Fractional-Rational Representation of the Frequency Spectrum of the Scattered Field for Localized Surface Plasmon of a Metal Nanowire

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Abstract—**The paper discusses the problem of determining the eigenfrequencies of surface plasmons for metal nanowire over the frequency spectrum of the scattered field. To determine the eigenfrequencies a fractional-rational approximation of the frequency spectrum based on continued fractions was used. Q-factors for lower and higher modes of the localized surface plasmons are investigated.**

Keywords—plasmon resonance; localized surface plasmon; fractional-rational approximation; Q-factor

I. Introduction

Recently, the study of surface plasmon of the nanoobjects is an actual and important topic in nanoplasmonics [1, 2]. Various devices and elements working on plasmons such as sensors probe microdroplets [3], surface plasmon resonance sensor [4], active waveguides [5] and smart phone platforms [6] have been studied currently. The plasmonic properties of nanowires and nanoparticles have recently been investigated using a variety of methods. However, there is a lack of investigations in terms of eigenfrequencies and Q-factor of plasmons. Many authors find surface plasmons by investigating resonance peaks in Scattering Cross Section (SCS). This study cannot be considered as a complete one, because in this way only 'bright' plasmons can be seen, 'dark' plasmons that do not couple efficiently to incident wave cannot be discovered in such a description. In paper [7] researchers developed nonquasistatical expressions for the eigenvalues of surface plasmons that includes finding of eigenfrequencies and Q-factor. Using this approach all possible plasmons can be found and investigated, including 'dark' and multipole ones.

Approximation of the frequency spectrum by a fractional-rational model also makes it possible to determine the eigenfrequency values. The use of the additive pole model for these purposes also makes it possible to determine the amplitude coefficient (residue) for each excited natural oscillation. This allows us to estimate the contribution of each natural oscillation of the surface plasmon (the brightness of the plasmon) to the response in the form of the SCS frequency spectrum.

To determine the eigenfrequency values a fractional-rational approximation of the frequency spectrum based on continued fractions [8-9] can be used. This approach has been successfully applied in [10-11] to process the frequency spectrum of various resonant structures.

The aim of this paper is to investigate the possibility of applying a fractional-rational approximation to determining the eigenfrequency and Q-factor of the localized surface plasmon in a single metal nanowire.

II. Statement of the Problem and Method of Solution

The problem of determining the eigenfrequencies of surface plasmons of a metal nanowire with the radius a over the frequency spectrum of the scattered field has been examined. The frequency dependent plasma permittivity is described by the Drude model

$$\varepsilon_p(\omega) = 1 - \frac{\omega_p^2}{\omega^2 - j\gamma\omega}, \qquad (1)$$

where ω_p represents the plasma frequency, γ characterizes decaying process. The field excited by a plane wave for the considered object is represented in the form of the expansion

$$H(\rho,\varphi)=\sum_{s=-\infty}^{\infty}A_s J_s(k_p\rho)e^{js\varphi}, \quad \rho\le a, \tag{2}$$

$$H(\rho,\varphi)=\sum_{s=-\infty}^{\infty}\overline{A}_s H_s^{(2)}(k\rho)e^{js\varphi}+e^{-j\rho\cos(\varphi-\alpha)}, \quad \rho>a, \tag{3}$$

where $k=\omega/c$ is the wave number of free space, $k_p=n_p k$ is wave number in the plasma determined by the value $n_p=\sqrt{\varepsilon_p}$, α is the angle of incidence of a plane wave. The coefficients of the expansion A_s and $\overline{A}_s$ are determined from the boundary condition as

$$A_s=-\frac{2jn_p}{\pi a F_s}e^{-js(\alpha+\pi/2)}, \tag{4}$$

$$\overline{A}_s=\frac{V_s}{F_s}e^{-js(\alpha+\pi/2)}. \tag{5}$$

Here

$$F_s=H_s^{(2)}(ka)J_s(k_pa)\left[\frac{1}{n_p}\frac{J_{s+1}(k_pa)}{J_s(k_pa)}-\frac{H_{s+1}^{(2)}(ka)}{H_s^{(2)}(ka)}-s\frac{1-\varepsilon_p}{\varepsilon_p ka}\right], \tag{6}$$

$$V_s=J_s(ka)J_s(k_pa)\left[\frac{1}{n_p}\frac{J_{s+1}(k_pa)}{J_s(k_pa)}-\frac{J_{s+1}(ka)}{J_s(ka)}-s\frac{1-\varepsilon_p}{\varepsilon_p ka}\right]. \tag{7}$$

Since under the condition $ka>>1$ the asymptotic representation is valid

$$H_s^{(2)}(k\rho)\approx\sqrt{\frac{2}{\pi k\rho}}e^{-j(k\rho-\pi/4-s\pi/2)}, \tag{8}$$

then the field scattered by the metal nanowire in the domain $\rho>a$ can be written as

$$H(\rho,\varphi)\approx\sqrt{\frac{2}{\pi k\rho}}e^{-j(k\rho-\pi/4)}\sum_{s=-\infty}^{\infty}\overline{A}_s e^{js(\varphi+\pi/2)}. \tag{9}$$

The far-field normalized by the field of an infinitely thin wire will take the form

$$H(\varphi)=\sum_{s=-\infty}^{\infty}\overline{A}_s e^{js(\varphi+\pi/2)}=\sum_{s=-\infty}^{\infty}\tilde{A}_s e^{is(\varphi-\alpha)}, \tag{10}$$

where we used $\tilde{A}_s=\overline{A}_s e^{is(\alpha+\pi/2)}$ for excluding the dependence on the incidence angle of the exciting plane wave from the expansion coefficients. Further consideration of the frequency properties of the scattered field will be investigated for the case $\varphi=\alpha$. We will consider the frequency spectrum which are defined as

$$H(\omega)=\sum_{s=-\infty}^{\infty}\tilde{A}_s. \tag{11}$$

To determine the eigenfrequencies in the considered metal wire, the approximation of the investigated spectrum by a fractional-rational model

$$H_M(\omega)=g\frac{\prod_{m=1}^{M}(\omega-z_m)}{\prod_{m=1}^{M}(\omega-p_m)}=r_0+\sum_{m=1}^{N}\frac{r_n}{\omega-p_m} \tag{12}$$

is used. The parameters of this model are the values of the poles $\mathbf{p}=\{p_1,p_2,\ldots,p_M\}$ and zeros $\mathbf{z}=\{z_1,z_2,\ldots,z_M\}$ or residues $\mathbf{r}=\{r_0,r_1,\ldots,r_M\}$ of spectrum. To solve the problem of approximation of the resonant frequency response by a fractional-rational function a continued fraction of the order $L=2M+1$ is used. The values of the poles $\mathbf{p}$ and zeros $\mathbf{z}$ are determined by the parameters of the continued fraction approximating the considered spectrum [8-9].

For single-pole model $H_1(\omega)=r_0+r_1/(\omega-p_1)$ at frequency $\omega=\operatorname{Re}p_1$ when $r_0\to 0$, its frequency response will be determined by the quantity $R_1=jr_1/\operatorname{Im}p_1$. Therefore as the amplitude coefficient for the eigenfrequency p_m ($m=1,2,\ldots,M$) we will use the normalized value of the residue $R_m=jr_m/\operatorname{Im}p_m$ ('plasmon brightness').

III. Numerical Results

In this examination for the convenience of analyzing the eigenfrequencies following normalized values were used: $w_p=\omega_p a/c$ is normalized plasma frequency, $f=w/w_p=\omega/\omega_p$ is normalized frequency (where $w=ka$) and $a'=a\,\omega_p/c$ is normalized radius of wire. The real part of the eigenfrequency will be denoted by w_0, imaginary part as δ and we will also normalize them to the plasma frequency.

The possibility of determining the eigenfrequencies of the surface plasmon of a metal wire from the frequency spectrum of the scattered field by means of its fractional-rational approximation has been studied in several examples. Figure 1 shows the frequency spectrum of the scattered field for a single metal wire with a normalized value of radius $a'=1$ (for the case $\gamma=0.001\cdot\omega_p$) and the result of its fractional-rational approximation. The estimations of parameters of the model

(12) are present in the inset. The spectrum and fractional-rational approximation agree with graphical accuracy, error of approximation $\rho = \|H(\omega) - H_M(\omega)\|^2 \big/ \|H(\omega)\|^2$ was equal to $5.7 \cdot 10^{-14}$ %. Figure 2 shows the additive pole representation of the considered frequency spectrum: components of the model (12) are represented by separate lines of different colors.

Analysis of the presented results shows that this approach can be successfully used for determination of the eigenfrequencies of the lowest modes which in the spectrum are initially represented by separate resonance peaks gradually merging into one peak and have a nonzero amplitude coefficient $R_m = j\, r_m \big/ \operatorname{Im} p_m$ (normalized value of residue). The higher modes have practically zero amplitude and are located nearer each other. Therefore it is difficult to determine the eigenfrequencies for them by using of fractional-rational approximation and their contribution to the total frequency response does not make sense.

For a larger radius of wire the first components of the spectrum are more separated from each other and have a larger amplitude coefficient. Therefore the fractional-rational approximation of their scattering frequency spectrum requires the use of a larger order of model. Figure 3 reports the results of a fractional-rational approximation of the frequency scattering spectrum for a metal nanowire with a large radius equal to $a' = 5$. Figure 4 shows the corresponding additive pole representation of the spectrum (with an indication of the contribution of each spectral component).

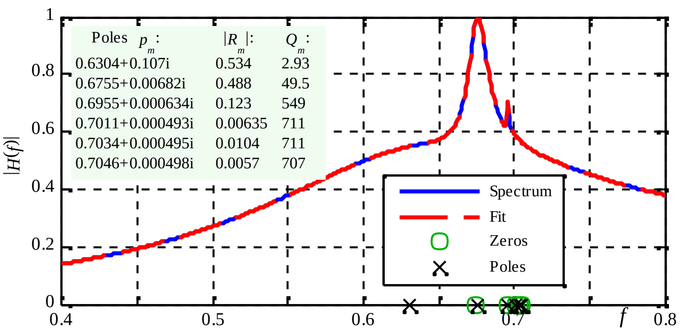

Figure 1. Fractional-rational approximation of the frequency spectrum of scattering of nanowire with radius $a' = 1$.

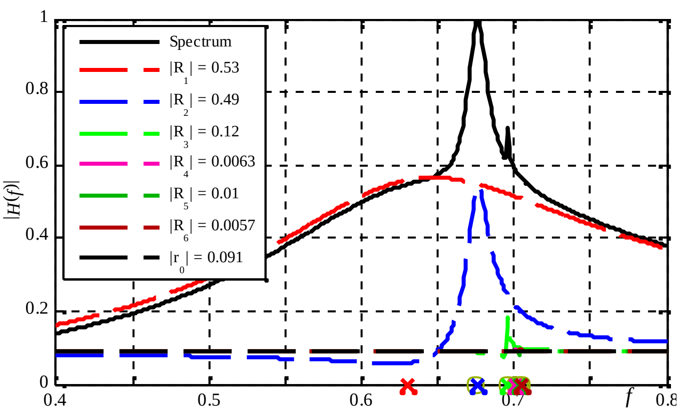

Figure 2. The pole representation of the frequency spectrum of the scattering of nanowire with radius $a' = 1$

We see that for the considered case the height of the pole peaks increases and then as we approach the frequency of the surface plasmon resonance for plane case $f_{SP} \approx 1/\sqrt{2}$ is falls sharply. Figure 5 shows the spectrum of the amplitude coefficients of the expansion of the scattered field $\overline{A}_s$ (spectrum is represented by a dashed line). This spectrum has the same characteristics. In this case the amplitude coefficients of the expansion of the internal field of the wire A_s monotonically increase with increasing their number. Figure 6 presents their spectrum for wire with radius $a' = 5$.

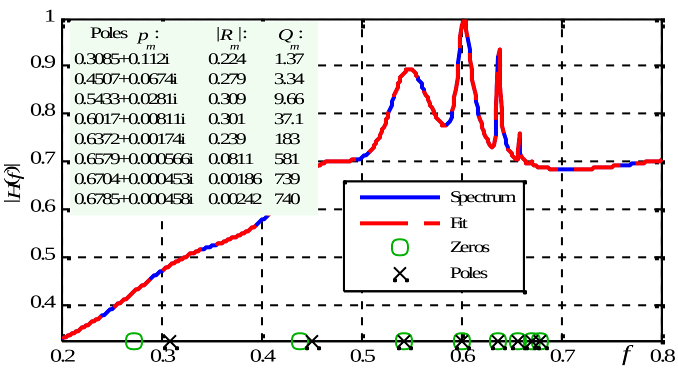

Figure 3. Fractional-rational approximation of the frequency spectrum of scattering of nanowire with radius $a' = 5$.

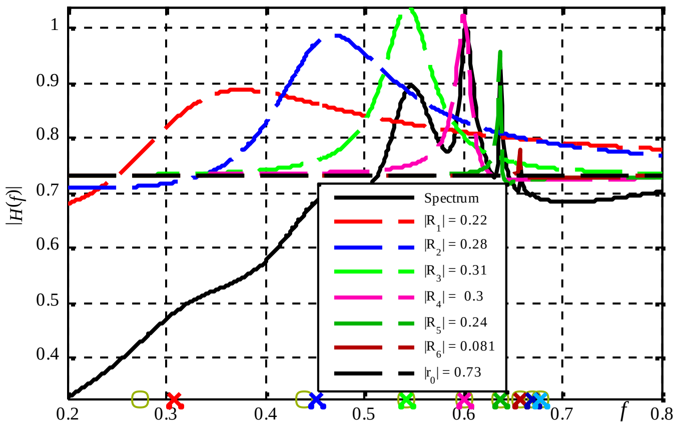

Figure 4. The pole representation of the frequency spectrum of the scattering of nanowire with radius $a' = 5$

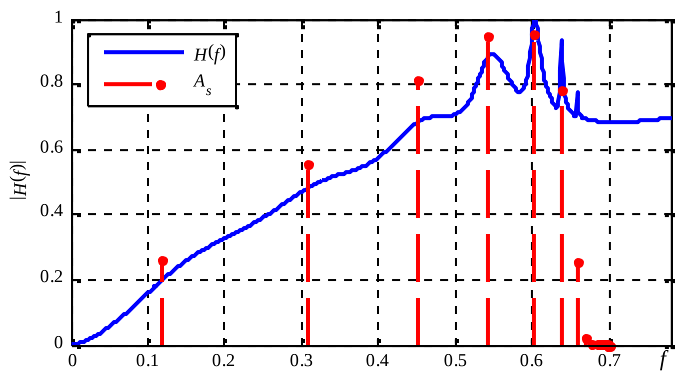

Figure 5. The spectrum of the coefficients of the expansion for the scattered field by nanowire with radius $a' = 5$

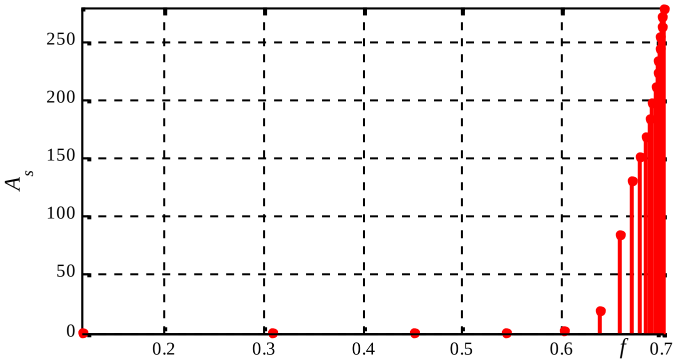

Figure 6. The spectrum of the coefficients of the expansion for the internal field of nanowire with radius $a' = 5$

When considering the values of the eigenfrequency of surface plasmon in nanowire we compare them with the eigenfrequency of the surface plasmon for a plane interface which is defined as

$$\omega_{\text{SP}} = \frac{\omega_p}{\sqrt{2}} \sqrt{1 - \frac{\gamma^2}{2\omega_p^2}} + j\frac{\gamma}{2} . \tag{13}$$

Hence, the Q-factor of such surface plasmon can be defined as $Q_{\text{SP}} \approx \omega_p / \gamma\sqrt{2}$.

Figures 7-8 shows the dependence of the eigenfrequencies on the mode number s for the three different values of radius of the metal wire $a' = \{0.5, 1, 2\}$. A finite part of the graphs corresponding to the large mode numbers is shown in the inset with gray background. We see that regardless of the wire radius the normalized value of the real part of the eigenfrequency with increasing mode number tends to the normalized value of the frequency of the surface plasmon $f_{\text{SP}} = \omega_{\text{SP}} / \omega_p \approx 1/\sqrt{2}$. The imaginary part of eigenfrequency decreases to order $\operatorname{Im}\omega_{\text{SP}} / \omega_p = \gamma / 2\omega_p$ determined by the coefficient of absorption in the medium $\gamma = 0.001 \cdot \omega_p$.

With reducing the radius value the frequency of the lowest mode tends to the limiting value $f_{\text{SP}} = 1/\sqrt{2}$ and its losses tend to the minimum reached level. In this case for losses depending on the radius for a given number of mode reaches a minimum. We see that an increase of the radius value of nanowire leads to an increase in the depth of this minimum.

Figure 9 presents the dependence of the Q-factor of the eigenoscillations of the considered metal wire against the number of mode. We see that the lower modes have a low Q-factor. With the growth of the mode number a rapid increase in the Q-factor occurs to a practically constant level due to the decrease of radiation losses (to the level of the intrinsic (unloaded) Q-factor $Q_0 = Q_{\text{SP}} \approx \omega_p / \gamma\sqrt{2}$ in this case equal to 707). We see that an increase of the radius of nanowire leads to an increase of the number of mode which is required to reach this level.

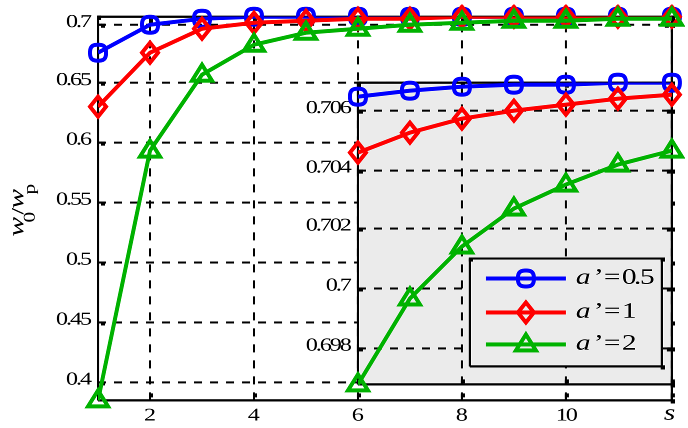

Figure 7. Dependence of value of the real part of the eigenfrequency vs the number of mode.

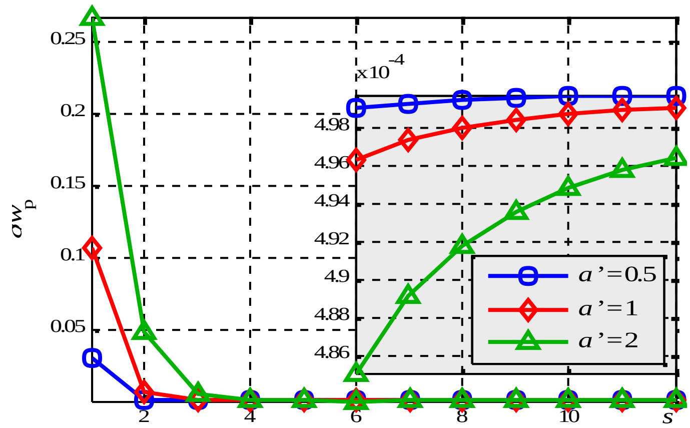

Figure 8. Dependence of value of the imaginary part of the eigenfrequency vs the number of mode.

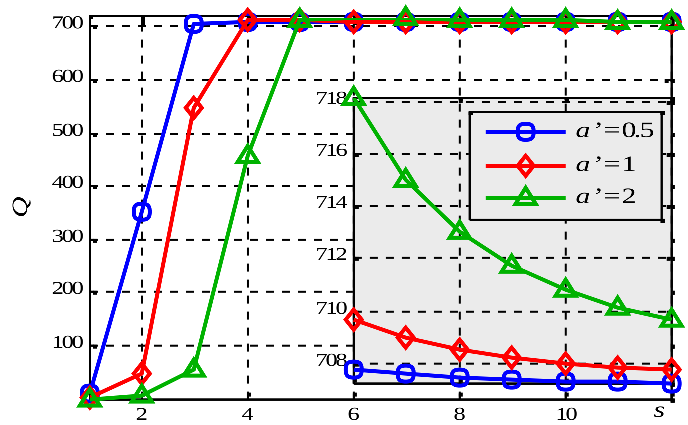

Figure 9. Dependence of the Q-factor of the eigenmodes vs the number of mode.

If we assume approximately that the considered resonances are determined only by the surface wave propagated along the interface to the plasma (in this case along a circle of radius a), then on the resonance frequency the condition $\operatorname{Re} k_S a = s$ must be satisfied. Here

$$k_S = \frac{\omega}{c}\sqrt{\frac{\varepsilon_p(\omega)}{\varepsilon_1 + \varepsilon_p(\omega)}} = \frac{\omega}{c}\sqrt{\frac{1-\omega_p^2/(\omega^2 - j\gamma\omega)}{2-\omega_p^2/(\omega^2 - j\gamma\omega)}} \qquad (14)$$

is the propagation constant of the surface wave that are propagating along the interface between two media with permittivities $\varepsilon_1 = 1$ and $\varepsilon_p(\omega) = 1 - \omega_p^2/(\omega^2 - j\gamma\omega)$. To exclude the influence of the dispersion of the surface plasmon against the dependence of the eigenfrequencies of the metal wire on the mode number it is possible to use the velocity (deceleration) factor

$$n_S = \frac{k_S}{k} = \sqrt{\frac{1-\omega_p^2/(\omega^2 - j\gamma\omega)}{2-\omega_p^2/(\omega^2 - j\gamma\omega)}}. \qquad (15)$$

In this case, the real part of the eigenfrequency can be determined from the condition $\mathrm{Re}\, n_S w_0 = s$. The dependence of the normalized value of the real part of the eigenfrequency $w_S = w_0 \,\mathrm{Re}\, n_S$ on the mode number *s* is shown in Figure 10. It confirms that for large wire radius the linear dependence $w_S = s$ is valid. As the radius decreases, this dependence takes place up to some number $s_{\max}$ after which the values of w_S practically cease to change and become equal $s_{\max}$. In this case, the value of $s_{\max}$ decreases in proportion to the decrease in the wire radius *a*. For *a'* = 0.1, the value of $s_{\max}$ approaches to 1. With a further decrease in the wire radius, the linear dependence of $w_S = s$ ceases to be observed, in this case for all mode numbers the equation $w_S \approx \mathrm{const} < 1$ becomes valid.

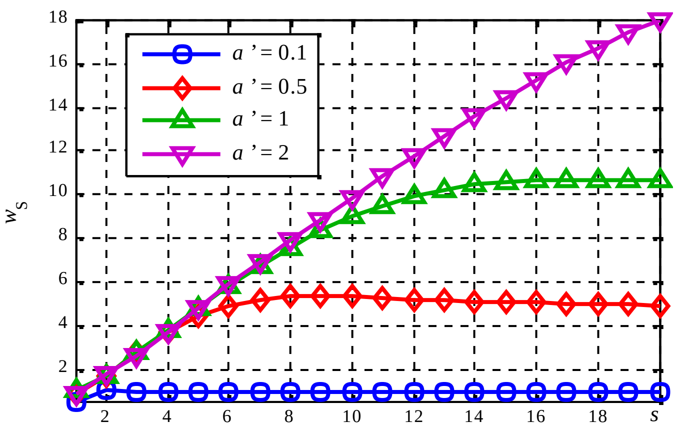

Figure 10. Dependence of normalized value of the real part of the eigenfrequency vs the number of mode.

IV. Conclusions

The problem of determining the eigenfrequencies of surface plasmons for metal nanowire over the frequency spectrum of the scattered field are studied. The realization of the fractional-rational approximation of the frequency spectrum of the scattered field of a metal wire on the basis of continued fractions makes it possible to obtain correct estimates of the complex eigenfrequency and Q-factor for our structure.

References

[1] D.M. Natarov, “Modes of a core-shell silver wire plasmonic nanolaser beyond the Drude formula,” J. Opt., vol. 16, no 7, pp. 075002/6, 2014.

[2] N.P. Stognii and N.K. Sakhnenko, “Theoretical study of plasmon excitation of a Drude metal nanowire coupled with optically dynamic shell,” Proc. In. Conf. Electron. Nanotechnol. (ELNANO-2017), pp. 205-208, Kiev, Ukraine, 18-20 April, 2017.

[3] J. Schutt, B. Ibarlucea, R. Illing, F. Zorgiebel, S. Pregl, D. Nozaki, W.M. Weber, T. Mikolajick, L. Baraban, and G. Cuniberti, “Compact nanowire sensors probe microdroplets,” Nano Lett., vol. 16, no 8, pp. 4991–5000, 2016.

[4] H. Nishi, S. Hiroya, and T. Tatsuma, “Potential-scanning localized surface plasmon resonance sensor,” ACS Nano, vol. 9, no 6, pp. 6214–6221, 2015.

[5] B. Piccione, L.K. Vugt, and R. Agarwal, “Propagation loss spectroscopy on single nanowire active waveguides,” Nano Lett., vol. 10, no 6, pp. 2251–2256, 2010.

[6] Y. Liu, Q. Liu, S. Chen, F. Cheng, H. Wang, and W. Peng, “Surface plasmon resonance biosensor based on smart phone platforms,” Scient. Rep. 5, vol. 5, 12864, 2015.

[7] N. Stognii and N. Sakhnenko, “Plasmon resonances and their quality factors in a finite linear chain of coupled metal wires,” IEEE J. Select. Topics Quant. Electron., vol. 19, no 3, 4602207, 2013.

[8] M.V. Andreev, V.F. Borulko, O.O. Drobakhin, and D.Yu. Saltykov, “Determination of parameters of fractional-rational model using interpolation by continued fraction,” Proc. In. Conf. Math. Meth. Electr. Th. (MMET-2006), pp. 264-266, Kharkiv, Ukraine, 26-29 June, 2006.

[9] M.V. Andreev, V.F. Borulko, O.O. Drobakhin, and D.Yu. Saltykov, “Determination of complex eigenfrequencies of resonators by means of fractional rational approximation by continued fractions,” Bull. Univ. Dniprop.: Series Physics. Radio Electron., vol. 15, no. 12/1, pp. 5-10, 2007 (in Russian).

[10] M.V. Andreev, V.F. Borulko, O.O. Drobakhin, V.S. Miroshnichenko, and Ye.B. Senkevich, “Determination of oscillation parameters of open resonator systems using fractional-rational approximation by continued fraction,” Proc. In. Kharkov Sympos. Physics Engin. Microwaves (MSMW-2007), pp. 334-336, Kharkov, Ukraine, 25-30 June, 2007.

[11] M.V. Andreev, O.O. Drobakhin, and D.Yu. Saltykov, “Determination of the resonant frequency and quality factor of a semi-solid dielectric resonator by means of fractional-rational approximation,” Radiophys. Radio Astron., vol. 18, no 4, pp. 362-372, 2013 (in Russian).