Tailoring the photonic band splitting in metallodielectric photonic crystal superlattices

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We experimentally and theoretically investigate the influence of a structured supercell on the band splitting of one-dimensional metallodielectric photonic crystal superlattices. We show that the splitting of the photonic bands can be modified by periodic structuring of the elementary unit cell of the photonic crystal. For our investigation we constructed metallic photonic crystal superlattices by creating supercells from standard photonic crystal building blocks and arranged them at certain distances apart. The optical properties were obtained by conventional angle-resolved white-light transmission measurements.

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I. INTRODUCTION

Photonic devices based on periodically structured materials are an interesting alternative to conventional electronic devices. Enhanced speed of operation, reduced size, and lower heat losses are some of their potential advantages. The operation principle is based on a photonic band gap that can occur in photonic crystal structures.[1] It was shown that a large contrast of the refractive index and a specific structure are required to form a complete band gap in photonic crystals.[2] For modifying the photonic band edges or increasing the photonic band gap, intense theoretical and experimental work has been carried out over the last years.[3–5] Meanwhile, specific designs have been suggested to increase the photonic band gap further.[6–8] Full control over the size of the photonic band gap is mandatory for applications based on novel integrated photonic devices such as optical filters or sensors as well as for nanostructures which take advantage of slow light effects.

So far, technological problems still restrict the fabrication of high-quality three-dimensional (3D) photonic crystals for the visible frequency range. Therefore, especially 1D structures have been extensively studied, not only in the fields of nano-optics and photonic crystals but also in the field of microwave engineering, where they are called "1D photonic crystal slabs."[9,10]

In this work, we investigate the influence of periodically structured unit cells and lattice defects on the splitting of the photonic bands in 1D metallodielectric photonic crystal slabs. To advance previously published results on metallic photonic crystal superlattices (compare Ref. 11), we perform *angle-resolved* white-light transmission measurements in order to determine the dispersion relation at the center of the first Brillouin zone and deduce the size of the band gap.[12,13] This kind of photonic crystals is composed of metallic nanostructures, which can support localized electronic resonances in the form of particle plasmon polaritons as well as photonic resonances such as modes of a dielectric waveguide slab, simultaneously.[12,14] We show that the photonic band splitting of the optical modes in metallic photonic crystals can be tailored and engineered by appropriate structuring of the superlattice unit cell.

The paper is organized as follows. In Sec. II we start with the description of the sample geometries and fabrication and introduce the optical measurement technique. In Sec. III we first discuss the experimental results for transverse electric (TE) polarization. In order to exclude effects on the band splitting which are due to a modified effective refractive index, we next concentrate on a disordered grating structure as well as an incommensurable superlattice. The section is completed with the results for transverse magnetic (TM) polarization where plasmonic resonances are included. Finally, in Sec. IV we conclude our findings.

II. SAMPLES AND EXPERIMENTAL TECHNIQUES

For investigation of the photonic band splitting of 1D metallic photonic crystal superlattices, we fabricated gold nanowire arrays with a size of 100×100 μm^2 on top of a dielectric hafnium dioxide (HfO_2) slab wave guide by electron beam lithography. The HfO_2 layer ($\epsilon = 1.9$) had a height of 180 nm and was deposited on a quartz substrate. For the gold nanowire cross section we chose a height of 20 nm and a wire width of 100 nm. This geometry supports localized surface plasmon polaritons at a photon energy of $\approx$1.75 eV with dipole moments perpendicular to the wires and parallel to the surface of the waveguide slab.

The optical properties of the samples were characterized by a standard white-light transmission setup with aperture angles below 0.2°.[12] In this configuration the gold nanowires act as a grating coupler for the incidence light field with the quasiguided modes in the HfO_2 layer. The transmission of the samples is measured in an angular range of up to 4° for light propagating normal to the slab surface in the positive z direction (see Fig. 1). If the electric field of the incoming light is polarized parallel to the nanowires (TE), these modes are characterized by sharp spectral features in the extinction spectrum.

In TM polarization, where the electric field is perpendicular to the wires, the light field can excite an additional collective oscillation of the conduction band electrons in the gold nanowires. These localized electronic resonances of the compound system are so-called particle plasmon polaritons and appear as a broad peak in the extinction spectrum.

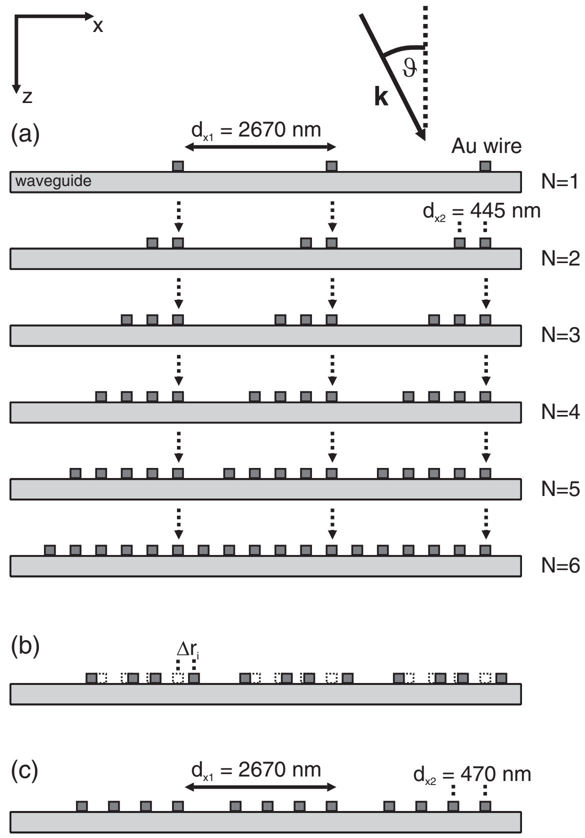

FIG. 1. Schematic view of the lattice geometry used. Gold nanowires (dark gray) are deposited on top of a dielectric slab waveguide made of HfO_2 (light gray). (a) While the superperiod $d_{x1} = 2670$ nm and the subcell period $d_{x2} = 445$ nm are kept constant in the whole sample series, the number of nanowires in each supercell is increased stepwise from one to six. The light incidence is normal to the sample surface and the angle ϑ is changed according to the sketch. (b) In the disordered structure the wires are displaced by Δr_i, while the superperiod is kept constant. (c) The incommensurable structure has the same superperiod, $d_{x1} = 2670$ nm, but a larger subcell period, $d_{x2} = 470$ nm.

However, for TM polarization this kind of 1D photonic crystal structure supports not only electronic resonances in the form of particle plasmons but also photonic resonances in the form of quasiguided TM modes in the dielectric waveguide slab. As shown by Christ *et al.*, a spectral overlap of these resonances can lead to a strong coupling among them, resulting in the formation of a waveguide plasmon polariton.[12]

A schematic view of the sample structure is shown in Fig. 1. In contrast to a simple grating structure[12,15] with one single wire per unit cell (with period d_{x2}), the superlattice unit cell (supercell) is now composed of a set of N wires.[11] By changing the number of nanowires per supercell or the subcell distance d_{x2} or by introducing defects (displacement of a wire), it is possible to change the supercell structure without changing the superperiod of the lattice.

In the first step, we investigate the band splitting of the excited modes at the center of the Brillouin zone for TE and TM polarization by increasing the number of nanowires per supercell. In this series, the superperiod d_{x1} is chosen as a multiple of the perfect subcell distance d_{x2} and the structure becomes commensurable. We show that the increased band splitting is a direct consequence of the subcell periodicity, that is, the structure factor of the lattice. To confirm this, we investigate a structure where defects in the wire positions are introduced in a second step. The metallic photonic crystal structures used are singly periodic with a superperiod d_{x1}, whereas the periodicity of the subcell d_{x2} is destroyed by inserting defects (displacement or missing of nanowires). The degree to which the subcell periodicity is destroyed can be effectively controlled by the relative strengths of the inserted defects.[11] In a further confirmation step we change the subcell distance so that the superperiod d_{x1} is no longer a multiple of d_{x2} and the structure becomes incommensurable.

To determine the photonic band splitting of the excited modes, which can be identified by peaks in the extinction spectrum, we changed the angle ϑ of incidence of the light from 0° to 4°. Although the smallest gap between the waveguide mode bands appears for normal light incidence, it is not possible to extract the spectral position of the antisymmetric band-edge eigenstate for the excited quasiguided waveguide mode because it cannot be excited at normal light incidence.[12] However, a small variation of the angle of incidence is sufficient and the antisymmetric mode appears in the spectrum. As an example, the measured and calculated extinction spectra for a superlattice structure with four nanowires per supercell ($N = 4$ in Fig. 1) are shown in Fig. 2. For normal light incidence ($\vartheta = 0°$) and TE polarization, only a single peak in the extinction spectrum is visible in the displayed spectral region. In comparison to Ref. 11 this peak appears due to the excitation of the symmetric band-edge eigenstate of the sixth Bragg resonance of the superlattice. A second peak, that is, the antisymmetric band-edge eigenstate, immediately arises below the resonance when ϑ is increased to 0.5°. For TM polarization the quasiguided TM mode of the waveguide slab and the particle plasmon polaritons in the gold nanowires form a waveguide plasmon polariton which is characterized by the two strong peaks at 1.65 and 1.9 eV in the lowermost spectrum in Fig. 2(c). The third peak, at 1.55 eV, is due to the excitation of the fifth Bragg resonance of the superlattice. Since the

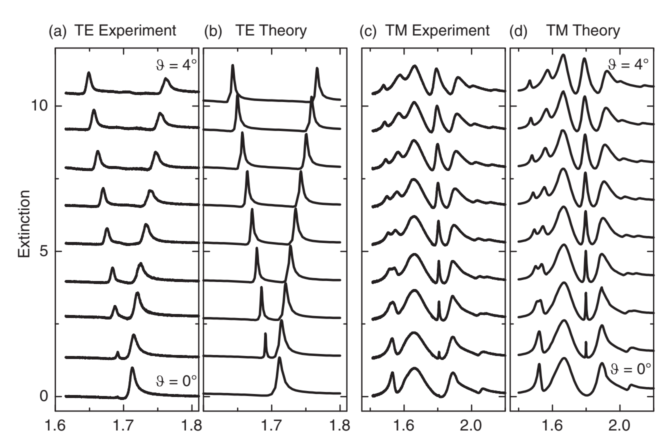

FIG. 2. Measured (a,c) and calculated (b,d) extinction spectra for a superlattice structure with $N = 4$ nanowires per supercell. From bottom to top, the angle of incidence ϑ was changed from 0° to 4° in steps of 0.5°. The spectra are shifted for better visibility.

energy of this mode is off resonant to the plasmon modes at 1.9 eV, it couples only weakly to the localized plasmons for normal incidence. Coupling of the particle plasmon polaritons with the two-band-edge eigenstate of the quasiguide TM slab mode results in the formation of three new eigenstates (dressed states), whereas only two are visible for normal light incidence. However, the third mode becomes visible for angles ϑ which are nonzero. For a detailed description of this behavior, see Ref. 12. All theoretical spectra in this work are obtained using a scattering matrix formalism.[16]

III. RESULTS AND DISCUSSION

A. TE polarization

We start the discussion with the superlattice structures shown in Fig. 1. For this series it is important to mention that the superperiod d_{x1} is an exact multiple of the introduced subcell distance d_{x2} and the structure is commensurable. By adding single nanowires into the supercell we change the structure factor of the elementary unit cell and hence the overall interaction of the quasiguided modes in the slab with the wires within one supercell.[11] As discussed in Sec. II, the influence of the structure factor on the mode splitting is not apparent for normal light incidence. Consequently, we measured the extinction of the samples for several angles of incidence and extracted the positions of the modes by taking the peak positions in the extinction spectrum. Since the peaks in the extinction spectra correspond to resonances with a Fano lineshape,[17] the spectral position of the underlying mode does not exactly match the maximum in the extinction.[18] However, the error is small compared to the linewidth and the coupling strength of the resonances in our system. Due to a limitation of our white-light transmission setup, the smallest angle change we can resolve is $\vartheta = 0.5^\circ$.

The results of the measured peak positions for TE polarization in dependence on the angle of incidence are shown in Fig. 3. We limit our discussion to the small angle region of $\vartheta \leqslant 4^\circ$ because the smallest band gap between the quasiguided modes occurs for angles near 0 at the center of the Brillouin zone. Due to the mirror symmetry of the lattice, only the values for positive angles are shown in Fig. 3. For only one single nanowire per supercell ($N = 1$) and $\vartheta = 0.5^\circ$, the band gap between the modes is around 13 meV. If the number of nanowires per supercell is increased, also the splitting between the modes increases. For $N = 6$ the splitting between the modes at $\vartheta = 0.5^\circ$ has more than doubled. In contrast to small angles around 0, the splitting of the modes for angles above 2° seems to be unchanged. For larger angles the mode position is determined by the dispersion relation. Only at the center and the edge of the Brillouin zone, where the modes would have the same energy, does the splitting of the modes due to coupling become visible. Additionally, we calculated the extinction spectra for $\vartheta = 0.1^\circ$ to estimate the mode splitting and therefore the real photonic band-gap size. The results are shown as the shaded region in each curve. One can clearly see that the band splitting of the TE bands strongly depends on the structure of the supercell. The slight shift in the mode positions to higher energies for larger N is due to a change in the effective refractive index of the waveguide slab when additional gold nanowiresd are added.

For the complete sample series, the measured and calculated band splitting at the center of the Brillouin zone for the TE modes and $\vartheta = 0.5^\circ$ are shown in Fig. 4. It is obvious that the splitting increases with the number of wires per supercell, although the superperiod of the lattice is constant. This is related to the changed structure factor of the lattice geometry. In analogy to the nearly free electron model in the band structure theory of solids, the new structure factor leads to an increased overall interaction of the quasiguided modes with the wires within one supercell and hence a stronger splitting of the bands in the metallic photonic crystal. All calculated values for the splitting at $\vartheta = 0.5^\circ$ are in good agreement with the measurements. Minor mismatches can be explained by imperfections of the real grating structure (small variations in the period by fabrication tolerances and surface roughness) and the limited number of illuminated supercells ($\approx$20) due to the finite beam diameter in the experiment. All these effects will lead to a reduced interaction of the modes with the wires, that is, to a changed structure factor in comparison with a perfect lattice.

Figure 4 additionally shows the calculated splitting of the TE bands for $\vartheta = 0.1^\circ$, which gives a good approximation of the band gap in our structures. The splitting between the modes increases linearly with the number of the nanowires in the supercell. Compared to the structure with $N = 1$, the band gap is increased by a factor of nearly 5 for the

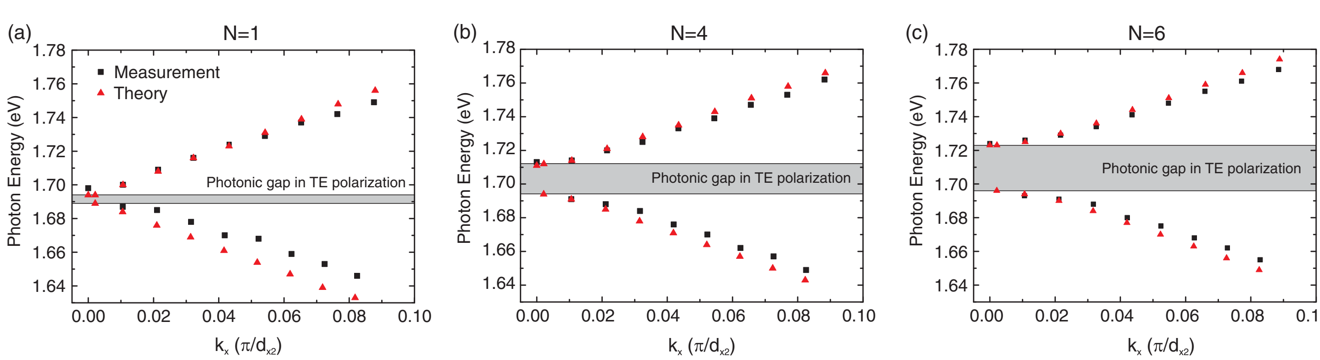

FIG. 3. (Color online) (a–c) Measured (squares) and calculated (triangles) positions of the extinction spectra maxima of the lowest energy TE modes of the metallic photonic crystal superlattice structure with $N = 1$, $N = 4$, and $N = 6$ nanowires per supercell. The shaded region marks the photonic band gap for each structure.

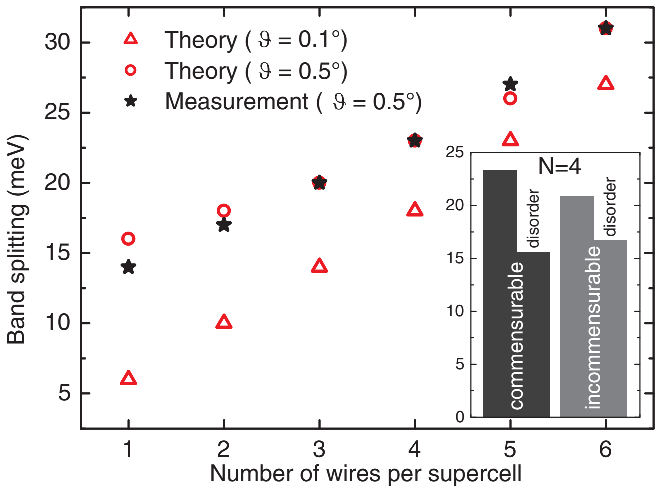

FIG. 4. (Color online) Measured (stars) and calculated (circles) photonic band splitting of TE modes for an angle of incidence of $\vartheta = 0.5^\circ$. For an approximation of the splitting for nearly normal light incidence, the calculated values for $\vartheta = 0.1^\circ$ are shown (triangles). Inset: Comparison of the band splittings for $N = 4$ wires according to Table I.

supercell with $N = 6$. Such an increase in band splitting was expected from the simple empty lattice approximation calculations [see Fig. 2(b) in Ref. 11]. However, with the presented angle-resolved measurements, this increased band splitting can indeed be observed.

B. Disordered and incommensurable structures

To exclude that the variation in band splitting in our structures is due to the modified effective index contrast based on the changed filling ration of gold nanowires on top of the waveguide surface, we measured and calculated the splitting for a second series of structures with varied positions of the nanowires. Therefore we chose the superlattice geometry with four wires per supercell and introduced periodic defects (random displacements) in the nanowire positions [see Fig. 1(b)].[11,19] One set of four random displacements Δr_i ($i = 1,2,\ldots,4$) of the wires from its original position was calculated by $\Delta r_i = 0.5 d_{x2}\mathrm{RND}(i)$, where RND is a random number of a uniform distribution (-1 to 1). The maximum displacement was limited to half a period of the subcell in order to avoid a crossing of the nanowires. The same set of Δr_i was used for each supercell in the whole structure. For this special kind of periodic defects the subcell periodicity d_{x2} is destroyed, whereas the supercell period d_{x1} and the grating filling factor are unchanged.

For the structure with four wires per supercell and a subcell period $d_{x2} = 445$ nm (which makes the structure commensurable and d_{x1} a multiple integer of d_{x2}), we found that the splitting of the TE bands is reduced by a factor of 1.5 when the subcell period is destroyed. The values for the TE band splitting are listed in Table I.

In the next step we used the slightly changed subcell period of 470 nm [Fig. 1(c)]. The number of nanowires and the supercell period were kept fixed ($N = 4$, $d_{x1} = 2670$ nm). Now the supercell period was no longer a multiple of d_{x2} and the structure was incommensurable. The calculated spectra indicate that the splitting for this structure was reduced by ≈10% compared to the structure with $d_{x2} = 445$ nm. Again, we introduced the same periodic defects (displacements) in the positions of the wires. We found that the splitting was further decreased by ≈20%. Table I and the inset in Fig. 4 summarize the values obtained for the band splitting. Because the same number of nanowires (same filling factor of the metal grating) and the same supercell period were used, the effective index contrast is constant in all four structures. Therefore, the change in the photonic band splitting has to be caused by the modified structure factor of the supercells.

TABLE I. Measured and calculated band splitting for TE polarization, a superperiod of $d_{x1} = 2670$ nm, $\vartheta = 0.5^\circ$, and four wires per supercell.

Subcell period d_{x2} (nm)	Commensurable	Disorder	TE splitting (meV) Expt.	TE splitting (meV) Theory
445	Yes	No	23.4	23.4
445	Yes	Yes	15.6	15.5
470	No	No	20.9	20.1
470	No	Yes	16.8	16.7

C. TM polarization

Finally, we investigate the splitting of the bands for TM polarization, where the electric field of the incoming light is perpendicular to the gold nanowires. For this polarization the coupling of the quasiguided modes to the particle plasmon polariton resonances leads to a triplet of eigenstates at the center of the Brillouin zone, where two branches of the polariton are visible as peaks in the extinction spectrum for normal light incidence (for a detailed discussion see Refs. 12 and 15).

All measurements were conducted by changing the angle of incidence again between 0° and 4°, with a resolution of 0.5°. The excitation and the splitting of the quasiguided TM modes of the waveguide slab are analogous to those in the TE case described above. For this reason, we focus our discussion on the coupling efficiency between the resonances and hence on the splitting of the polariton branches in the spectrum.

As shown by Christ *et al.*, a complete in-plane band gap in such a 1D metallic photonic crystal can be obtained by appropriate structuring of the sample.[12] Thereby, the important fact is the extremely large Rabi splitting between the polariton branches that can be spectrally overlapped with the existing band gap in TE polarization. The splitting of the polariton depends on the coupling strength of the quasiguided modes with the particle plasmon polaritons in the nanowires. One possibility for altering the coupling between the resonances is to change the mode overlap of the particle plasmon polaritons with the quasiguided modes.[20] This can be easily done by modifying the structure factor of the nanowire lattice.[11]

For experimental verification of the modified coupling strength we once more used the superlattice structure shown in Fig. 1. Now the extinction spectra are recorded for TM

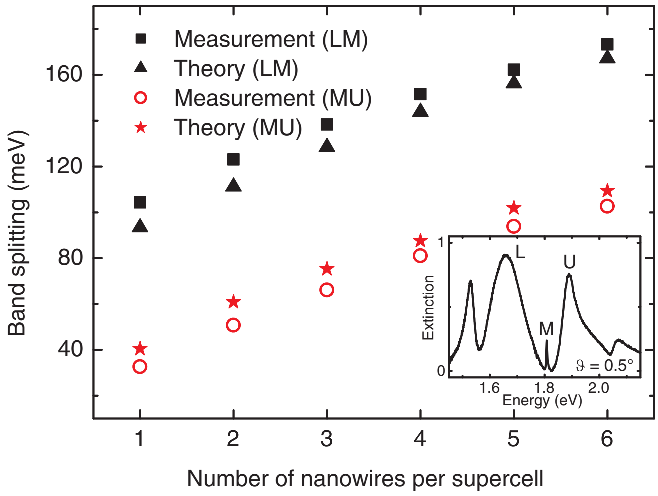

FIG. 5. (Color online) Measured and calculated photonic band splitting of the three polariton branches in TM polarization for an angle of incidence of $\vartheta = 0.5^\circ$: see the legend. Inset: Measured extinction spectrum in TM polarization for $N = 4$ together with the labels of the three polariton branches.

polarization. Figure 5 shows the extracted spectral positions of the extinction maxima for an angle of incidence of 0.5°. We plot the size of the band splitting between the lower and the middle polariton branch (LM) as well as the gap size between the middle and the upper polariton branch (MU). We observe the same behavior as in TE polarization. The gap between the branches increases nearly linearly with the number of wires in the unit cell. For six wires in the unit cell the MU gap is increased by a factor of 2 compared to the single-wire subcell. The size of the band gap in TM polarization is a direct consequence of the mode overlap of the particle plasmon polaritons in the gold wires and the electric field in the waveguide. Since the coupling of the two fundamental modes is proportional to the mode overlap, the band gap increases linearly with the number of wires.[13,21] The simulations again agree well with the experimental data, although the gap size is always slightly larger in the simulations, possibly due to the fabrication tolerances and higher loss in the system.

IV. CONCLUSION

In this paper we have shown how the band gap in a 1D metallic photonic crystal superlattice structure can be tailored by changing the structure of the unit cell. The band gap increases nearly linearly with the number of wires in the unit cell in both TE and TM polarization. In a control experiment using disordered and incommensurable structures, we verify that the band gap increase is not due to effective refractive index changes. We confirm all our results by scattering matrix calculations. Our investigations show a different approach to the design of optical band-gap structures based on plasmonic crystals and might help in the future design of all-optical integrated photonic devices such as optical filters, slow light devices, and sensors.

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