in order to study the effect of different metals on absorption. In all the cases, the lattice constant is 0.25 microns and the metallic scatterers are surrounded by air.

We utilize the frequency-dependent dielectric functions $\epsilon_1(\omega),\epsilon_2(\omega)$ for these metals that have been directly measured by Ordal et al. 11 from near-infrared to optical frequencies (1-20000 cm⁻¹). This provides a very realistic base for the photonic response of metallic structures composed of such elements. To aid the numerical calculation, the measured real and imaginary dielectric functions have been interpolated with a Drude model to yield the desired value of (ϵ_1, ϵ_2) at any frequency. The Drude dispersion model offers an excellent fit to the measured data over a wide frequency range,11

$$\epsilon_1(\omega) = \epsilon_\infty - \frac{\omega_p^2}{\omega^2 + \omega^2},\tag{1}$$

$$\epsilon_{1}(\omega) = \epsilon_{\infty} - \frac{\omega_{p}^{2}}{\omega^{2} + \omega_{\tau}^{2}}, \tag{1}$$

$$\epsilon_{2}(\omega) = \frac{\omega_{p}^{2} \omega_{r}}{\omega^{3} + \omega \omega_{\tau}^{2}}. \tag{2}$$

The plasma frequency ω_p and the damping frequency ω_τ have been tabulated in Ref. 11 by fitting the Drude dispersion model to experimental measurements. The values for ω_n and ω_{τ} are ¹¹ 3570/19.4 THz (Al), 1914/8.34 THz (Cu), 2175/6.5 THz (Au), and 2175/4.35 THz (Ag). These values fit the experimental data for (ϵ_1, ϵ_2) over frequencies from 30 to

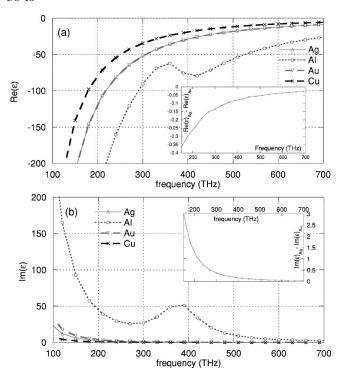


FIG. 1. Dispersion relations for Al, Ag, Au, and Cu. (a) Real part of the dielectric constant. (b) Imaginary part of the dielectric constant. The inset in both plots shows the small difference between Ag and Au.

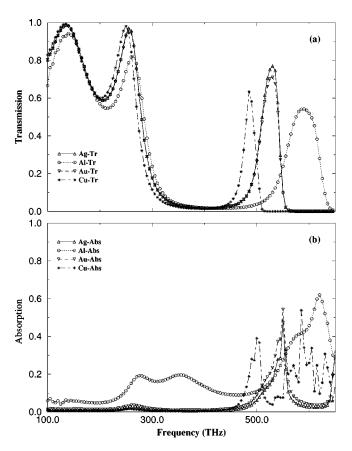


FIG. 2. Transmission and absorption for a simple-cubic structure consisting of isolated metallic cubes. The filling ratio of the cubes is 29.5%. The propagation is along the 100 direction and the structure is three unit cells thick.

900 THz, which covers the entire range of interest. The resulting dispersion relations for the real and imaginary parts of the dielectric constants of the above four metals are shown in Figs. 1(a) and 1(b).

The metallic photonic crystals studied here are the three-dimensional counterparts of frequency-selective surfaces (FSSs). These are two-dimensional arrays of metallic patches or aperture elements that have frequency filtering properties. FSSs have been studied in great detail because of their application as filters, bandpass radomes, polarizers, and mirrors in a microwave region. Most FSS work has focused on single-layer metal patterns.

We use the transfer-matrix method (TMM), introduced by Pendry and MacKinnon,¹³ to calculate the EM transmission through the PBG materials. In the TMM, the total volume of the system is divided into small cells and the fields in each cell are coupled to those in the neighboring cells. Then, the transfer matrix can be defined by relating the incident fields on one side of the PBG structure with the outgoing fields on the other side. Using the TMM, the band structure of an infinite periodic system can be calculated, but the main advantage of this method is the calculation of the transmission and reflection coefficients for EM waves of various frequencies incident on a finite thickness slab of the PBG material. In that case, the material is assumed to be periodic in the directions parallel to the interfaces.

The TMM has been used to simulate the reflection and transmission from a simple-cubic structure with metallic

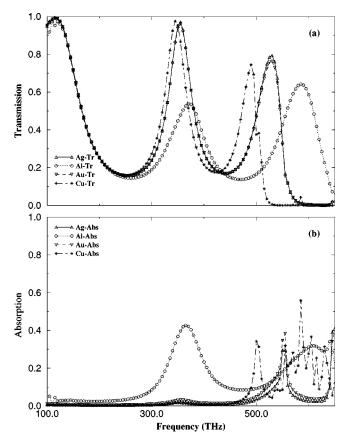


FIG. 3. Transmission and absorption for a simple-cubic structure consisting of isolated metallic cubes. Defects have been introduced in the structure by reducing the size of the cubes in the second layer. The filling ratio of the cubes is 21%. The propagation is along the (100) direction and the structure is three unit cells thick.

cubes at the lattice sites, occupying a filling fraction of 29.5%. Three unit cells are used for the thickness of the slab. The unit cell is discretized into 12 divisions, so that the three-unit-cell structure is described by a $12 \times 12 \times 36$ mesh. This mesh accurately describes the present cubes. We have checked the convergence of the calculation and found the high-frequency results to be well converged for this choice of discretization.

Figure 2 shows the transmission and absorption of a three-unit-cell-thick structure consisting of metallic cubes of 29.5% filling ratio. There is a broad drop in transmission around 400 THz for all metals. The gap is wider for aluminum where the real part of the dielectric function $|\epsilon_1(\omega)|$ has the largest absolute value at these frequencies. 11 In contrast, copper exhibits a narrower gap because it has the smaller value of $|\epsilon_1(\omega)|$. The absorption $\epsilon_2(\omega)$ is higher for aluminum generating the larger absorption feature in Fig. 1(b). The absorption for gold and copper is less than 5% for all the frequencies below the upper edge of the gap. For higher frequencies, there are peaks in the absorption which indicate that the wave penetrates more in the metal. Usually, a peak appears in the absorption close to the frequency where a peak appears in the transmission. Aluminum, however, displays a greater amount of absorption over the frequency range of the gap.

We also studied defects in a simple-cubic structure consisting of metallic cubes. Defects are introduced by reducing

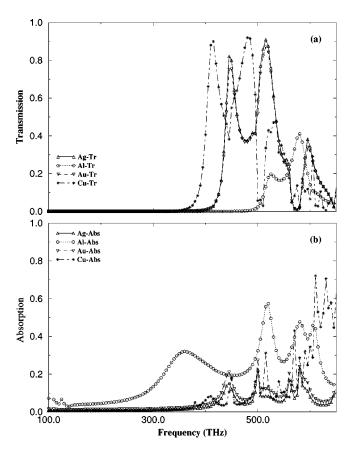


FIG. 4. Transmission and absorption for a simple-cubic structure consisting of interconnected metallic square rods. The filling ratio of the metal is 26%. The propagation is along the 100 direction and the structure is three unit cells thick.

the size of the cubes in the middle layer by 50%. This defect creates a new peak in the transmission within the gap region (Fig. 3). The origin of this peak may be a displacement of the peak at the low-frequency side of the gap [250 THz in Fig. 1(a)] to higher frequencies. The transmission at the top of the peak is 0.97, 0.95, 0.95, and 0.52 for copper, gold, silver, and aluminum, respectively. The lower transmission for aluminum is due to the higher absorption at the defect peak (Fig. 3), which is as high as 0.42 for aluminum while being less than 0.05 for copper, gold, and silver.

Figure 4 shows the transmission and absorption for the case where the metal forms a network of square rods connecting nearest neighbors in a simple-cubic lattice. The filling ratio of the metallic rods is 0.26. In that case there is a gap from zero up to a cutoff frequency in accordance with previous studies.⁵ The cutoff frequency is at 410, 510, and 520 THz for copper, gold/silver, and aluminum, respectively. This trend is again related to the real part of the dielectric constant; the higher its absolute value, the higher is the corresponding cutoff frequency. On the other hand, the absorption is higher for aluminum and smaller for copper due to the higher (lower) value of the imaginary part of the dielectric constant for aluminum (copper). For aluminum rods, there is a broad absorption feature around 375 THz, similar to the case for isolated cubes, which arises from the greater losses in aluminum compared to the other metals.

Defects in the interconnected structure are introduced by removing the metal inside a cube centered on the lattice

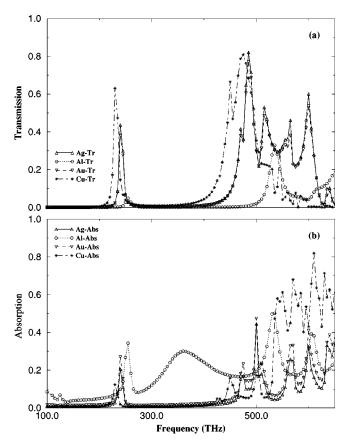


FIG. 5. Transmission and absorption for a simple-cubic structure consisting of interconnected metallic square rods with defects. The defects are created by removing the metal which is inside a cube centered in the lattice points of the second layer. The filling ratio of the metal is 21%. The propagation is along the (100) direction and the structure is three unit cells thick.

points of the second layer. Defect peaks appear in the transmission (Fig. 5) around 230 THz. The transmission on top of the peaks is 0.62, 0.43, 0.37, and 0.05 for copper, silver, gold, and aluminum, respectively. In contrast, there is an opposite trend for the absorption which is 0.1, 0.28, 0.2, and 0.35 for copper, gold, silver, and aluminum, respectively. Both of these trends are related with the higher (lower) value of the imaginary part of the dielectric constant of aluminum (copper). We found higher absorption for the connected-rods case rather than in the isolated metallic cubes. This is an expected result since the interconnected structures longrange conduction currents are induced which lead to higher losses. ¹⁴ Some improvement may be expected to use dielectric structures coated with a thin layer of metal, ¹⁵ which can lead to promising structures with gaps. ¹⁵

In conclusion, we studied metallic photonic crystals at near-infrared and optical wavelengths with the transfer-matrix method. We focused on the absorption of these structures, thus we studied the simple-cubic structure. This structure does not give the widest possible gaps but it is the simplest possible structure. We expect that our conclusions regarding the absorption will hold to any other metallic structures. By comparing the results for different metals, we found that copper gives the lowest possible absorption in all the cases. Gold gives slightly higher absorption. Aluminum

is very lossy and is not recommended for optical photonic crystals. Isolated metallic scatterers have lower losses than the interconnected metallic networks. The most promising configuration for an optical photonic crystal is the isolated metallic scatterers composed of copper. Both silver and gold are acceptable although slightly lower in performance. De-

fects in this structure introduce a narrow defect band that acts as a frequency-selective filter.

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¹For a recent review, see the articles in J. Lightwave Technol. **17**, 1728 (1999); M. M. Sigalas *et al.*, *Photonic Crystals, Encyclopedia of Electrical Engineering* (Wiley, New York, 1999), Vol. 16, p. 345.

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