Analysis of the resonance characteristics of surface plasmon polariton modes at air-metal interfaces in the ultraviolet, visible and infrared regions

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Abstract. Excitation of surface plasmon polariton (SPP) modes results in the appearance of resonance line shapes observed in the attenuated total reflection spectra of layered structures in the Otto or Kretschman configurations. The sensitivity of the resonance characteristics of the propagating modes to changes in optical characteristics of the environment is widely used in sensor devices to determine qualitative and quantitative changes in the environment, as well as low concentrations of substances adsorbed on the surface. In the present work, we analyze the resonance characteristics of SPP modes based on the optical properties of plasmonic materials. Interfaces of metal-dielectric structures support the propagation of SPP modes. Estimation of the dispersion dependences of the propagation constant of the SPP mode, sensitivity to changes in external conditions, enhancement of the near field on the surface is carried out within the electromagnetic theory based on approximations of asymmetric shapes of spectral resonance lines of SPP by Fano formulas in the ultraviolet, visible, and infrared regions.

1. Introduction

In the last decade, many research works in nanophotonics have been devoted to study of propagating eigenmodes in optical structures. Resonance effects associated with modes excitation, such as field enhancement (FE) and narrow resonance lines in spectra, are of great interest both for fundamental and for applied research [1]. Thus, resonance effects are observed in spectra of planar layered metal-dielectric structures that support modes of surface plasmon polaritons (SPP) propagating along the metal-dielectric interfaces [2]. The modes of metal-dielectric structures in the visible region are characterized by large energy losses associated with absorption in the metal. Due to their low Q-factor, wide resonances were detected in the past century in the spectra of attenuated total reflection (ATR) of layered planar plasmon structures in Otto and Kretschman configurations. The demands for high-
resolution measurements and higher electromagnetic FE imply the research on structures with high-Q resonances. Studies on the FE and resonance phenomena at the metal-insulator interfaces are important for various applications, such as nanoscale local light sources, integrated optical circuits, amplification and attenuation of single molecules fluorescence. The applications of resonance effects in the infrared (IR) region, which is characteristic for the excitation of vibrational modes of molecules of organic compounds, attracted considerable interest [3].

Previously, resonance spectra in three-layer structures in the Kretschmann configuration based on exact electromagnetic (EM) theory were analyzed to obtain the resonance characteristics of SPP modes in the ultraviolet (UV), visible and near-IR regions [4, 5]. It was shown that the sensitivity of the resonance position to the changes in the environment, width and height of the resonances determine the resolution of sensing structures. However, the rigorous numerical calculations require heavy data processing. Recently, Fano approximations of asymmetric surface plasmon resonance line shapes in spatial spectra of bilayer and three-layer plasmonic structures were obtained using both EM and coupled mode theories [6]. In this study, we analyze the resonance characteristics of SPP modes of a bilayer air-metal structure using the Fano approximation.

2. SPP modes of a bilayer structure

It is well known that a system of two semi-spaces with permittivities \( \varepsilon_1 = \varepsilon_1' + i\varepsilon_1'' \) and \( \varepsilon_2 = \varepsilon_2' + i\varepsilon_2'' \) can support propagating surface plasmon polariton (SPP) modes in the case of satisfying the conditions \( \varepsilon_1' < 0, \varepsilon_2' > 0, \varepsilon_1'' + \varepsilon_2'' < 0, \varepsilon_1'' \varepsilon_2'' = \varepsilon_1' \varepsilon_2' \) [2]. The materials with \( \varepsilon_1' > 0 \) and \( \varepsilon_2' < 0 \) are supposed to have properties of dielectric and metal, respectively. The considered two-layer dielectric-metal structure is schematically shown in figure 1.

![Figure 1. Excitation of SPP modes by the external evanescent field \( H \) in a bilayer dielectric-metal structure.](image)

The SPP mode of the bilayer structure is defined as \( \psi(x, z) = \psi(z) \exp(i\gamma_{SPP} k_0 x) \), where \( \gamma_{SPP} k_0 \) is the propagation constant of the mode, \( k_0 \) is the free-space wavevector. The expression for \( \gamma_{SPP} = \gamma_{SPP}' + i\gamma_{SPP}'' \) of SPP mode can be found as:

\[
\gamma_{SPP} = \sqrt{\frac{\varepsilon_1 \varepsilon_2}{\varepsilon_1 + \varepsilon_2}}.
\]

(1)

Here, \( \gamma_{SPP}' \) corresponds to the effective refractive index of the SPP mode, \( \gamma_{SPP}'' \) is the coefficient of SPP mode damping. The dispersion relation \( \gamma_{SPP}(\lambda) \) can be calculated using experimentally obtained values \( \varepsilon_1(\lambda) \) and \( \varepsilon_2(\lambda) \).

Under the conditions of SPP mode excitation, the external evanescent field \( H \) is partly outcoupled from the interface and partly couples into the SPP mode, which is supported by the dielectric-metal interface. The overall near-field enhancement (FE) of the outcoupled wave at the dielectric-metal interface is defined as \( |r_{12}|^2 = |H_\text{tot}|^2 / |H|^2 \), where \( H_\text{tot} \) is the total outcoupled evanescent wave and \( H \) is the incoupling evanescent wave. The enhancement of the outcoupled near field \( |r_{12}|^2 \) due to the SPP mode excitation results in the resonant absorption enhancement and in the appearance of the asymmetric resonance line shape in the near-field enhancement spectra. Recently we demonstrated that these asymmetric SPP resonances can be approximated by the Fano formula [6]:

\[
|r_{12}|^2 \approx \left| r_{tot} \right|^2 \frac{(\alpha - \gamma_{SPP}')(\alpha - \gamma_{SPP}'')}{(\alpha - \gamma_{SPP}')(\alpha - \gamma_{SPP}'')}.
\]

(2)
where $|r_{12}|^2$ is the approximation of $|t_{12}|^2$ at the dielectric-metal interface; $\alpha k_0$ is the in-plane propagation constant; $\gamma_{\text{pole}} = \gamma_\text{SPP}$ and $\gamma_{\text{zero}} = \gamma_\text{SPP} + 2\gamma_\text{SPP}^2 / (r_{12}(\varepsilon_2 - \varepsilon_1))$ are the pole and zero of function (2), respectively; $r_{12}^\prime = (\varepsilon_2 - \varepsilon_1) / (\varepsilon_2 + \varepsilon_1)$ is the component of the non-resonant near-field enhancement. The near-field enhancement maximum can be estimated at the position $\alpha = \gamma_{\text{SPP}}^\prime$ as $|t_{12}|^2_{\text{max}} = (\gamma_{\text{SPP}}^\prime - \gamma_{\text{zero}}^\prime)^2 + \gamma_{\text{zero}}^\prime)^2 / \gamma_{\text{SPP}}^2$. The resonance width is determined as $\Gamma = 2\gamma_{\text{SPP}}^\prime \gamma_{\text{SPP}}$ [6].

3. Results and discussions

In this work, we used the values of the refractive index of silver (Ag), gold (Au), copper (Cu) from [7] and aluminum (Al) [8]. Dielectric permittivity of air is assumed to be $\varepsilon(\lambda) = 1.0$ over the entire wavelength region. Simulations were carried out in the wavelength region from 124 to 9919 nm, which corresponds to the UV, visible and IR region of frequency spectra.

The dispersion relations of $\gamma_{\text{SPP}}^\prime(\lambda)$ are calculated by equation (1) and demonstrated in figure 2. For the air/Ag structure, the values of $\gamma_{\text{SPP}}^\prime$ decrease monotonously from 1.4 RIU at the wavelength of 350 nm with increase in the wavelength. For the air/Al structure the decrease in $\gamma_{\text{SPP}}^\prime$ is observed from the wavelength of 150 nm. Decrease in the $\gamma_{\text{SPP}}^\prime$ values is observed in the wavelength region from 500 to 9919 nm and in the region from 600 to 9919 nm for the structure air/Au and air/Cu, respectively. With the increase of wavelength from 600 to 10000 nm the value of $\gamma_{\text{SPP}}^\prime$ approaches $n_2$ for all considered bilayer structures. Therefore, excitation of SPP modes is supported in the wavelength regions above 400, 300, 300 and 150 nm at the air/Ag, air/Au, air/Cu, and air/Al interfaces, respectively.

Figure 3 shows the wavelength dependencies of the SPR width $\Gamma$. SPP mode supported at air/Al interfaces is characterized by narrow resonances in the UV wavelength region from 150 to 350 nm and next in the visible and IR regions. SPP modes supported by the air/Au and air/Cu structures are characterized by similar values of the resonance width in the wavelength region from 600 to 9919 nm. Values of width decrease for all observed structures in the all entire wavelength region except a local maximum of the width of $5 \cdot 10^{-3}$ RIU for the air/Al structure at the wavelength of 900 nm.
The maximal FE $|r_{\text{max}}|^2$ is plotted in figure 4 as a function of the wavelength. It achieves its maximal values at different wavelengths for considered metals. In particular, the $|r_{\text{max}}|^2$ maximal values exceed $2.9 \times 10^4$ for the air/Ag interface in the wavelength region from 600 nm to 2000 nm. For the air/Au and air/Cu interfaces the FE is higher than $1.0 \times 10^4$ in the wavelength region from 600 nm to 2000 nm. The FE at the interfaces achieves its maximal values for the Ag, Cu, and Au cases at the wavelength of around 1000 nm. The magnitude of the FE for the air/Al interface does not exceed 1000 in the considered wavelength region and achieves its maximal value in the UV region at the wavelength near 150 nm and in the IR region near 1500 nm. With increasing wavelength FE decreases from its maximum values for the all considered structures in the wavelength region from 1000 to 9919 nm.

Figure 4. Maximum FE at the air-metal interface.

4. Conclusion
In this work, we studied the resonance characteristics of SPP modes supported by air/metal interfaces for Ag, Cu, Au, and Al using the Fano approximation approach. We confirmed that SPP modes can be excited at the air/Au, air/Ag, air/Cu, air/Al interfaces in the UV, visible, and IR regions. The width values of the SPR line shape decreases with the wavelength for all the considered metals. The high values of FE and narrow resonance line shapes for Ag, Au, and Cu interfaces are achieved in the near- and mid-IR regions. The results obtained in the present work justify their application as high sensitivity sensors based on SPR technique. The implemented approximation approach can be further extended to analyze the resonance characteristics of SPP modes in multilayer sensing structures.

5. References
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