Bragg reflector enhanced attenuated total reflectance

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We model the effects of a quasibound photonic state that can exist within a substrate/metal film/Bragg reflector/air structure. The photonic state is confined as a result of total internal reflection at the air interface coupled with the effect of the photonic band gap of the Bragg reflector. The presence of the thin metallic film ensures that distinctive features are observable in the associated reflectivity spectrum. With an appropriately chosen metal layer thickness, light is able to penetrate into the structure but is then effectively trapped, leading to a greatly increased field intensity at the air interface and an associated sharp feature in the reflectivity. The sensitivity of the reflectivity feature to structural details and angle of incidence and the property of substantial field enhancement suggest that the structure could be of use in sensor/detector technology and nonlinear optics applications. © *2009 American Institute of Physics*. [doi:10.1063/1.3265436]

I. INTRODUCTION

In recent work, the authors in concert with others have theoretically[1] predicted and experimentally[2] demonstrated the existence of Tamm plasmon polaritons (TPPs), a form of photonic-related surface excitation, in structures in which the presence of a metal layer and Bragg reflector (BR) was crucial. A simple phase-matching prescription, employed as an aid in the investigation of such states in BR-based structures, has also been described[3] in the case where indium tin oxide forms the metallic layer. This work was a development of that of Kavokin *et al.*[4] who theoretically predicted the existence of lossless Tamm states at the interface between two different periodic dielectric structures and then went on to show how such states might be utilized in the construction of a polariton laser.[5] In turn, these activities were inspired by the much earlier efforts of both Tamm[6] and Ritchie[7] who considered electronic surface states and the later optical state studies of Yeh *et al.*[8,9] An additional novel characteristic of these BR-metal layer structures is that they make possible the existence of TPPs above the bulk plasma frequency.[10] The utilization of resonant cavity or interface states associated with a photonic band gap (PBG) structure on the surface of a prism has previously been proposed[11] for potential use in attenuated total reflectance (ATR) and other optical applications, but in that case the existence of a metallic layer at the upper interface was not considered and this has crucially important implications for the behavior of the system, as we shall demonstrate.

In this work, we employ a standard transfer matrix approach together with support from the phase-matching technique, which will be briefly described here, in order to investigate the nature of and calculate the reflectivity spectrum of a particular substrate-metal-BR-air photonic structure that has potential for practical applications. All calculations relate only to TM polarization in which the magnetic field is perpendicular to the plane of incidence with the magnetic *H*-field entirely parallel to the interfaces.

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II. BASIC STRUCTURE

Figure 1 illustrates the basic structure considered in this work, consisting of a substrate (taken to be SiO_2 with a refractive index of 1.47) with a thin overlayer of silver (the precise nature of the metal and its properties are not crucial to the form of the basic results) topped by a 40-layer SiO_2/TiO_2 BR, with a SiO_2 layer adjacent to the silver film. The TiO_2 is taken to have a refractive index of 2.37. (See, e.g., Lee and Yao[12] for an account of the dielectric properties of SiO_2 and TiO_2, which can be taken to be lossless and with fixed refractive indices in the infrared regime considered.) For the purposes of the calculations, we have somewhat arbitrarily considered a BR in which the PBG of the associated infinitely repeated Bragg structure is centered at 1 eV. For such a structure, to the nearest nanometer, the respective SiO_2 and TiO_2 layer thicknesses are 211 and 131 nm. We have employed the simple Drude expression

$$\varepsilon(\omega) = 1 - \frac{\omega_p^2}{\omega(\omega + i\omega_c)}$$

for the relative permittivity of the metallic layer. We employ silver as a suitable representative metal with a plasma frequency such that $\hbar\omega_p \equiv 7.2$ eV and with collision frequency, which determines the losses in the metal, given by $\hbar\omega_c \equiv 0.05$ eV.[13] We take the incident angle on the silver in the SiO_2 substrate to be $\theta=45°$ which, given that the SiO_2/air critical angle is 42.86°, ensures that the overall transmission

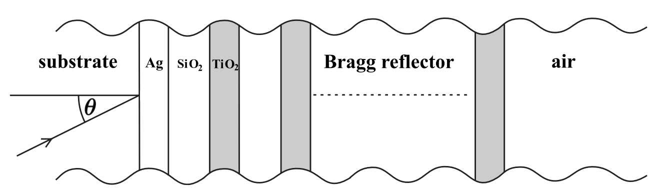

FIG. 1. The basic structure employed in most of the calculations, consisting of a left-hand substrate (SiO_2 in this case) with a thin silver (Ag) overlayer and a 40-layer SiO_2/TiO_2 BR (20 layer pairs) on top. For the reflection coefficient calculations light is incident at an angle θ from the left.

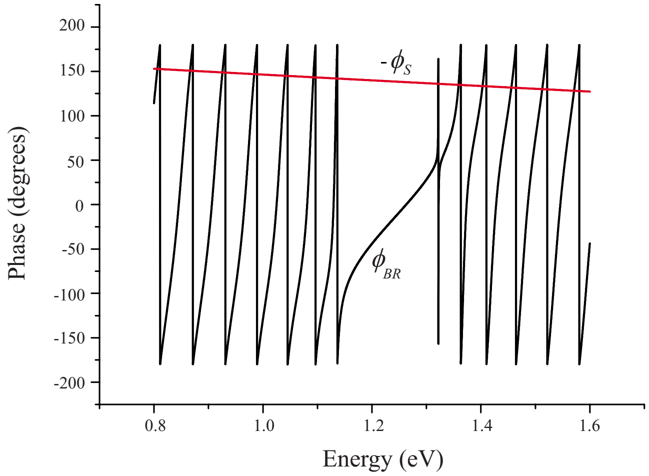

FIG. 2. (Color online) The phases ϕ_{BR} and $-\phi_S$ as a function of the energy of the incident light at an incident angle of $\theta=45°$ within the substrate. The crossing points indicate the energies at which "bound" photonic states are to be expected. (The vertical solid lines are an artifact of the plotting routine: at these points the phase shifts discontinuously from +ve to −ve values and hence these sections do not define crossing points.)

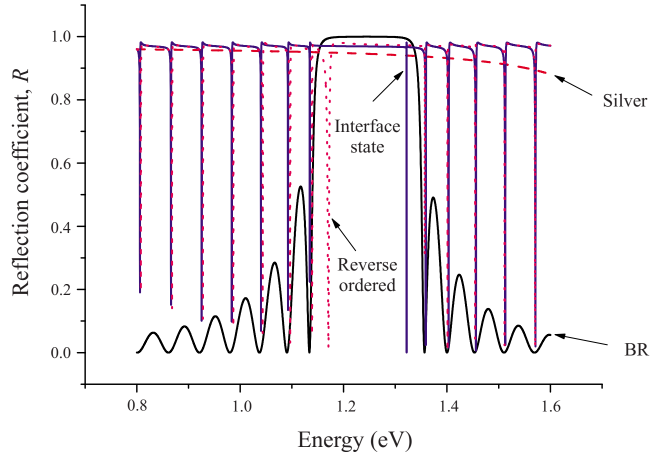

FIG. 3. (Color online) The reflection coefficient as a function of energy with light incident from the SiO_2 substrate at an angle of $\theta=45°$. The plot labeled BR corresponds to that for a 40-layer SiO_2/TiO_2 stack surrounded by SiO_2 on both the left and right. Results for light impinging on a single 57 nm layer of silver followed by air are shown by the dashed line. There are two other curves. One is for the model structure with a SiO_2 layer adjacent to the silver layer and clearly indicates the existence of the interface state at 1.32 eV. For comparison the results for the reverse-ordered BR structure consisting of a 40-layer BR with a high index TiO_2 layer adjacent to the silver are also shown.

through the structure is zero, independent of the detailed form of the intervening 1D layered system.

III. CALCULATIONS

As described more fully in Refs. 1 and 3, the existence of an interface state, or indeed any form of bound photonic eigenstate, in a 1D photonic structure can be predicted from the condition $\phi_{\text{left}}+\phi_{\text{right}}=0$. Here, ϕ_{left} and ϕ_{right} are the phases associated with the electric field amplitude reflection coefficients for light traveling from right to left, and left to right respectively at an imaginary interface at a point within any lossless region of the photonic structure. For our purposes, we take the interface to be just within the BR, an infinitesimal distance from the metal layer, and the phases are calculated using the transfer matrix method. We can then predict the energies at which any such states exist by, for example, plotting a graph of $-\phi_{\text{left}}$ and ϕ_{right} against energy and looking for the crossing points. This has been done for the structure detailed in Sec. II and the results are shown in Fig. 2. For the purpose of the calculations, the thickness of the silver layer was set at 57 nm. In this case, $\phi_S=\phi_{\text{left}}$, which relates to light impinging on the silver layer to the left of the BR, and $\phi_{\text{BR}}=\phi_{\text{right}}$, which relates to light impinging on the BR in the reverse direction. As can be seen, there are a number of crossing points over the range of energy considered. Most of the associated states, as will be demonstrated, are derived from simple resonance states of the associated Bragg structure, but one of them, at about 1.32 eV, is an interface state with potentially useful applications. We note that truly bound photonic states would only exist within this structure in the case of an infinitely thick, lossless metallic region, or an infinite BR on the left together with an infinite air region on the right, so in practice all states are only quasibound. A finite metallic layer is employed so that the presence of the photonic states can be readily detected with the use of reflectivity experiments in a configuration similar to that employed in a standard ATR study. Without the presence of the metallic layer, in which there are losses, the reflectance spectrum would otherwise be featureless in the absence of any transmission through the structure.

The transfer matrix approach has been employed to perform a number of power reflection coefficient (R) calculations and these are detailed in Fig. 3. First, R was calculated for the BR structure alone, bounded on either side by SiO_2. For the 40-layer structure (effectively a 39 layer symmetric structure given that the first layer is the same composition as the substrate) a fairly well defined high reflectivity PBG region is clearly visible centered at about 1.25 eV. The surrounding series of fairly broad minima in R are, of course, associated with light transmission to the right-hand side via resonance states of the overall BR structure. The field envelopes of these states have one or more maxima within the BR. If the SiO_2 at the right-hand side of the BR is instead replaced by air, because the incident angle is above the critical angle, a featureless spectrum in which $R=1$ at all energies is obtained. If the BR is omitted and a simple structure consisting of a 57 nm layer of silver between the substrate and air is considered there can be no overall transmission through the structure but a gradually reducing value of R with energy can be observed due to losses within the silver layer. We note that, for this standard ATR structure, a distinct feature due to the associated surface plasmon polariton can be observed closer to the critical angle but this is at an energy significantly below the range illustrated in the figure.

The reflection coefficient for the full model structure shows a distinctive new feature. The series of sharp minima in R on both sides of the initial PBG region are related to the original resonance states, but are shifted slightly upwards in energy due to their increased localization. The thin silver layer provides some additional confinement of the states within the structure to form very sharp quasibound photonic states while allowing just enough access to the structure to

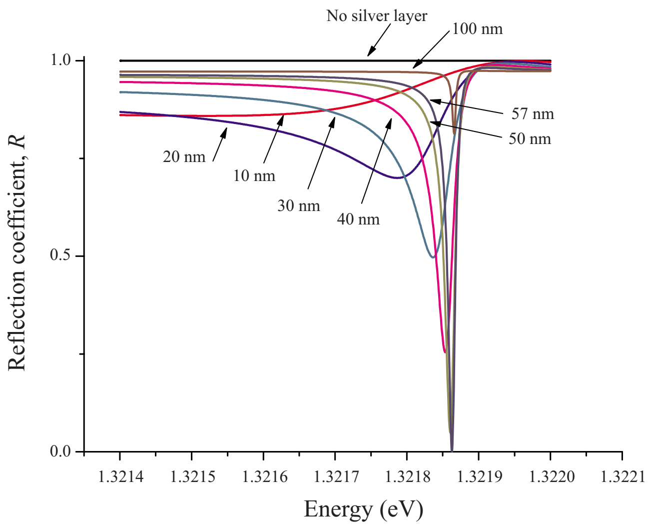

FIG. 4. (Color online) The change in reflectivity near the interface state energy as a function of silver layer thickness. A 57 nm wide layer of silver leads to a situation in which there is almost no detectable reflected wave from the structure and the system is tuned such that virtually all of the incoming energy is dissipated within the metallic layer. Further increase in metal layer thickness leads to a more confined quasibound interface state but it becomes more difficult to access the state and so the reflectivity increases. Layers thinner than 57 nm give rise to an increase in reflectivity, decreased confinement and a broadening of the reflectivity feature.

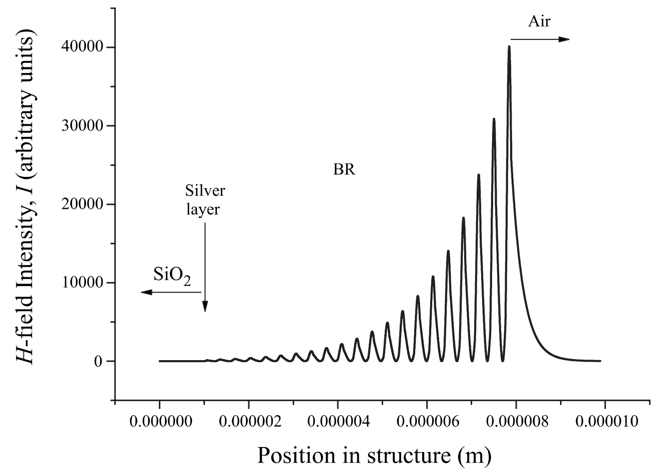

FIG. 5. The time-averaged *H*-field intensity associated with the 1.32 eV interface state. The region considered is composed of 1000 nm of SiO_2 substrate, 57 nm of silver, 20 pairs of SiO_2/TiO_2 layers giving a 6833 nm wide BR with a 2000 nm region of air on the right.

produce the associated distinctive reflectivity features. However, in addition to the resonance-related states which are clearly identifiable due to the close correspondence with those of the BR structure alone, there is an additional sharp feature at about 1.32 eV which is just below the upper edge of the PBG of the infinite BR. In practice, the positions of all of the sharp dips in reflectivity agree with the predictions of the phase-matching results of Fig. 2 to about 0.0001 eV. The state within the PBG has a half height width of about 2×10^{-5} eV and is noticeably narrower than the original resonance-related dips. The thickness of the silver layer has been chosen to approximately minimize the reflectivity ($R < 0.0002$) associated with the 1.32 eV feature (see Fig. 4), but we note that it also leads to low reflectivity for the BR-related resonances. The nature of this state can be revealed by plotting the associated *H*-field intensity profile (time-averaged H^2), as shown in Fig. 5, clearly demonstrating that this is an interface state localized toward the right-hand side of the BR. For comparison, in Fig. 6 the equivalent plot for the BR resonance-related state near 1.13 eV is also shown.

For the purposes of the transfer matrix calculation, the incoming *H*-wave has an amplitude such that the intensity at the interface between the substrate and the silver layer is $I = 1$ in arbitrary units in the absence of a reflected wave. For all the states considered, the field profile in the region of the silver layer is very similar. However, for the interface state, I rises from a value near unity at the substrate/silver interface to a peak value of about 100 at the right-hand edge of the silver layer and this state has a much higher peak intensity than that of any of the BR resonance states. In addition, the intensity of the interface state can be readily increased further by judicious alteration of the structure and angle of incidence θ, leading to an even narrower feature.

It is important to emphasize that states similar in form to those shown in Figs. 5 and 6 exist even in the absence of the silver layer as was realized by Nelson and Haus,[11] but without the presence of the crucial silver layer such states only produce a change in the *phase* of the reflectance spectrum, and not the distinctive reflectivity feature reported here. Also, the field intensity for the states is reduced by orders of magnitude compared to that with the silver layer present, and this is of great importance with regard to potential nonlinear optics applications. Although the use of a somewhat different value for the loss term ω_c has no significant effect on the energy, it is clear that it can substantially affect the conditions for experimental detection of the interface state. If ω_c is set to zero, there can then be no losses or transmission through the structure and thus $R = 1$ at all energies. With a given loss term, appropriate adjustment of the metallic layer thickness is required in order to obtain the most advantageous enhancement of the features in the reflectivity spectrum and the field intensity at the external interface.

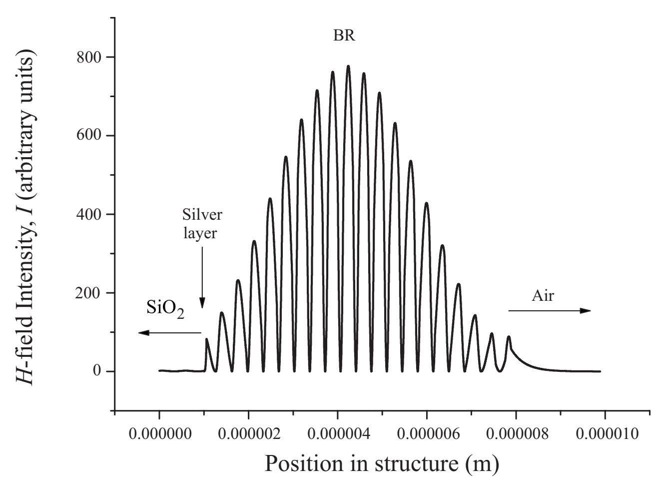

FIG. 6. A similar plot to that in Fig. 5 showing the profile of the 1.13 eV BR resonance state. The initial section of the plot, within the silver layer, is essentially the same as that for the interface state shown in Fig. 5 but is too small to be distinguishable in that figure due to the greatly enhanced field at the BR/air interface.

Due to the high field intensity associated with the state at the BR/air interface, we propose that this structure may have potential uses as a sensor/detector or in nonlinear optics applications. For example, in the case of this particular structure, if the refractive index on the right hand side is progressively increased from that of air to 1.0394 then the distinctive reflectivity feature shifts to lower energy, narrows, and then vanishes as eventually the incident angle $\theta = 45°$ is no longer above the critical angle and the interface state disappears. Alternatively, in the case of air on the right, the reflectivity feature becomes progressively sharper then disappears if the angle of incidence is reduced toward the critical angle of 42.86°. In practice, the structure acts as a very narrow notch filter in which effectively all of the incoming energy is absorbed at the design wavelength/energy in the thin metallic layer. The consequences of the associated energy absorption at the tuned wavelength might also have applications.

For comparison, a calculation of the reflection coefficient has also been carried out for the situation in which the ordering of the layers within the BR is reversed. In that case, with a high refractive index TiO_2 layer at the interface with the silver layer and the low index SiO_2 bordering the air region on the right of the structure, an interface state is still present, as can be seen from the associated reflectivity feature at about 1.17 eV in Fig. 3. However, this feature is significantly broader than those of even the resonance-like states and is localized at the internal interface at the opposite silver/BR side of the structure (within the silver the I profile is again very similar to that of the other states with the same incoming wave amplitude). This state is very similar in nature to that revealed in experiment by Sasin *et al.*[2] and, due to its localization at the left BR interface, it is insensitive to the details of the material to the right-hand side of the BR. Essentially, the same reflectivity feature, at the same energy is obtained if, say, SiO_2 rather than air is on the right-hand side of the structure, although the rest of the reflectivity plot is significantly altered. Due to the localization of this state at the internal BR interface, it does not offer the same potential for sensor and other applications as the state localized at the opposite interface.

Any practical implementation of the proposed structure will incorporate layer width variations, due to fabrication errors, which could, in principle, affect the results. The consequences can be rather subtle, due to the exponential form of the field profile associated with the interface state. However, we note that in the context of the present work, a 5% change in the width of the first layer, adjacent to the silver, produces no significant alteration in the position or form of the reflectivity minimum. A similar alteration in the width of the final layer, adjacent to the air, produces an energy shift several hundred times larger of about 0.01 eV while retaining an essentially zero value for the reflection coefficient. As positive and negative changes compared to the idealized layer widths lead to opposite shifts with respect to the position of the reflectivity minimum, the net effect of random layer thickness variations is expected to be small.

IV. CONCLUSIONS

In conclusion, we have proposed a Bragg-reflector-related structure in which the associated quasibound photonic state leads to a distinctive narrow feature in the reflectivity spectrum and a high field intensity at the externally accessible interface. This feature is much sharper and gives rise to a much greater field intensity than would be experienced in the case of a standard ATR experiment without the BR, or with the BR in the absence of the metal layer. This suggests that the structure may have applications for sensor/detector or nonlinear optics applications, as the nature of the resultant interface state and the consequent features in the reflectivity are sensitive to conditions at the external interface. The structure acts as a highly selective notch filter which can be designed to absorb virtually all of the incoming energy at a particular energy and this may also have useful applications. The materials employed and thicknesses of all layers in the structure, as well as the angle of incidence considered, can be adjusted in order to tune the response of the structure.

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