

Substantial enlargement of angular existence range for Dyakonov-like surface waves at semi-infinite metal-dielectric superlattice

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Abstract. We investigated surface waves guided by the boundary of a semi-infinite layered metal-dielectric nanostructure cut normally to the layers and a semi-infinite dielectric material. Using the Floquet-Bloch formalism, we found that Dyakonov-like surface waves with hybrid polarization can propagate in dramatically enhanced angular range compared to conventional birefringent materials. Our numerical simulations for an Ag-GaAs stack in contact with glass show a low to moderate influence of losses. © 2012 Society of Photo-Optical Instrumentation Engineers (SPIE). [DOI: [10.1117/1.JNP.6.063525](https://doi.org/10.1117/1.JNP.6.063525)]

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1 Introduction

Ultrathin optical multilayers fabricated as periodic superlattices of two or more different materials have continually been a focus of interest for both engineers and theorists for decades.¹ The possibility to relatively simply fabricate laminar structures with the thickness of their strata in the nanometer range allowed for the fabrication of a plethora of different practical structures, from antireflection layers and dielectric mirrors to various kinds of coatings and filters. A new boost to this field arrived with the advent of plasmonics.^{2,3} New areas of investigation have emerged, such as electromagnetic metamaterials, negative refraction, near-perfect near-field focusing, subwavelength imaging, transformation optics including cloaking devices and superconcentrators,⁴⁻⁶ to mention just a few. Practical applications include chemical and biological sensing, optical interconnects and waveguides, solar cell enhancement, etc.

A variety of different electromagnetic waves appear in ultrathin layered structures.⁷ An especially important group is one-dimensional (1-D) noble metal-dielectric subwavelength nanostructured planar multilayers. Such superlattices represent plasmonic metamaterials with optical properties similar to uniaxial crystals with positive birefringence. They are also sometimes denoted as 1-D subwavelength plasmonic crystals, in analogy with photonic crystals. Due to the presence of metallic nanolayers, such superlattices are dispersive and dissipative. A unit cell of a 1-D subwavelength plasmonic crystal comprises one metal and one dielectric layer. In addition to conventional propagating Floquet-Bloch (FB) modes, various in-plane plasmon-polariton modes may appear at the interfaces between metal and dielectric strata,⁸⁻¹⁰ the presence of metal being responsible for the excitation of surface plasmon-polariton resonances. Both transverse magnetic (TM) and transverse electric (TE) polarized surface modes may exist in

such anisotropic metamaterials,¹¹ contrary to the conventional single-interface situation where only TM modes are supported. The subwavelength stratified metal-dielectrics can be structurally tailored in different manners in order to obtain the desired dispersion characteristics, including those supporting fast light, slow light and left-handed modes.⁹

In the situation when an interface exists between two dielectric media, when one of them is anisotropic and the other is isotropic, surface electromagnetic waves that are not based on plasmon-polariton resonance may appear. These waves are termed Dyakonov waves after the researcher who first envisioned them.^{12,13}

If the anisotropic material is a uniaxial crystal with the optical axes in the plane of interface, it becomes necessary for birefringence to be positive. At the same time, permittivity of the bordering isotropic dielectric must fulfill certain conditions. In contrast to metal-dielectric superlattices, nondissipative all-dielectric multilayers always have negative birefringence, and therefore, no Dyakonov modes can exist on their surface.

Contrary to the surface plasmon polaritons that are strictly TM polarized, Dyakonov waves are hybrid with both TE and TM polarization components involved. Nevertheless, their most interesting property is that they can propagate without losses and within a certain angular range with respect to the optical axes. However, these waves were experimentally demonstrated only recently,¹⁴ over 20 years after Dyakonov's prediction, due to the fact that naturally anisotropic materials have extremely small birefringence that leads to exceedingly narrow angular domain of existence of Dyakonov modes. Some authors proposed widening the angular domain utilizing the Pockels effect.¹⁵ A widening of the angular domain for hybrid surface modes utilizing weakly dissipative metal-dielectric laminar structures was described using the effective medium theory (EMT).^{16,17} However, while EMT is a widely used and often accurate tool for simplified calculation of electromagnetic properties of nanocomposites, it naturally has its inherent limitations^{18,19} and in some situations gives only rough approximations or even completely fails.^{19,20}

In this paper we utilize the exact FB approach to consider the general case of the wave propagation along the interface between a semi-infinite isotropic dielectric and a semi-infinite metallodielectric binary superlattice cut normally to the layers.^{16,21} We report on the existence of hybrid surface waves with both TE and TM polarizations involved, provided certain conditions are fulfilled. Since we consider modes that are dispersive and dissipative, we introduce the term Dyakonov-like surface modes, to make a distinction with the original Dyakonov modes, which are described for purely lossless case. We compare the obtained results with those determined by EMT. We show that by careful choice of the structural parameters, a substantial enlargement of the angular range of existence of Dyakonov-like waves can be obtained.

2 Formulation of the Problem

We consider a binary plasmonic superlattice (laminar metal-dielectric) made of metal and dielectric layers alternatively stacked along the z axis and cut normally along the y - z plane so that it reveals a surface with alternating metal and dielectric regions toward the environment, as shown in Fig. 1. The unit cell of the 1-D lattice integrates a transparent material layer with a relative dielectric permittivity ϵ_d and a slab width w_d followed by a metal layer with the corresponding parameters ϵ_m and w_m . The plasmonic metamaterial is located in the semi-space $x > 0$, while an isotropic material with a relative dielectric permittivity ϵ is placed adjacent to the cut surface of the periodic medium in the semi-space $x < 0$ (Fig. 1). In this work, we consider two kinds of glass substrates as that dielectric material, N-BAK1 with dielectric constant $\epsilon = 2.43$, and P-SF68 (SCHOTT) with dielectric constant $\epsilon = 3.8025$. We denote the relative permittivity measured along the optical z -axis by ϵ_{\parallel} , while the permittivity in the transversal direction is ϵ_{\perp} . The metal filling factor is defined as

$$f = \frac{w_m}{w_d + w_m}. \quad (1)$$

Besides absorption losses, there is a strong time dispersion in metals that gives rise to a frequency dependence of metal permittivity. This can be described by the well-known Drude model. However, for the purpose of this paper, we keep the wavelength (frequency) constant at $\lambda_0 = 1.55 \mu\text{m}$. That allows us to study space dispersion only, and avoid study of time

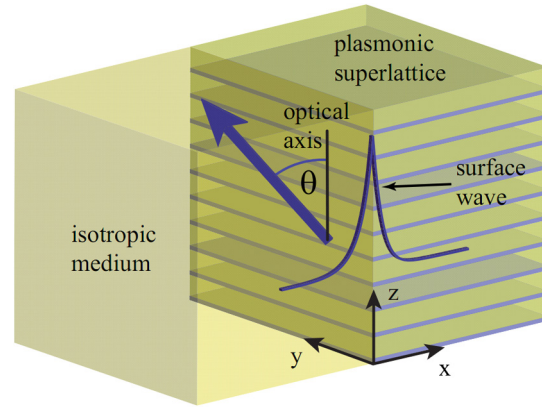


Fig. 1 Schematic setup under study consisting of a semi-infinite Ag-GaAs superlattice ($x > 0$) and an isotropic cover ($x < 0$), either N-BAK1 or P-SF68 (SCHOTT).

dispersion. In our numerical simulations we set $\epsilon_d = 12.4$ and $\epsilon_m = -103.3 + i 8.1$, corresponding to GaAs and Ag, respectively, at a wavelength of $\lambda_0 = 1.55 \mu\text{m}$.^{22,23}

The optical properties of multilayers are often described by the EMT, also known as optical homogenization theory,²⁴ provided that the radiation wavelength is much greater than the dimensions of a unit cell of the multilayer. The EMT may be useful in describing both propagating volume and surface modes instead of the accurate transfer-matrix solutions.^{25,26} It furnishes relatively simple expressions and is computationally undemanding. However, caution is necessary when utilizing EMT, especially for metal-dielectric structures.^{18,27} The limitations of the theory have been investigated variously for weakly dissipative metamaterials¹⁹ and 1-D laminar gratings,^{11,18} but also for complex nanocomposites, including those with fractal patterns.²⁸ An isofrequency, or space dispersion relation of light propagation in both all-dielectric and metal-dielectric nanostructured multilayers can significantly differ from the results of the EMT due to high nonlocalities.²⁹⁻³¹ For 1-D subwavelength plasmonic crystals EMT is valid if $k_d w_d \ll 1$; $k_m w_m \ll 1$, and $k_z(w_d + w_m) \ll 1$, where k_x , k_y , and k_z are the wavevector components, while

$$k_d = k_0 \sqrt{\epsilon_d - (k_x^2 + k_y^2)/k_0^2}; \quad k_m = k_0 \sqrt{\epsilon_m - (k_x^2 + k_y^2)/k_0^2}; \quad k_0 = 2\pi/\lambda_0.$$

The isofrequency surfaces in the three-dimensional space of wavevectors for $\epsilon_{\perp} > 0$ and $\epsilon_{\parallel} > 0$ obtained by the EMT are spheroid for ordinary modes that correspond to TE-polarization, while extraordinary modes that correspond to TM polarization are described by an ellipsoid. In this case our plasmonic metamaterial qualitatively behaves like a uniaxial crystal with positive birefringence. If $\epsilon_{\perp} < 0$ and $\epsilon_{\parallel} > 0$ the isofrequency surface becomes a hyperboloid. A consideration of the EMT applied for the case of surface modes in laminar metal-dielectrics can be found in Ref. 11, and its application to the case of Dyakonov waves in Refs. 16 and 17.

By applying the continuity of fields as the standard boundary conditions at $x = 0$, one can see that both ordinary (TE) and extraordinary (TM) evanescent modes in metal-dielectric superlattice must become coupled with the evanescent wave in the isotropic dielectric medium. Contrary to the standard surface plasmon polaritons that are widely studied in plasmonics and are exclusively TM-polarized, such surface modes become necessarily hybrid in polarization and propagate obliquely with respect to the optical axes. This was precisely Dyakonov's conclusion in 1988 for the case of planar interface between isotropic and anisotropic dielectrics.¹² Dyakonov equation for space dispersion reads

$$(\kappa + \kappa_e)(\kappa + \kappa_o)(\epsilon \kappa_o + \epsilon_{\perp} \kappa_e) = (\epsilon_{\parallel} - \epsilon)(\epsilon - \epsilon_{\perp})k_0^2 \kappa_o, \quad (2)$$

where κ_e (extraordinary) and κ_o (ordinary) are the imaginary wavevector components normal to the boundary (x -direction), while k_0 is the wavevector in free space.

Strictly speaking, Dyakonov Eq. (2) is applicable only if EMT is valid. However, within the regions of existence of Dyakonov-like surface waves, the FB solutions for TM and TE

modes can be approximated with high accuracy by ellipses and circles. That procedure allows for Dyakonov Eq. (2) to be employed.

According to Eq. (2), Dyakonov waves can propagate in a narrow angular domain $\Delta\theta = \theta_{\max} - \theta_{\min}$. Here θ stands for the angle between the two-dimensional wavevector \vec{q} ($k_y = q \sin \theta$; $k_z = q \cos \theta$) and the optical axis. The angular domain is proportional to the birefringence of material determined by the difference between refractive indices in the z-direction and transversal to it, $\Delta n = \sqrt{\varepsilon_{\parallel}} - \sqrt{\varepsilon_{\perp}}$.

Assuming that all dielectric constants (ε , ε_{\parallel} and ε_{\perp}) are positive and imposing that all decay rates involved must be positive, the following additional restriction for the existence of Dyakonov surface waves becomes valid

$$\varepsilon_{\parallel} > \varepsilon > \varepsilon_{\perp}. \quad (3)$$

As a consequence, positive birefringence is mandatory to ensure the existence of surface waves. In addition, the value of the dielectric permittivity of the isotropic media has to be between the parallel and the perpendicular ones with respect to the optical axes of the plasmonic metamaterial. Therefore, such a layered superlattice cannot be formed by all-dielectric materials, since their birefringence is always negative.

To consider the full-wave solution of Maxwell's equations in bulk 1-D-periodic media with binary unit cell it becomes necessary to use the exact transfer-matrix method.²⁵ As a result, two FB dispersion equations can be obtained for TE-polarized (ordinary) and TM-polarized (extraordinary) modes that can propagate within the periodic Ag-GaAs structure illustrated in Fig. 1^{25,26}

$$\cos(k_z L) = \cos(k_m w_m) \cos(k_d w_d) - \eta_{o,e} \sin(k_m w_m) \sin(k_d w_d), \quad (4)$$

where k_z represents the pseudo-moment of a Bloch wave, $L = w_m + w_d$ is the unit cell thickness, while $\eta_o = (k_d^2 + k_m^2)/2k_d k_m$ and $\eta_e = (\varepsilon_m^2 k_d^2 + \varepsilon_d^2 k_m^2)/2\varepsilon_m \varepsilon_d k_d k_m$ are coefficients for TE (ordinary) and TM (extraordinary) waves, respectively. Finally, $k_d^2 = \varepsilon_d k_0^2 - k_x^2 - k_y^2$ represents the dispersion equation for bulk waves within GaAs, and $k_m^2 = \varepsilon_m k_0^2 - k_x^2 - k_y^2$ is the corresponding equation for silver.

It is worth noting that the dispersion equations for EMT for 1-D subwavelength plasmonic crystal¹¹ can be obtained as a special case of the FB Eq. (4) using a corresponding Taylor expansion for the case when $k_d w_d \ll 1$; $k_m w_m \ll 1$ and $k_z L \ll 1$.

In some cases, the propagation of Dyakonov-like waves can be prevented due to high absorption that can be described by energy attenuation length $l = [2\text{Im}(q)]^{-1}$. Because of that we utilize a figure of merit $\text{FOM} = \text{Re}\{q\}/\text{Im}\{q\}$ describing the influence of absorption losses. Obviously, high values of FOM are desirable.

3 Results and Discussion

A consideration of the two FB Eq. (4) shows that their solutions are periodic in k_z with a period $2\pi/L$, contrary to EMT solutions. They are dependent on the unit cell thickness $L = w_m + w_d$ for a fixed filling factor f , since nonlocalities and retardation effects are not neglected, as is the case with the EMT. Nonlocalities must be taken into account for metallic layer thickness of the order of the metal skin-depth or lower. For silver, we estimate $\lambda_s = c/\omega_p \approx 24$ nm, where ω_p is the plasma frequency. Notice that in practice, metallic strata less than 10 nm thick are rarely used. In some cases, the solutions of FB equations reveal dual elliptic-hyperbolic periodic isofrequency curves.³⁰

The calculated birefringence of the Ag-GaAs laminar structure is $\Delta n > 3.7$. For comparison we quote $\Delta n = 0.0084$. for crystalline quartz and $\Delta n = 0.22$ for liquid crystal BDH-E7.³² Thus our plasmonic superlattice has a birefringence greater by more than an order of magnitude.

The isofrequency curves for various Ag layer thicknesses w_m , but for a fixed filling factor f , obtained from the FB Eq. (4) (for $k_x = 0$), in the case of negligible losses, are shown in Fig. 2 together with the corresponding EMT solution. We observe that the EMT is sufficiently accurate for $w_m \leq 3$ nm only.

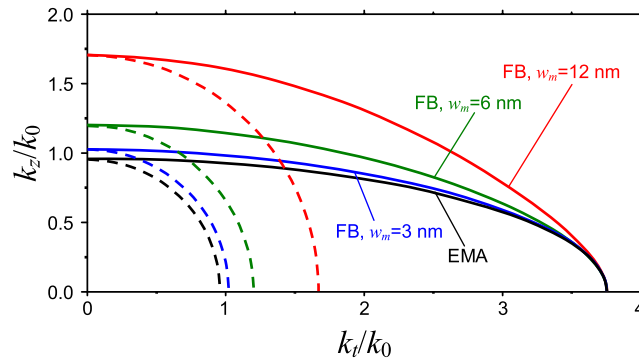


Fig. 2 Isofrequency curves (spatial dispersion) for Ag-GaAs metal-dielectric superlattice by using Floquet-Bloch equation (blue, red, and green) and EMA (black), for various metallic layer thickness. Dashed lines: TE—polarization; full lines: TM—polarization. Losses in Ag layers are neglected.

The contours for $w_m = 6$ nm (green), and $w_m = 12$ nm (red) are ellipse-like (solid), and circle-like (dashed) curves, but they are not the true ellipses and circles, respectively. Apparently Eq. (13) is in good agreement with the EMT in the vicinity of $k_z = 0$ for TM waves. In contrast, propagation along the z -axis, where $k_y = 0$, results in larger discrepancies, as the Bloch wave number k_z increases for higher w_m . This effect is observed simultaneously for TM and TE waves. Consequently the form birefringence displayed by TM waves is reduced (see Fig. 3). For TE waves, isotropy of the isofrequency curve is practically conserved, e.g., $n_{\perp} = 1.70$ and $n_{\parallel} = 1.67$ for $w_m = 12$ nm. At the same time, ϵ_{\perp} increases with w_m . Figure 3(b) shows the angular range of existence for Dyakonov-like surface waves obtained by FB.

Nonlocal effects can substantially impact the existence of Dyakonov-like surface waves. Increasing ϵ_{\perp} by decreasing f leads to a significant modification of the isofrequency curve

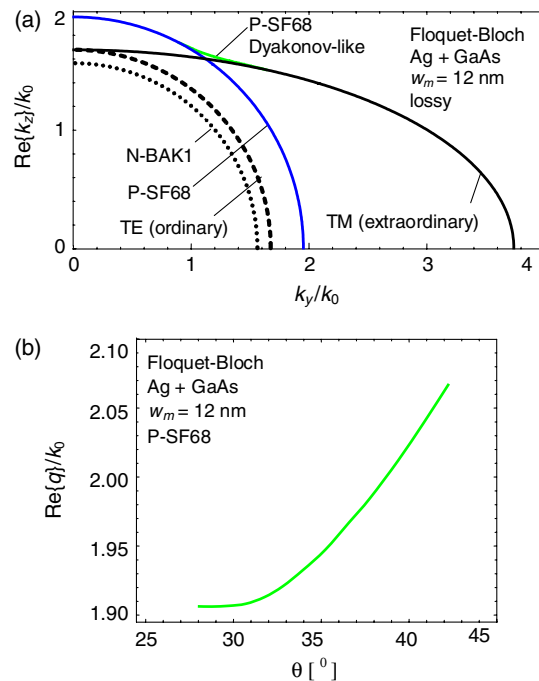


Fig. 3 (a) Spatial dispersion (isofrequency curves) of Dyakonov-like surface waves (green) at the interface of Ag-GaAs superlattice and P-SF68 (blue) substrate utilizing Floquet-Bloch equation; $f = 0.10$ and $w_m = 12$ nm. (b) Angular range of existence for Dyakonov-like surface waves at the interface of Ag-GaAs and P-SF68 substrate by using Floquet-Bloch equation. Realistic losses in Ag are included.

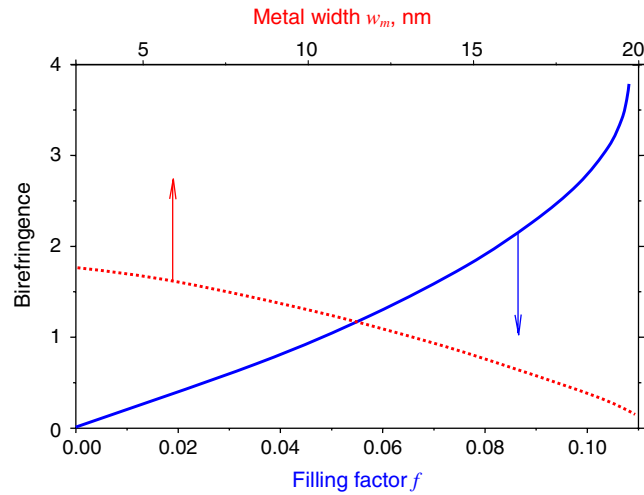


Fig. 4 Birefringence for Ag-GaAs superlattice as a function of filling factor (blue), and as a function of metallic layer thickness with a constant filling factor $f = 0.10$ (red).

derived from Eq. (2). According to Eq. (3) it may entirely prevent the existence of surface waves. In Fig. 4 we present the form birefringence as a function of the filling factor f (solid blue line), and as function of metallic layer width w_m for a fixed filling factor $f = 0.1$ (dotted red line).

As it can be seen, the birefringence increases with the filling factor up to $f = f_0$, which is 1.07 in our case. However, the birefringence decreases with the metallic layer thickness for a fixed filling factor $f = 0.1$. Consequently, the angular range of existence of Dyakonov-like waves $\Delta\theta$ will decrease.

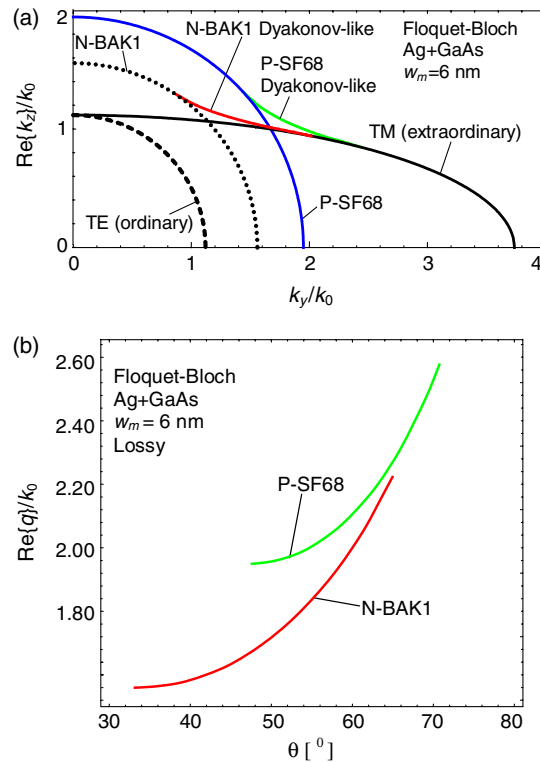


Fig. 5 (a) Spatial dispersion (isofrequency curves) of Dyakonov surface waves at the interface of Ag-GaAs superlattice and N-BAK1 (red), or P-SF68 (green) substrate utilizing Floquet-Bloch equation; $f = 0.1$ and $w_m = 6$ nm. (b) Angular range of existence for Dyakonov-like surface waves for the same substrates by using Floquet-Bloch equation; losses in Ag layers are included.

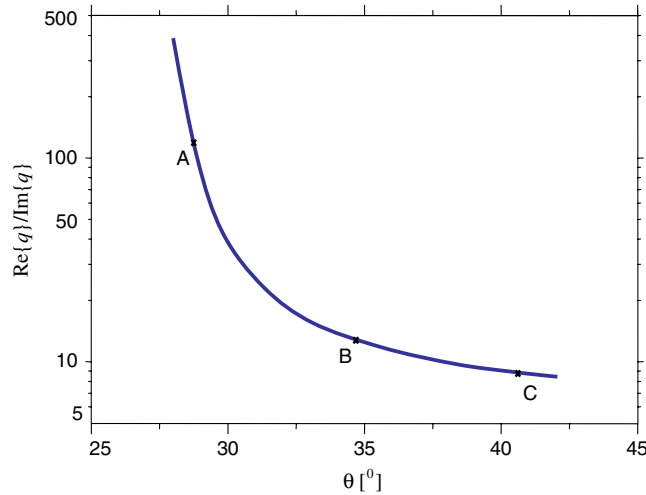


Fig. 6 Figure of merit (FOM) as a function of angle of propagation corresponding to Dyakonov-like hybrid surface waves at the boundary between a semi-infinite P-SF68 (SCHOTT) substrate and a plasmonic Ag-GaAs superlattice with $f = 0.10$ and $w_m = 12$ nm. Points A, B, and C correspond to high, moderate and low FOM, respectively.

To further study Dyakonov-like surface waves at the Ag-GaAs interface, we have used FB Eq. (4) with $w_m = 6$ nm and $w_m = 12$ nm, and a filling factor of $f = 0.1$. The dissipative effects in metallic layers have been included, too. Since the imaginary part of ϵ_m is not neglected, k_z becomes complex. Furthermore, we impose that the real parts of the parameters κ , κ_o and κ_e in Eq. (2) are all positive, which is correlated with the requirement that the field decays exponentially from the surface, thus remaining confined near $x = 0$. We evaluate numerically k_z for a given k_y and plot $\text{Re}\{k_z\}$ as a function of k_y . The results are presented in Fig. 5(a) for $w_m = 6$ nm; $f = 0.1$, for N-BAK-1 (red line), and P-SF68 (green line) substrates, respectively.

In Fig. 5(b) we present $\text{Re}\{q\}/k_0$, as a function of $\theta = \text{Re}\{\arctan(k_y/k_z)\}$ for the same parameters and substrates. As can be seen, the angular range of existence is $\Delta\theta \approx 32$ deg with $\theta_{\min} = 33$ deg for N-BAK1, and $\Delta\theta \approx 23$ deg with $\theta_{\min} = 47.4$ deg. Generally, as the substrate permittivity ϵ increases, the angular domain of existence of Dyakonov-like waves decreases and moves toward higher angles.

The situation when $w_m = 12$ nm and all other parameters are kept the same is presented in Fig. 3(a) and 3(b). Now, there are no Dyakonov-like surface waves for N-BAK1 substrate, because of violation of Eq. (3). The angular range of existence becomes smaller, $\Delta\theta \approx 14$ deg with $\theta_{\min} = 28$ deg, but shifted toward lower angles.

In Fig. 6 we plot FOM as a function of k_y , in the range of existence of the surface waves. The boundaries of such a curve are established according to the ability of the electromagnetic field to be confined in the neighborhood of $x = 0$, which leads to a certain inaccuracy from the computational grounds. For paraxial surface waves with low k_y , we observe that $\text{Im}\{q\} \ll \text{Re}\{q\}$, or high FOM. This is caused by a large shift of the intensity maximum toward the transparent isotropic medium. In this case, $\text{Re}\{\kappa\} \rightarrow 0$. On the other hand, nonparaxial waves with high k_y are characterized by deep energy penetration inside the plasmonic superlattice, and

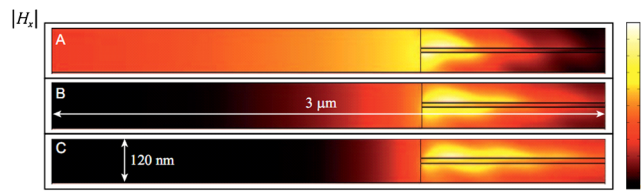


Fig. 7 Three contour plots of magnetic field $|H_x|$ in the points A, B, C as given in Fig. 6, evaluated by the finite element method. Left: P-SF68 [SCHOTT] glass, right: plasmonic Ag-GaAs superlattice with $f = 0.10$ and $w_m = 12$ nm.

$\text{Re}\{\kappa_e\} \rightarrow 0$. As a consequence, losses in metal are manifested by significantly higher values of $\text{Im}\{q\}$, or low FOM.

To complete our analysis, we determined field profiles near the interface between the AgGaAs superlattice and the P-SF68 (SCHOTT) substrate. For that purpose numerical simulations were performed using a commercial software package (COMSOL Multiphysics) based on the finite element method. Notice that our computer simulations have not revealed surface waves for N-BAK1 substrate ($n = 1.56$), as expected. Clearly, this is because of the violation of Eq. (3) in that case. However, for P-SF68 (SCHOTT) substrate this inequality is not violated. The corresponding field profiles that are presented in Fig. 7 are fully consistent with the FOM analysis given in Fig. 6.

Finally, it is worth mentioning that the above analysis is valid for a fixed value of wavelength of $\lambda_0 = 1.55 \mu\text{m}$. Results at other wavelengths are expected to qualitatively differ from those presented here.

4 Conclusion

We conclude that oblique surface waves may propagate at an interface between a plasmonic bilayer superlattice and an isotropic transparent material. These modes are not TM-polarized, since all three spatial components of the electric, as well as of the magnetic, field are involved, i.e., these modes are hybrid in polarization. Our numerical simulations prescribe the use of substrate materials with higher refractive index for the existence of surface waves. A large increase of the angular range of Dyakonov-like surface waves is attainable with large to moderate energy attenuation lengths. Thus, somewhat counter-intuitively, the introduction of weak absorption losses actually increases the angular domain of existence for hybrid surface waves. Finally, we point out that the properties of the resulting bound states change rapidly with the refractive index of the surrounding medium (cover), which suggests potential applications for chemical and biological sensors.

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