Resonant Bragg quantum wells in hybrid photonic crystals: optical properties and applications

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Abstract

The exciton–polariton propagation in resonant hybrid periodic stacks of isotropic/anisotropic layers, with misaligned in-plane anisotropy and Bragg photon frequency in resonance with Wannier exciton of 2D quantum wells is studied by self-consistent theory and in the effective mass approximation. The optical tailoring of this new class of resonant Bragg reflectors, where the structural periodicity of a multi-layer drives the in-plane optical \( \hat{C} \)-axis orientation, is computed for symmetric and asymmetric elementary cells by conserving strong radiation–matter coupling and photonic band-gaps. The optical response computation, on a finite cluster of \( N \)-asymmetric elementary cells, shows anomalous exciton–polariton propagation and absorbance properties strongly dependent on the incident wave polarizations. Finally, the behaviour of the so-called intermediate dispersion curves, close to the unperturbed exciton resonance, and located between upper and lower branches of the first band gap, is studied as a function of the in-plane \( \hat{C} \)-axis orientation. This latter optical property is promising for storing exciton–polariton impulses in this kind of Bragg reflector.

Keywords: polaritons, hybrid photonic crystals, Bragg cavity

1. Introduction

The manipulation of optical properties in order to obtain coherent radiative coupling among a collection of emissive species was proposed by R.H. Dicke [1] in 1954. The Wannier exciton is intrinsically a giant dipole excitation, since the microscopic dipole transitions of the elementary cells of a semiconductor are coherently coupled in a volume determined by its Bohr radius [2]. Moreover, if \( N \) emitters (excitons) are arranged periodically in an homogeneous dielectric background, with emission wavelength equal to twice the spatial periodicity, a new collective coherent state (superradiance mode) originates in the system for \( N \) from one to a critical value, where the \( N \)-oscillator strengths come to be redistributed on all the levels of the system [3–5], called the resonant photonic Bragg reflector (RPBR). Since in the super-radiant regime the strength of \( N \)-oscillators concentrates in a single state, the radiation–matter interaction increases by increasing the number of quantum wells, and therefore polariton splitting energy can overcome the total broadening of the system giving the so-called strong coupling regime [5–15].

The study of anisotropic photonic crystals, obtained by alternating different uniaxial layers (or isotropic/anisotropic layers), is largely present in the recent literature due to new interesting optical properties [16, 17]. For instance, in a periodic system obtained by alternating uniaxial bilayers, with different orientation of the in-plane optical \( \hat{C} \)-axis, it was demonstrated that a band gap can be opened inside the Brillouin zone [17]. In fact, while the destructive interference between forward and backward propagation of ordinary or extraordinary waves still remains at the border of the Brillouin zone, the interference between different kinds of waves can be located in a different position and, in this case, the band curvature indicates the possibility of negative refraction [17].

Recently, the RPBR has becomes an important tool for the control and manipulation of light. Yang et al[12] proposed the stopping, storing and releasing of light in these systems; this effect is based on the parametric manipulation of the exciton resonance, and practical limitations for its
realization, due to the large number of quantum wells present in the cluster \((N > 200)\), were also discussed.

The recent improvements on plasma-assisted molecular-beam epitaxy [18] allowed the growth of structures with in-plane optical \(\hat{C}\)-axis: In fact, on a substrate of \(\gamma\)-LiAlO\(_2\)(100) was deposited a buffer of 1 \(\mu\)m of GaN (1100) and 15 quantum wells of AlGaN/GaN with in-plane optical \(\hat{C}\) axis. Moreover, it is well known that isotropic Bragg structures also become optically anisotropic when submitted to an intense mechanical constrain and, an hybrid material can be obtained also by encapsulating liquid crystals in a solid isotropic periodic structure. In conclusion, the present technology is not very far from realizing complex multilayer with in-plane \(\hat{C}\)-axis orientation.

The present work is devoted to studying the optical response of a new class of resonant hybrid Bragg reflectors, where two periodicities, the background dielectric constant modulation and the optical \(\hat{C}\)-axis modulation, are present. These systems can combine the optical properties of the isotropic resonant quantum confined systems (super-radiance, strong radiation–matter interaction, spatial dispersion effects, etc) with those observed in anisotropic multilayers (high photon density of states, negative refraction, photonic gap inside the Brillouin zone, etc).

The aim of the present work is twofold: (a) to study, for selected physical parameter values, the exciton–polariton propagation in resonant hybrid Bragg reflector stacks with N-symmetric and-asymmetric elementary cells under strong radiation–matter interaction, and (b) to investigate the dispersion curves, as a function of \(\hat{C}\)-axis orientation, in the lowest energy photonic stop band, in order to elucidate the behaviour of the so-called intermediate exciton–polariton dispersion curves (IDC) close to the unperturbed exciton resonance.

The plan of the work is summarized in the following sections. In section 2 the procedure for computing the optical response of resonant hybrid Bragg reflectors is presented. In section 3 the optical response for a finite resonant hybrid Bragg reflector, with in-plane \(\hat{C}\)-axis, is computed and photonic band gaps are observed for symmetric and asymmetric elementary cells. In the present calculation we study the absorbance properties of the so-called ‘high quality’ quantum wells (QWs) at low temperature \((T < 10 \text{ K})\), due to the radiative and non-radiative homogeneous broadening contributions. In section 4, the dispersion curves \((N \rightarrow \infty)\) are presented for non-radiative broadening value \(\Gamma_{nr} \rightarrow 0\) and the behaviour of the IDC will be discussed in comparison with the correspondent isotropic case [3, 5, 9]. The conclusions are summarized in section 5.

2. Theory

The exciton–polariton propagation is computed for a resonant hybrid Bragg reflector, of \(N\) elementary cells composed by a 2D quantum well located in an isotropic \(\lambda/4\) layer, and by two uniaxial layers (left and right) of equal \(\lambda/8\) thicknesses, with in-plane \(\hat{C}_\alpha\)-axis \((\alpha = L, R)\), as schematically reported in figure 1. Notice that in the cluster two surface quantum wells are also present.

The study of photonic dielectric gap and super-radiant exciton–polariton mode building up is performed by self-consistent calculation and in the effective mass approximation [2, 5, 15]. A standard method based on Green functions and the transfer matrix approach is adopted for numerical calculation, and all formulas, explicitly given in the appendices, are of analytical form since the calculations are based on the simple \(4 \times 4\) matrices algebra. Notice that for the angle between the two optical axes different from \(\alpha = n\pi/2\) \((n = 0, 1, 2, \ldots)\), giant transmission band resonance and degenerate band edge can be observed [16]; moreover the direct energy gaps can be located inside the Brillouin zone [17].

In the present study the use of a non-local self-consistent framework is mandatory for a correct estimation of the radiative self-energy, whose imaginary part, complemented with non-radiative homogeneous broadening (usually derived from the experiments), allows us to assess the reach of the strong coupling regime in the radiation–matter interaction [2]. Moreover, it gives a quantitative estimation of the absorbance spectra in ‘high quality’ quantum wells at low temperature, where the non-homogeneous broadening is negligible.

In order to obtain a heavy-hole optically isotropic Wannier exciton in the anisotropic super-lattice, we have to minimize the envelope function penetration depths into the uniaxial layers and also the effect of the image potential on the exciton dipole, due to the presence of different uniaxial layers at both sides of the quantum well [19] (see figure 1). The former requirement is accomplished by considering a heavy-hole Wannier exciton perfectly confined into a 2D quantum well, and clad between two rather large, with respect to the exciton Bohr radius, isotropic barriers. The latter requirement is obtained by taking the background dielectric

![Figure 1](image-url)
constant equal for the well and isotropic barriers \((\varepsilon_b = \varepsilon_w)\), and moreover, is not very different in value from the orthogonal \((\varepsilon_L)\) and parallel \((\varepsilon_i)\) dielectric constants of the uniaxial layers.

The most interesting optical properties of anisotropic photonic crystal are due to the possibility of rearrangement of band structures by the misalignment of the optical axes; moreover, for in-plane optical axes, the direct absolute gaps drop inside the Brillouin zone, and this strongly influences the resonant exciton–polariton propagation, as will be demonstrated by the calculations in finite hybrid multilayer stacks with \(N = 32\) asymmetric elementary cells. The optical response in finite clusters will be also compared with the corresponding dispersion curves (for \(N \rightarrow \infty\)). In order to simplify the optical tailoring, in a periodic hybrid multilayer with asymmetric elementary cell, we have chosen equal layer thicknesses \(\lambda/4 = \pi \hbar / (2 \sqrt{\varepsilon_i} E_{\text{ex}}(0))\), and symmetric background dielectric constant values \((\varepsilon_\perp < \varepsilon_b < \varepsilon_i)\) and \(\varepsilon = (\varepsilon_\perp + \varepsilon_i)/2 \approx \varepsilon_b\). Notice that while the first condition \((\varepsilon_\perp < \varepsilon_b < \varepsilon_i)\) determines the uniaxial symmetry (the so-called 'positive optical group'), the second one can be removed, without strong qualitative variation on the optical properties.

In the present calculation we use parameter values largely present in the literature. The quantum well parameters are close to the InGaAs/AlGaAs/GaAs(001) semiconductor materials, namely: exciton total mass \(M = 0.524\), exciton Bohr radius \(a_B = 8.047\) nm and background dielectric constants: \(\varepsilon_w = \varepsilon_b = 10.24\). In all the cases the used well width is \(L_w = 10\) nm.

The exciton transition energy is computed as \(E_{\text{ex}}(K_i) = E_{\text{ex}}(0) + \hbar^2 K_i^2/2 M\), where \(K_i\) is the centre-of-mass wave vector that, in the present calculation, has been chosen parallel to the \(x\)-axis while \(E_{\text{ex}}(0) = 1.418\) eV is the variational energy of the exciton confined between infinite potential barriers.

The homogeneous non-radiative broadening \(\Gamma_{\text{NR}}\) is chosen close to the value experimentally observed in high-quality quantum wells at rather low temperature \([15]\): \(\Gamma_{\text{NR}} = 0.25\) meV for \(T \approx 10\) K. Finally, in order to minimize the Fabry–Perot oscillations due to the vacuum/semiconductor background dielectric mismatch, which strongly perturb exciton–polariton propagation \([5, 9]\), the 1D cluster is clad between two isotropic semi-infinite bulk materials with \(\varepsilon_b\) background dielectric constant. Notice that the same result can be obtained experimentally by an anti-reflection coating deposited on both surfaces of the sample.

### 3. Optical response of photonic hybrid cluster

Let us consider the optical response of a resonant hybrid Bragg reflector, composed by \(N = 32\) elementary cells with \(z\)-axis along the periodicity and \((x, y)\) in-plane coordinates, for incident wave polarized \(S\) and \(P\), and in-plane optical \(\hat{C}\)-axis of the uniaxial slabs \((\alpha_L, \alpha_R)\) as shown in figure 1. At first, we have taken \(n_L = n_b = 3.2\) and \(n_I = 3.5\) respectively, and both the \(\hat{C}\)-axes parallel \((\alpha_L = \alpha_R = \alpha)\), in order to obtain a symmetric elementary cell; this preliminary choice elucidates the role of the \(\hat{C}\)-axis orientation and makes simple the optical tailoring. For normal incident \(P\)-polarized wave and \(\hat{C}\)-axes of the two uniaxial layers parallel to the \(x\)-axis, the Bragg energy \(\hbar\omega_0\) of the reflection stop band is in resonance with the exciton energy \((\hbar\omega_0 \approx E_{\text{ex}}(0) = 1.418\) eV) if the thicknesses of the isotropic layers are set equal to \(\lambda/4 = \pi \hbar/(2\omega_{\chi w} n_i)\) and those of the uniaxial layers equal to \(\lambda/8 = \pi \hbar/(4\omega_{\chi w} n_i)\) respectively.

In figure 2(a) we observe a reflection central deep, very close to the exciton energy, an intense absorbance peak \((I_\alpha \approx 88\%)\), and a broad photonic stop band of \(\Delta \omega(q_y = 0) = 101\) meV (full width at half maximum) \([4, 5]\) since the dielectric resonant modulation of the multilayer is due to the \(\varepsilon_i\) dielectric constant and to the dispersive component of the exciton susceptibility. In figure 2(b), given in enlarged energy scale, the spectrum is computed for \(\hat{C}\)-axis orientation along the \(y\)-axis \((\alpha = \pi/2)\): in this case, for the \(P\)-wave the multilayer results are homogeneous \((\varepsilon_i = \varepsilon_b)\), the reflection band disappears, and only the normal exciton–polariton absorbance spectrum is present, which shows a double peak with two maxima separated in energy of about 1.7 meV.

Notice that the orientation of in-plane \(\hat{C}\)-axis of the uniaxial bilayer stack with respect to the incident radiation determines the reflection intensity from 0% to 100% in the two limiting cases of figures 2(b) and (a) respectively, while the line-shape remains unchanged. This behaviour is confirmed in figure 2(c) where the optical response for \(\alpha = \pi/4\) is reported, and, since the same variation, due to the contribution of ordinary and extraordinary waves, is expected, the reflection spectrum intensity reaches 50% and the transmission spectrum, close to the borders of the reflection stop band, maintains its high intensity value \((I_\alpha \sim 100\%)\). For the \(S\)-polarized incident wave, due to the symmetry of the system \([17]\), the optical response with \(\alpha\) orientation of the \(\hat{C}\)-axis is the same of that computed for the \(P\)-polarized incident wave with \(\alpha' = \pi/2 - \alpha\) orientation.

Now, let us consider an asymmetric elementary cell where the right uniaxial layer has the optical axis oriented along the \(x\)-axis \((\alpha_R = 0)\), and the left one varying on the \(x\)-\(y\) plane \((0 \leq \alpha_L \leq \pi/2)\). For the dielectric constant values we adopt the choice already discussed in the theory, \(\varepsilon_\perp < \varepsilon_b = \varepsilon_W < \varepsilon_i\) where \(\varepsilon_W = 8.24\) and \(\varepsilon_b \approx (\varepsilon_\perp + \varepsilon_i)/2\). Both the uniaxial layers have equal thickness values \((\lambda/8)\) computed by using the background dielectric constant \(\varepsilon_b\). Notice that in the case \(\alpha_L = \alpha_R\) the cell is still symmetric but the thicknesses of the two uniaxial layers are in resonance neither with \(\lambda/4\) computed by using \(n_i\) nor with that computed by using \(n_W\) values, while if \(\alpha_L = \alpha_R\) the elementary cell is asymmetric and we have to distinguish between forward and backward optical response.

The optical response for a multilayer in the limit of symmetric elementary cell \((\alpha_L \rightarrow \alpha_R = 0)\) is shown in figures 3(a) and (b) for the \(P\)- and \(S\)-incident polarization respectively; in the pictures two well-shaped reflection stop bands can be observed at opposite energy sides of the exciton.
Figure 2. P-polarized optical response, at normal incidence, of a resonant hybrid Bragg reflector \((N = 32)\), computed for different \(\alpha\) values. Reflectivity: dashed line (red online); transmission: dotted line (blue online) and absorbance: solid line (green online).

Figure 3. Linear-polarized optical response, at normal incidence, of a resonant hybrid Bragg reflector \((N = 32)\), computed for different \(\alpha_L\) values. Reflectivity: dashed line (red online); transmission: dotted line (blue online) and absorbance: solid line (green online).
absorption peak, and moreover an exciton–polariton double peak is present in the absorption spectra.

By increasing the $\alpha_L$ value (taking constant $\alpha_R = 0$), the forward optical spectra for the P- and S-polarizations show slightly deformed stop bands that move in opposite directions, towards the exciton energy value attained for $\alpha_L = \pi/4$ as shown in figures 3(c) and (d) respectively. In fact for the former $\alpha_L$ value, a well-formed photonic stop band ($\Delta \omega(0) \approx 57$ meV) in resonance with exciton energy is present for S-polarization. For the P-polarization the optical spectrum shows a very broad reflection band ($\Delta \omega(0) \approx 114$ meV) not centred on the exciton energy; nevertheless the Bragg energy shown in the dispersion curve of figure 6(b) is in resonance with the exciton energy, and this fact underlines that the large reflection shoulder, at the lower-energy side of figure 3(c), is not due to the absolute gap of the sample. This is confirmed by the absorbance computation for a cluster with $N \gg 32$ cells (not reported here), which shows two absorption side-bands, located at the opposite energy side with respect to the main exciton peak, whose energy distance is close to the right value (57 meV) of the band gap.

It is well known that, when the two $\tilde{C}$-axes of a rather large cluster of non-absorbing photonic crystals are perpendicular, the optical response gives the same reflectance/transmission spectra for S- and P-polarization [17]. This property is due to the fact that, under the former conditions, S- and P-waves feel the same sequence of dielectric constants in the elementary cell of the multilayer, except for their order. In fact, for $\alpha_L = \pi/2$ two photonic band gaps, with Bragg energies in resonance with the exciton energy ($\Delta \omega(0) \approx 103$ meV), are shown in figures 4(a) and (b) for both polarizations. The two spectra coincide, as underlined before, except for photon energies very close to the exciton transition energy, where exciton absorptions show rather different intensities as a function of the polarization, while in an enlarged intensity scale (see figure 4(c)) the pattern of three peaks in perfect agreement with stop band width is retained. The dependence of the absorbance intensities from the polarization of the incident waves is due to the asymmetry of the elementary cell, as could be easily verified by observing that S- and P-absorption spectra exchange their intensities by exchanging forward with backward in the exciton–polariton propagation. Finally, let us underline that the former properties can be easily verified by computing an ‘analogous’ isotropic and asymmetric Bragg reflector.

It is well known that in dielectric Bragg reflectors, where only the background dielectric modulation is present, the building up of the reflection stop bands is usually reached at a rather small number of dielectric $\lambda/4$ bi-layers ($N \approx 20 \div 40$), while for quantum wells Bragg reflectors in a bulk, the building up of the reflection stop bands and the transition from super-radiance to the Bloch exciton–polariton show the same behaviour and both saturate at higher number ($N \approx 150 \div 300$) of $\lambda/2$ Bragg quantum well [3–5, 9]. Moreover, when the exciton and dielectric background periodicities are both present, the reflection stop band is given by the background dielectric periodicity and the dispersive part of the exciton non-local dielectric function [4, 5].

In figure 5 the full width at half maximum of the absorbance spectra for the S- and P-polarizations of the incidence wave is reported. The parameter values of the system are the same as in figures 3(c) and (d) for the S- and P-polarization respectively. Notice that a pure super-radiant rather linear behavior, with only one broad peak in the absorbance line-shape, is observed for S-polarization at low number of elementary cells ($N = 2 \div 32$), while in the transition zone ($N = 32 \div 64$), which connects super-radiance and the so-called saturation zone of energies ($N \gg 64$), the absorbance line-shape becomes rather complex showing a few maxima and/or shoulders. Finally, in the saturation zone, where exciton oscillator strengths are redistributed on more than one polariton mode and Bloch exciton–polaritons propagate, only two maxima are present for photon energies close to the unperturbed exciton energy, and their splitting energy is of the order of a few meVs, as will be fully discussed in the next section.

Figure 4. Optical response, at normal incidence, of a resonant hybrid Bragg reflector ($N = 32$). Reflection: dashed line (red online); transmission: dotted line (blue online) and absorbance: solid line (green online). (c) Shows the absorbance spectra of the system of (a) (dotted line) and (b) (solid line) in enlarged scale of intensity.

(a) P polarization $\alpha_L = 90^\circ$, $\alpha_R = 0^\circ$
(b) S polarization $\alpha_L = 90^\circ$, $\alpha_R = 0^\circ$
(c) S and P polarizations $\alpha_L = 90^\circ$, $\alpha_R = 0^\circ$
In the present paper we have chosen to discuss in detail a system with not a very large number of quantum wells ($N = 32 + 2$), in order to operate in the strong coupling regime of the radiation–matter interaction, but also in the presence of a well-shaped photonic stop-band ($N = 32$ isotropic/anisotropic bi-layers). Obviously, this reasonable number of quantum wells should also facilitate sample realization [18, 20].

4. exciton–polariton dispersion curves

In order to go a bit deeper in understanding the exciton–polariton propagation in the hybrid periodic system with asymmetric elementary cells, the dispersion curves, with the same parameter values of figures 3(c) and (d) ($\alpha_L = 0$, $\alpha_R = \pi/4$), computed in the limits $N \rightarrow \infty$ and $\Gamma_{NR} \rightarrow 0$, are shown in figure 6. In figure 6(a) the photonic energy gaps are located inside the Brillouin zone, as clearly observed in the second and third gap of the picture, and this is a rather general property of resonant hybrid Bragg reflectors with in-plane optical axis as discussed before. In the lowest energy gap of figure 6(a) an IDC, close to the unperturbed exciton energy, is also reported. This feature, which is present also in isotropic Bragg quantum wells [4, 5], characterizes the exciton–polariton propagation and is promising for optical applications [12, 20]. In fact, its rather constant behaviour in energy supports zero polariton group velocity, therefore a trapped light in the resonant hybrid Bragg reflector could be obtained if this property is maintained in the whole Brillouin zone as discussed for isotropic RPBR in [12]. In figure 6(b) the first gap is shown in an enlarged energy scale and very close to the boundary of the Brillouin zone. The lower and upper dispersion curves of the absolute photonic gap show a strong deformed behaviour, with respect to the normal parabolic one, that denotes high polariton density of states, and this property is also related with the high transmission band edge resonances [16, 20]. Moreover, two IDC are present in the gap, whose energies are very close to the unperturbed exciton energy, except for quasi-momentum $K$-values in correspondence to the direct gap, where the interaction with the lower and upper photonic dispersion curves removes the degeneracy and therefore they show an energy separation as large as $\Delta \omega \approx 5.0$ meV. The former energy splitting between the two IDC is due to four bands interaction, which in the present case is essentially reduced to the repulsion between the upper and lower photonic dispersion curve with the lower-energy IDC, and between the lower dispersion curve with the upper-energy IDC [20], as will be demonstrated by using $q_\parallel \neq 0$ (see figure 8). For $\alpha = \pi/2$ then two IDC curves recombine in a two-fold curve (see the inset of figure 6(b)) and the band structures become degenerate for both polarizations [17]; therefore the two-fold IDC becomes constant in energy in the whole Brillouin zone, since the interaction between the upper and lower photonic branches and the two IDC are strongly reduced due to the increasing of the energy gap ($\Delta \omega(0)$ changes from about 57 meV to about 90 meV). Moreover, the band gap moves to the border of the Brillouin zone and shows a rather normal quadratic behaviour.

The possibility of opening or closing the window of $\Delta \omega \approx 5.0$ meV by different orientation of the $\hat{C}$-axis is promising for studying the light-storing effect in resonant hybrid Bragg reflectors. In fact, at variance of an analogous isotropic case discussed in [12], where the switch on/off is based on the dynamical Stark effect, in the present system the switch is obtained by a linear renormalization of the photonic gap. Figure 7 shows the maximum splitting value between the two IDC bands as a function of $\hat{C}$-axes misorientation, and the possibility to obtain a large energy deformation of the two IDC bands as a function of the $\hat{C}$-axis orientation is the most interesting result of the present paper. Moreover, in order to enlarge the zone of the $K$-values, where the IDC degeneracy is removed, we will have to take very different values for the uniaxial dielectric constants ($\varepsilon_L \ll \varepsilon_P$) and also use higher-energy stop bands, where the direct gaps are not very close to the border of the Brillouin zone.

Since the removal of the degeneracy between the two IDC bands can be obtained also for non-normal incidence propagation, let us consider the dispersion curves computed as in the case of an incident angle $\theta = 10^\circ$. In this case, while the energy shift of the exciton centre-of-mass is negligibly small ($\hbar^2 q_0^2/2 M \approx 6.7$ $\mu$eV), the shift, due to the longer path of light in the multilayer, is clearly observed for $\alpha_L = \pi/4$ (see figure 8). In fact, the direct polaritonic gap changes from $\Delta \omega(0) \approx 52$ meV to $\Delta \omega(q_0) \approx 42$ meV, and the top of the lower photonic band shifts in energy of $\hbar [\omega_p(q_0) - \omega_p(0)] = 33.3$ $\mu$eV, coming close to the exciton resonance. Notice that while the energy splitting between the two IDC bands increases with respect to the former case (about $\Delta \omega_p \approx 10$ meV), the lower IDC is rather unperturbed, at variance of the higher IDC, since the upper polariton
branch now is rather higher in energy than the symmetric case (see figure 6).

Finally, we have computed the dispersion curves for the same structural system discussed before, but with stronger dielectric contrast in the uniaxial bilayer ($\varepsilon_1 = 13.00$ and $\varepsilon_2 = 2.25$). Notice that the asymmetric background dielectric constant values increase the optical asymmetry of the uniaxial layers, but, as underlined before, the differences with the former case are rather expected. In figure 9(a) larger energy gaps are present and very far from the high-symmetry points of the Brillouin zone; therefore, for exciton energy close to one of these photonic gaps an anomalous exciton–polariton propagation could be present [16, 17]; moreover, also in this case, due to the shift of the photonic band gap, two IDC, close to the top of the first optical valence band, are observed.

In figure 9(b) the first energy gap is shown in an enlarged energy scale and with this resolution an indirect absolute photonic gap is observed ($\Delta\omega(q_x = 0) \approx 119.2$ meV). In a further enlarged energy scale (see the inset of figure 9(b)), the former pattern looks rather symmetric with respect to the maximum of the lower photonic band energy. Two dispersion curves are present in the photonic gap with strongly different behaviour, namely one dispersion curve is a rather unperturbed and shows a negligible group velocity till very close to the boundary of the Brillouin zone [17], while the second curve shows strong distortion due to the repulsion with the top of the lower photonic band.
In conclusion, the hybrid isotropic/anisotropic resonant photonic crystals seem a rather promising class of metamaterials, with respect to the isotropic multilayers, enlarging the possibilities of optical tailoring for fundamental studies and device applications.

5. Conclusions

In the present work, the non-local optical response of a resonant hybrid Bragg reflector is computed for a cluster of $N = 32$ cells in the symmetric configuration (same orientation of the in-plane optical axis of the two uniaxial layers, $\alpha_L = \alpha_R$) and in the asymmetric one ($\alpha_L \neq \alpha_R$) by self-consistent calculations and in the effective mass approximation. The non-radiative homogeneous broadening value is taken coherently with those adopted for the so-called ‘high quality’ quantum wells at rather low temperature ($T < 10$ K).

The tailoring of the optical response for asymmetric elementary cells is performed under the conditions $\varepsilon_L < \varepsilon_R = \varepsilon_\perp$ and $(\varepsilon_\parallel + \varepsilon_\perp)/2 \approx \varepsilon_R$ and the misalignment of the optical axes determines a strong rearrangement of the band structure. For $\alpha = \pi/2$ a strong difference in the exciton–polariton absorbance intensity is observed for S- and P-polarization. Moreover, a rather broad reflection band in P-polarization (about two times the corresponding S-polarization) is observed, when both ordinary and extraordinary contributions are present ($\alpha = \pi/4$). The former effect is explained by discussing the corresponding dispersion curves (figure 6(b)).

Investigating the exciton–polariton propagation and/or localization in the asymmetric elementary cell systems, the dispersion curves evidence two IDC in the lowest gap, very close to the unperturbed exciton energy: their energy splitting as a function of $\hat{C}$-axes misorientation is also reported (figure 7). The possibility of opening or closing the energy window by different orientation of the left $\hat{C}$-axis is promising for studying the light-storing effect in resonant hybrid Bragg reflectors.

Finally, dispersion curves computed for an asymmetric elementary cell with stronger uniaxial dielectric asymmetry $\varepsilon_L \ll \varepsilon_\perp$ are shown and the indirect optical gap and anomalous exciton–polariton propagation is discussed.

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Appendix A. Exciton–polariton model in a 2D quantum well

The study of exciton–polariton propagation in semiconductor materials, requires the solution of the Maxwell equation:

$$\nabla \times \nabla \times \mathbf{E}(R; \omega) = q^2 \varepsilon_{0} \mathbf{E}(R; \omega) + 4\pi \mathbf{P}_{ex}(R; \omega)$$  \hspace{1cm} (A.1)

where $q = \omega/c$, $\mathbf{P}_{ex}(R; \omega)$ is the nonlocal linear polarization vector:

$$\mathbf{P}_{ex}(R; \omega) = q^2 S_{ex} \Psi(r, R) \int_{-L/2}^{L/2} \mathrm{d}R' \Psi^*(r, R') \mathbf{E}(R'; \omega)$$  \hspace{1cm} (A.2)

and $\Psi(r, R)$ is the exciton envelope function computed for $r = 0$.

In isotropic material we can choose Cartesian coordinates with the Z-axis perpendicular to the surface plane (x, y) and,
for the cylindrical symmetry of the quantum well, we can adopt mixed coordinates \((K_z, R)\) for the motion of the exciton centre-of-mass. In this case the exciton function can be written as

\[
\Psi(r, R) = N\varphi(r, z)e^{iK_lr} \tag{A.3}
\]

where \(r = (\rho^2 + |z_c - z|^2)^{1/2}\). For a 2D heavy hole Wannier exciton, perfectly confined between infinite potential barriers, \(\varphi(r, Z)\) can be written as a two-subbands variational envelope function [21, 22]:

\[
\varphi(r, Z) = N_{ex} \cos \left( \frac{\pi z_c}{L_w} \right) \cos \left( \frac{\pi z}{L_w} \right) e^{-i\alpha_{ex}}. \tag{A.4}
\]

As is well known, the solutions \(E_\beta(\beta = x, y)\) of equation (A.1) can be obtained by the solutions \(E_{\beta,ex}\) of the corresponding homogeneous part \(\left( P_{ex} = 0 \right)\), combined with a solution of the heterogeneous equation (see, for instance [2, 22]), namely:

\[
E_\beta(\omega, z) = E_{\beta,ex}^0(\omega, z) - \frac{q}{c_e} S_{ex}(\omega, q_x) \\
\times \int_{-L_z/2}^{L_z/2} dz'' \left[ \Psi_{ex}^*(z'') \right] \left[ \Psi_{ex}(z) \right] \\
\times \int_{-L_z/2}^{L_z/2} dz' \Psi_{ex}(z') E_\beta(\omega, z') \tag{A.5}
\]

where \(G_{\beta,ex}^0(\omega, z'')\) is the Green function. Notice that we have embodied all the different normalization constants [22], of the Green function into the coefficient \(\tilde{q}_{ex}\) that assumes the values: \(\tilde{q}_{ex}^x = K_x^2/c_w\) and \(\tilde{q}_{ex}^z = \omega^2/c_z^2\) respectively. Therefore, the Green functions become the same for both \(x\)- and \(y\)-components:

\[
G_{\omega}(\omega, z') = \frac{e^{i|\omega|z'-\omega t}}{i2q_w}. \tag{A.6}
\]

All the energy dependence is contained in the quantity:

\[
S_{ex}(\omega) = \frac{S_{ex}(\omega)}{E(K) - \hbar^2 \omega^2 - i2\hbar \omega \Gamma_{XRB}} \tag{A.7}
\]

where \(S_{ex}(\omega) = 4\pi \hbar \omega \epsilon /\omega m_o\) and \(E(K)\) the total exciton energy peak:

\[
E(K) = E_{gap} - E_{ex} + \frac{\hbar^2}{2M} K_z^2. \tag{A.8}
\]

\(E_K\) is the Kane energy \((E_K = 23 \text{ eV} \text{ in GaAs-based semiconductors})\), \(m_o\) the electron mass and \(g\) the spin-degeneracy that, in the present calculation, has been taken as a constant value \((g = 1)\).

Finally, by solving the Lippmann–Schwinger equation [2, 22], we can obtain the electric field into explicit form (with the factor exp \(i\omega_{ex}\) suppressed):

\[
E_\beta(\omega, z) = A_{\beta,ex} \left[ e^{i\omega_{ex}t} - g_{ex}(z) \varphi_{ex}(\omega; q_x) \tilde{q}_{ex}(q_x) \right] \\
+ B_{\beta,ex} \left[ e^{-i\omega_{ex}t} - g_{ex}(z) \varphi_{ex}(\omega; q_x) \tilde{q}_{ex}(-q_x) \right] \tag{A.9}
\]

\(\varphi_{ex}(q_x)\) is the Fourier transform of exciton envelope function \(\Psi_{ex}(r)\) computed for \(r = 0\): \(\rho = 0, z_e = z_h = z\):

\[
\varphi_{ex}(\pm k_{ex}) = \int_{-L_z/2}^{L_z/2} dz \Psi_{ex}(z)e^{iK_{ex}z} \tag{A.10}
\]

\[
\varphi_{ex}(\pm k_{ex}) = \frac{N_{ex}k_{ex}^2}{k_{ex}(k_{ex}^2 - k_{ex}^2)} \sin \left( \frac{k_{ex}L_w}{2} \right) \tag{A.11}
\]

where \(k_{ex} = 2\pi/L_w\).

We define now the integral function \(g_{ex}(z)\) computed at the slab interfaces:

\[
g_{ex}(z) = \int_{-L_z/2}^{L_z/2} dz' \Psi_{ex}(z') \tag{A.12}
\]

and the function:

\[
M_{ex}(\omega) = \int_{-L_z/2}^{L_z/2} dz \Psi_{ex}(z) g_{ex}(z) \tag{A.13}
\]

\[
M_{ex}(\omega) = \frac{N_{ex}^2}{4} \left[ L_w \left( \frac{1}{q_{ex}^2} - \frac{1}{2(k_{ex}^2 - q_{ex}^2)} \right) \right] \\
- iq_{ex} \left( \frac{1}{q_{ex}^2} + \frac{1}{k_{ex}^2 - q_{ex}^2} \right) \left( 1 - e^{i\omega L_w} \right) \tag{A.14}
\]

by means of that we write the new energy function \(S_{ex}(\omega, q_x)\):

\[
S_{ex}^3 = \frac{\tilde{q}_{ex}^2 S_{ex}(\omega)}{E_{ex}^3 - \hbar^2 \omega^2 - i2\Gamma_{XRB}/\omega + \tilde{q}_{ex}^2 S_{ex}(\omega)M_{ex}} \tag{A.15}
\]

and obtain the polariton self-energy \(\Sigma_{ex}\) in explicit form:

\[
\Sigma_{ex}(\omega, q_x) = \tilde{q}_{ex}^2 S_{ex}(\omega)M_{ex}(\omega). \tag{A.16}
\]

**Appendix B. Uniaxial crystal slab with in-plane optical \(\hat{C}\)-axis**

Let us consider an electromagnetic wave incident from an isotropic medium (vacuum or air) onto the left surface of a uniaxial multilayer. The Cartesian coordinate system is chosen such that the \(xz\) is the plane of incidence and the \(z\)-axis is normal to the reflecting surface. When passing through the uniaxial materials, the electromagnetic beam splits in two rays: the ordinary and extraordinary, to be mutually perpendicular polarized. The optical response of the uniaxial multilayer may be characterized by four reflection amplitudes \((R_{ex}, R_{op}, R_{pp}, R_{pp})\) and four transmission amplitudes \((T_{ex}, T_{op}, T_{px}, T_{pp})\), where the second suffix refers to the polarization, \(S\) or \(P\), of the reflected and transmitted waves, when the incident wave is in the polarization state of the first suffix [23, 24]. In order to calculate these amplitudes we employ the transfer-matrix method that connects the electromagnetic field amplitudes at both the interfaces of the layers.
Constitutive equations for uniaxial crystal in a Cartesian framework are:

\[
\begin{align*}
(q^2\varepsilon_{xx} - k_i^2)E_x + q^2\varepsilon_{yy}E_y + (q^2\varepsilon_{zz} + k_i k_i)E_z &= 0 \\
q^2\varepsilon_{xx}E_x + (q^2\varepsilon_{yy} - k_i^2 - k_i^2)E_y + q^2\varepsilon_{zz}E_z &= 0 \\
(q^2\varepsilon_{xx} + k_i k_i)E_x + q^2\varepsilon_{yy}E_y + (q^2\varepsilon_{zz} - k_i^2)E_z &= 0
\end{align*}
\] (B.1)

where \( q = \omega / c \) and \( \varepsilon_{xuv} \) \((\nu = x, y, z)\) are the components of the Cartesian symmetric dielectric tensor \( \varepsilon \), that, for uniaxial crystals with optical axis \( C \) in the reflecting plane \((xy)\) and forming an angle \( \alpha \) with the x axis, becomes:

\[
\varepsilon = \begin{pmatrix}
\varepsilon_1 + \frac{k_i^2}{\varepsilon}\varepsilon_2 & \varepsilon_{x1} & \varepsilon_{x2} & \varepsilon_{x3} \\
\varepsilon_{x1} & \varepsilon_1 & \varepsilon_{y1} & \varepsilon_{y2} \\
\varepsilon_{x2} & \varepsilon_{y1} & \varepsilon_1 & \varepsilon_{z1} \\
\varepsilon_{x3} & \varepsilon_{y2} & \varepsilon_{z1} & \varepsilon_1
\end{pmatrix}
\] (B.2)

where \( \varepsilon_1 \) and \( \varepsilon_2 \) are the dielectric constants, valued in the principal axes framework, that describe the electromagnetic response for solicitations along the directions parallel and perpendicular to the optical \( C \)-axis, respectively. \( \varepsilon_1 = \cos \alpha \) and \( \varepsilon_2 = \sin \alpha \) are the projections of \( C \) on the x- and y-axes. We take nonmagnetic materials for which the magnetic permeability value \( \mu = 1 \) is used throughout the whole layered medium.

In order to have nontrivial solutions of equation (B.1), the determinant of the matrix of the coefficients must vanish. This requires the solution of a fourth degree (in \( k_i \)) equation whose four roots are the wave vectors relative to the ordinary \((\pm k_o)\) and extraordinary \((k_c^\pm)\) rays:

\[
\pm k_o = \pm \sqrt{q^2\varepsilon_1 - k_i^2}, \quad k_c^\pm = \pm \sqrt{\frac{k_i^2}{\varepsilon_1} + \frac{k_i^2}{\varepsilon_2} \left[ \varepsilon_2 - \varepsilon_1 \right]} \quad \varepsilon_1
\] (B.3)

where \( k_i = (\omega / c) \sqrt{\varepsilon_{xuv}}, \) \( k_o = k_i = (\omega / c) \sqrt{\varepsilon_1} \) \( \sin \theta_i, \) \( \theta_i \) is the angle of incidence. Notice that the expressions in equations (B.3) and (B.4) are all independents of the polarizing state of the incident wave.

The corresponding twelve solutions of equation (B.1) are:

\[
E_{xx}^\pm e^{\pm ik_c^\pm y}, \quad E_{yy}^\pm e^{\pm ik_c^\pm y}, \quad E_{zz}^\pm e^{\pm ik_c^\pm y}
\] for the ordinary ray and

\[
E_{xx}^{(\pm)} = \pm s_i k_o, \quad E_{yy}^{(\pm)} = \pm s_i k_o, \quad E_{zz}^{(\pm)} = \pm s_i k_o
\]
for the extraordinary ray with:

\[
E_{xx} = \frac{1}{s_i k_o} E_{xx}^{(\pm)} , \quad E_{yy} = \frac{1}{s_i k_o} E_{yy}^{(\pm)} , \quad E_{zz} = \frac{1}{s_i k_o} E_{zz}^{(\pm)}
\] (B.5)

The \( E_i \) components \((\nu = x, y, z)\) of the electric field are computed as a linear combination of the corresponding four partial waves:

\[
E_i = (A_e E_{xx}^+ + B_e E_{xx}^- + B_e E_{yy}^- + A_e E_{yy}^+) e^{ik_c^+ y} + (A_e E_{xx}^- + B_e E_{xx}^+ + B_e E_{yy}^+ + A_e E_{yy}^-) e^{ik_c^- y}
\] (B.6)

and, finally, the magnetic field components can be obtained by the Maxwell equation \( \nabla \times E = i \omega j_{0} d_{0} B \).

Notice that for convenience, the tangential components of the electromagnetic field, from here on, will be written in matrix form as:

\[
\psi(z', \omega) = \begin{pmatrix}
E_x(z'; \omega) \\
E_y(z'; \omega) \\
H_x(z'; \omega) \\
H_y(z'; \omega)
\end{pmatrix}
\] (B.7)

The four coefficients \( A_e, B_e, A_e, \) and \( B_e \) are computed, for each layer of heterostructure, by imposing the continuity of the electric and magnetic tangential components at the boundaries of each layer, by means of the following propagation relation:

\[
\psi(z + l_j; \omega) = C_j \psi(z; \omega)
\] (B.8)

where \( z_j \) and \( l_j \) are the coordinate of the left interface and the thickness of the \( j \)-layer respectively.

The matrix \( C_j \), usually called the transfer matrix, is easily building up as:

\[
C_j = M_j U(L_j) M_j^{-1}
\] (B.9)

where:

\[
M_j = \begin{pmatrix}
E_{xx}^+ & E_{xx}^- & E_{xx}^+ & E_{xx}^- \\
E_{yy}^+ & E_{yy}^- & E_{yy}^+ & E_{yy}^- \\
H_{xx}^+ & H_{xx}^- & H_{xx}^+ & H_{xx}^- \\
H_{yy}^+ & H_{yy}^- & H_{yy}^+ & H_{yy}^-
\end{pmatrix}
\] (B.10)

\[
U(L_j) = \begin{pmatrix}
e^{ik_e^j y_j} & e^{ik_e^j y_j} \\
e^{-ik_e^j y_j} & e^{-ik_e^j y_j}
\end{pmatrix}
\] (B.11)

Thus, the transfer matrix \( C \) of the whole stack of \( n \) layers is computed as:

\[
C = C_n C_{n-1} \ldots C_1
\]

The refraction \( R \) and transmission \( T \) amplitudes are expressed as the ratio of the correspondent electric field components, of the reflected or transmitted waves, to the incident electric field. Finally we can write the following relations, between the incoming and outgoing electromagnetic fields, for S-polarized incident waves:

\[
\begin{pmatrix}
\cos \theta_i R_{sp} \\
1 + R_{sp}
\end{pmatrix} = \begin{pmatrix}
\cos \theta_i T_{sp} \\
T_{sp}
\end{pmatrix}
\] (B.12)

and for P-polarized incident waves:

\[
\begin{pmatrix}
\cos \theta_i (1 + R_{pp}) \\
k_1 \cos \theta_i R_{ps}
\end{pmatrix} = \begin{pmatrix}
\cos \theta_i T_{pp} \\
k_2 T_{ps}
\end{pmatrix}
\] (B.13)

where \( k_1 = q \sqrt{\varepsilon_1}, k_2 = q \sqrt{\varepsilon_2}, \) \( \theta_i \) and \( \theta_2 \) angles of incidence and transmission respectively. The reflectivity \( r \) and transmission \( t \) are computed as:

\[
r = R^2 R^* \quad \text{and} \quad t = (Z_2 / Z_1) T^* T
\]

where \( Z_1 \) and \( Z_2 \) are the characteristic optical impedances of the two external media respectively, while the absorbance is computed as:

\[
a = 1 - (r + t).
\]
From a theoretical point of view, the calculation of the photon–polariton dispersion curves involves the solution of the Maxwell equation (A.1) in periodic heterostructures, where the diffraction indexes have the full translational symmetry of the lattice. In principle, the electromagnetic field components \( \psi_0 \) must fulfill the condition of continuity at each interface of the multilayer, together with the periodicity condition at the boundaries of the unit cell. Moreover, as in any periodic potential problem, the overall solution must be of the Bloch form. All these conditions can be satisfied by using, as an electromagnetic field, Bloch-type functions:

\[
\psi(z; \omega, k_{BZ}) = \psi_0(z; \omega) e^{-ik_{BZ}z}
\]  

(B.14)

where the wave vector \( k_{BZ} \) defines a point inside the first Brillouin zone.

It is easy to show as, from the continuity and periodicity conditions, we can write the coupled matrix equations:

\[
\begin{bmatrix}
C \psi(z; \omega, k_{BZ}) = \psi(z + d; \omega, k_{BZ}) \\
e^{ik_{BZ}d} \psi(z; \omega, k_{BZ}) = \psi(z + d; \omega, k_{BZ})
\end{bmatrix}
\]  

(B.15)

where \( d \) is the period of the unit cell. Finally, from the above system, the following homogeneous equation is immediately obtained:

\[
(C - e^{ik_{BZ}d}I) \psi(z; \omega, k_{BZ}) = (0).
\]  

(B.16)

The couples of values of \( \omega \) and \( k_{BZ} \), for which the determinant \( |C - e^{ik_{BZ}d}I| \) vanishes, define the dispersion curves in the Brillouin zone. The solutions of the above determinant are obtained by the roots of the characteristic polynomial: 

\[
y^4 + py^3 + qy^2 + ry + s = 0 \quad (y = \exp[ik_{BZ}d]).
\]

Notice that, for the systems here studied, it results that \( p = r \) and \( s = 1 \). In this case the fourth degree, polynomial reduces to the second degree: 

\[
4 \cos^2(k_{BZ}d) + 2p \cos(k_{BZ}d) + (q - 2) = 0,
\]

from whose solutions we compute \( k_{BZ} \) as function of \( \omega \).

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