Negative refraction and polarization filtering in a photonic crystal of metallic nanoshells

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Abstract

The extraordinary refractive properties of an fcc crystal of metallic nanoshells are studied by the full-electrodynamic layer-multiple-scattering method. The calculated isofrequency surfaces and corresponding group velocities show that the crystal exhibits all-angle negative refraction, which originates from the excitation of collective plasmonic modes. A thorough analysis of band structure and transmission diagrams reveals the existence of a single band extending over a narrow frequency region, which is formed from dipole plasmon modes of the individual nanoshells and can be excited, predominantly, by *p*-polarized incident light, leading to negative refraction and polarization filtering.

1. Introduction

Metallic nanoshells, dielectric spheres covered by a thin metallic shell, are studied extensively in recent years, because they combine tunability of their plasmonic resonances with relatively easy fabrication. In such nanoparticles, plasmons at the outer and inner surfaces of the shell interact with each other, giving rise to two predominant dipole hybrid modes that can be tailored by an appropriate choice of the geometric parameters involved, i.e., particle size and shell thickness. Due to their rich, easily tunable optical response, metallic nanoshells, as well as periodic assemblies of such, have been considered in numerous applications (see for example [1] and references therein). In this article we focus on fcc structures of metallic nanoshells as optical metamaterials and, more specifically, we examine the possibility of negative refraction. This behavior cannot be ascribed to the simultaneous existence of an electric and a magnetic resonance or to anisotropy, but results from the excitation of collective plasmonic modes.

2. Results and discussion

Rigorous full-electrodynamic calculations for an fcc crystal of metallic nanoshells are carried out by the layer-multiple-scattering method [2]. The dielectric function of the metallic component is assumed to have the simple Drude form, $\varepsilon_{\rm m} = 1 - \omega_{\rm p}^2 / [\omega(\omega + i\tau^{-1})]$, ($\omega_{\rm p}$ is the bulk plasma frequency and τ the relaxation time of the conduction-band electrons), which introduces $\omega_{\rm p}$ as a natural frequency unit and $c/\omega_{\rm p}$, c being the velocity of light in vacuum, as a natural length unit. The nanoshells consist of a silica core ($\varepsilon_{\rm silica} = 2.13$) of radius $S_1 = 0.7c/\omega_{\rm p}$ covered by a metallic layer of thickness $D = 0.3c/\omega_{\rm p}$. The fcc crystal is built as a sequence of (001) planes, where the nanoshells are arranged on a square lattice defined by the primitive vectors $\mathbf{a}_1 = (a_0, 0, 0)$ and $\mathbf{a}_2 = (0, a_0, 0)$. The distance between successive (001) planes is $d = a_0\sqrt{2}/2$. We take $a_0 = 3c/\omega_{\rm p}$ and disregard absorptive losses ($\tau^{-1} = 0$) for now in order to simplify the subsequent analysis.



Fig. 1: Top diagrams: Photonic band structure of the crystal under study along its [001] direction, and the corresponding transmittance at normal incidence of a slab of it consisting of eight (001) layers. Thick and thin lines in the dispersion diagram correspond to doubly degenerate and non-degenerate bands, respectively. Bottom diagrams: Photonic band structure of the crystal for $\mathbf{k}_{\parallel} = (0.24, 0.18)\pi/a_0$ and the corresponding transmittance for *p*-(black line) and *s*-polarized (gray line) incident light.

The photonic band structure of the crystal along two different directions k in reciprocal space is depicted in Fig. 1. At low frequencies it is characterized by a linear, doubly degenerate dispersion curve, as expected for propagation in a homogeneous medium. This band interacts with a flat, doubly degenerate band originating from the dipole particle-plasmon modes of the individual nanoshells and gives rise to a hybridization gap [1] about $\omega \approx 0.4\omega_{\rm p}$. These plasmon modes give a threefold degenerate state at $\mathbf{k} = \mathbf{0}$, which splits into a doubly degenerate and a non-degenerate band along the [001] direction, corresponding to modes polarized in the x - y plane and along the z direction, respectively. The non-degenerate band cannot be excited at normal incidence because of the transverse nature of the electromagnetic field, and, therefore, transmittance is negligible in the frequency region where only this band exits, as shown in Fig. 1 for a slab of the crystal consisting of eight (001) layers. On the other hand, along an arbitrary direction, e.g., for $\mathbf{k}_{\parallel} = (k_x, k_y) = (0.24, 0.18)\pi/a_0$, all bands can in principle be excited by an incident wave of any polarization. This is indeed the case in the region below the hybridization gap, where, as shown in the lower panel of Fig. 1, even in a narrow range of frequencies where only one band exists, both p and s polarizations still produce measurable transmittance. Above the gap, however, the single band extending from $0.386\omega_{\rm p}$ to $0.417\omega_{\rm p}$ is associated with free-electron oscillations along the z direction and thus can be excited, predominantly, by an electric field with a non-zero z component. Therefore only p-polarized incident light yields appreciable transmittance, which implies that this band can act as a polarization filter. At the same time, it provides negative refraction as will be demonstrated below.

In order to study the refractive properties of the crystal we calculate its isofrequency surfaces, $\omega(\mathbf{k}) = const.$, at some frequencies in the region of interest. In Fig. 2 we present the projection of such surfaces on the $k_x - k_z$ plane in the region of the single band, which has negative group velocity about $0.4\omega_p$, together with the corresponding three-dimensional isofrequency surface. In the lower panel of Fig. 2 we show a standard analysis (see for example [3]) for the determination of the propagation directions of the reflected and transmitted waves for light impinging on an interface between air and the photonic crystal. Taking into account all the physical requirements that have to be fulfilled, we see that the transmitted wave has negative x component of the group velocity, i.e., there is negative refraction.

Absorptive losses in the metallic material can be taken into account by setting $\tau^{-1} \simeq 0.002\omega_{\rm p}$ in the Drude dielectric function, a value appropriate for silver. Then all bands become complex, in the sense that all values of the wave vector acquire a small imaginary part to account for dissipative losses. In our case, the imaginary part of $k_z d/\pi$ for the relevant bands is always smaller than 0.015. This implies a propagation length of about ten lattice constants along the propagation direction.



Fig. 2: Upper panel: Isofrequency contours in the $k_x - k_z$ plane for the frequencies denoted in ω_p units, decreasing from the center outwards. The shaded rectangle marks the projection of the reduced k zone on this plane. Only the black segments of the contours correspond to propagating waves in air. The three-dimensional isofrequency surface, at $0.4\omega_p$, is also depicted. Lower panel: Wave-vector diagrams in the $k_x - k_z$ plane, at $0.4\omega_p$, in air (left) and in the photonic crystal (right). The dashed horizontal line provides the conservation of the wave-vector component parallel to the interface. Short arrows represent the incident (dark grey), reflected (light grey) and transmitted (black) wave vectors, while dashed arrows denote the corresponding group velocities. Thin arrows indicate wave vectors for which causality is violated. Negative refraction in real space is displayed in the margin.

3. Conclusion

In summary, we demonstrated the existence of a single band that characterizes the photonic band structure of an fcc crystal of metallic nanoshells in the frequency region where negative refraction occurs. By analyzing the band structure, in conjunction with corresponding transmission diagrams for finite slabs of the crystal, we showed that this band couples predominantly with *p*-polarized externally incident light, thus providing negative refraction together with polarization filtering.

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