Studying localized surface plasmon resonances in the THz region for subwavelength spiral disks

V V Gerasimov1,2, S A Kuznetsov1,2,3, A G Lemzyakov1 and R R Hafizov1,2
1 Budker Institute of Nuclear Physics of the Siberian Branch of the RAS, 11, Ac. Lavrentieva ave., Novosibirsk, 630090, Russia
2 Novosibirsk State University, 2, Pirogova ave., Novosibirsk, 630090, Russia
3 Rzhanov Institute of Semiconductor Physics SB RAS, Novosibirsk Branch “TDIAM”, 2/1, Ac. Lavrentieva ave., Novosibirsk, 630090, Russia

v.v.gerasimov3@gmail.com

Abstract. Spoof localized surface plasmon resonances (LSPRs) in the THz range are promising for bio-sensing and spectroscopy. Using long spiral grooves allows improving the surface mode confinement of LSPRs in the long-wavelength region. Our numerical simulations of sub-wavelength spiral gold disks in the range of 0.04–6 THz have shown that in case of Drude conductivity and normal incidence of EM radiation only the first- and second-order dipole localized surface plasmon resonances (LSPRs) are excited. High order resonances arise at inclined incidence. The spectra and 2D distributions of the EM field at the resonant frequencies depend on the number of spiral arms and symmetry of the spiral structure.

1. Introduction
Localized plasmon resonance is resonant oscillation of the charge density of free electrons in conducting particles of sub-wavelength size in an oscillating external field, accompanied by enhancement of the near field at the surface of the particles [1]. Localized plasmon resonances exhibit strong spatial localization and amplification of electromagnetic field near the particle surface and depend on the shape, size, and conductivity of the particle and its environment. These properties have wide applications in the visible frequency range: in chemical sensors and biosensors [2], amplification of surface-enhanced Raman scattering [3], fluorescence amplification [4], second harmonic generation [5], solar batteries [6], and photocatalysis [7].

The terahertz (THz) spectral range (covering the frequency domain from 0.3 to 10 THz) is of great importance for biology because THz radiation is nonionizing, and the rotation and vibrational modes of complex intra- and extra-molecule bonds of biological substances lie in this region. Particularly, using plasmon resonances in the THz range is promising for sensing and spectroscopy. But the THz frequencies ($\omega_{\text{THz}} \sim 10^{12}$ Hz) are several orders lower than the plasma frequency of free electrons in metal ($\omega_p \sim 10^{16}$ Hz) and the collision frequency ($\omega_c \sim 10^{14}$ Hz [8]), and thus plasmon resonances cannot be excited in this region. To overcome these limitations, Pendry and his colleagues suggested making periodic modulation of flat surface [9], which leads to formation of bound surface states with high confinement of electromagnetic field, so called “spoof surface plasmon resonances”. It was shown that single sub-wavelength metal structures [10] are able to support spoof local surface plasmon...
resonances (LSPRs) in the long-wave region. SpooLSPRs have several advantages at low frequencies. Besides sub-wavelength confinement, which enhances light–matter interaction, LSPRs depend on geometry of corrugations, which provides flexibility in engineering the EM properties of the structures. Furthermore, the Ohmic loss, which is an obstacle in the visible range, can be neglected at low frequencies. Finally, the time-domain technique [11], which is applicable in the THz region, enables convenient collection of both the phase and amplitude information.

Azimuthally grooved cylinders (see figure 1 (A)) have been studied in the microwave region [10, 12]. The grooves are filled with a dielectric material with a refractive index \( n_g \), and the surrounding medium is air. For efficient confinement of the surface mode on the structure, the period of grooves at the outer radius \( R \) must be much less than the radiation wavelength in air \( d = 2\pi R \ll \lambda_0 \).

CST calculations were made in the THz region for a periodic structure of thin grooved gold disks on dielectric substrates [13 – 14]. It was shown that multipole LSPRs could be excited using a grooved disk combined with a C-shaped resonator or under oblique incidence of the electromagnetic wave. The resonance frequencies depend on the geometrical parameters of the disk and the incidence angle.

The grooved cylinder supports the LSPRs up to the asymptotic frequency \( \omega_a \), which corresponds to spoof surface plasmon polaritons that would propagate along a plane surface with similar grooves. The asymptote frequency depends on the groove depth \( h \) and the refractive index \( n_g \) as \( \omega_a = \pi c/2hn_g \) (for Drude-metal particles \( \omega_{p} = \omega_{p}/2 \)) [15]. An increase in the groove depth shifts the asymptote frequency (and the resonance spectrum) towards the lower frequencies and, consequently, enhances confinement of surface plasmon modes. Thus, the lowest resonance frequency is determined by the size of the disk. To improve the mode-confinement of spoof LSPRs, lately, it was suggested to use long spiral grooves (figure 1 (B)) [16]. Extension of the spiral length allows shifting the resonances of LSPRs for a wavelength exceeding by far the structure size, which results in strong EM field localization near the surface. Besides, high order resonances have high Q-factor and are more sensitive to a presence of a dielectric material on the structure, than dipole resonances, which is promising for sensing applications. Numerical calculations, theoretical analysis, and experimental tests with spiral grooves in the microwave region were reported in literature [15]. Meantime, similar structures have been studied insufficiently in the THz region.

In this work, we theoretically investigated the localized surface plasmon resonances on thin spiral grooves in the THz region. An appropriate design of spiral grooves (shape, number, length) and excitation conditions can give rise to multipole resonances in THz range.

2. Numerical simulations and selected results

A schematic drawing of a single spiral disk is presented in figure 1 (B). We model the logarithmic spirals using the following parametric equations in polar coordinates:

\[
x(t) = r \cdot e^{i\omega t(\beta)} \cdot \cos(t) \quad y(t) = r \cdot e^{i\omega t(\beta)} \cdot \sin(t),
\]

where \( r \) is the inner radius, \( R \) is the outer radius, \( \beta \) is the spiral angle, \( w \) is the width of the spiral, and \( N \) is the number of spirals. Using the results of studying similar structures in the microwave region [16], we took the parameters of the spiral disk rescaled to the THz region: \( r=2 \mu m \), spiral angle \( \beta = 80^\circ \), and
\( w = 0.5 \, \mu m \); the number of spiral arms varied: \( N = 2 - 12 \) (see figure 2). The lateral periodicity of spirals in \( x \)- and \( y \)-directions was chosen to be \( p = 60 \, \mu m \), in which the fields from adjacent disks do not affect each other (no “hybridisation effect”). The spirals were modeled as 0.3\( \mu m \)-thick gold layers with Drude conductivity patterned on a semi-infinite silicon substrate with the dielectric permittivity \( \epsilon = 11.703 (1 - j \cdot 1.17 \cdot 10^{-4}) \) \[17\].

The transmission spectra (figure 3) of the periodic array of spiral disks in the range of 0.04–6 THz were simulated using ANSYS Electromagnetics Suite R18.2, wherein the regime of Floquet ports and periodic boundary conditions applied to the structure’s unit cell was employed. In this regime oblique illumination of the examined structure is modelled by specifying a polar angle \( \theta \), which describes the angle between the wave-vector of the incoming wave and \( Z \)-axis.

At normal incidence \( \theta = 0^\circ \) of EM wave (see figure 3 (a)) there are several peaks corresponding to LSPRs. The brown dotted line at 1.46 THz correspond to the first diffraction order of the periodic structure on a Si substrate. The resonance frequency depends on the number of spirals. For two arms (non-connected and connected in the centre of the disk), the spectra for \( E_x \) and \( E_y \) polarizations are different since such geometries have asymmetry in the \( XY \) plane. The analysis of \( E_z \) field distribution near the spiral disk showed that at normal incidence all resonance frequencies matched the dipole resonances of the first or second order. The transmission spectra for a disk with six arms were calculated for Drude gold conductivity and perfect electric conductor (PEC) (see figure 3 (b)). For PEC disk the resonances are narrower and shifted to the higher frequencies compared with the Drude gold disk. The deep resonance at 0.614 THz is dipole resonance (see \( E_z \) field distribution in the upper
inset in figure 3 (b)). The $E_z$ field distribution for $\theta = 40^\circ$ at 4.08 THz correspond to the quadrupole surface mode. Thus, on spiral disk of subwave-length sizes the multipole resonances can be arisen at the inclined incidence of EM wave. High-order resonances must have high Q-factors, and we expected, that they will show more sensitivity for sensing applications compared with dipolar resonances and allow realise multi-channel biosensing.

3. Summary
The numerical simulations of subwavelength spiral grooved gold disks in the THz region have shown that in case of Drude conductivity and normal incidence of EM radiation only the dipole localized surface plasmon resonances (LSPRs) of the first and second orders are excited. High order resonances arise at inclined incidence. The spectra and distributions of the EM field in the resonances depend on the number of spiral arms and symmetry of the spiral structure.

4. References
[1] Maier S A 2007 Plasmonics: Fundamentals and Applications (Springer Verlag, New York)
[2] Anker J N, et al. Biosensing with plasmonic nanosensors 2008 Nature Materials 7 442–453
[3] Stiles P L, Dieringer J A, Shah N C & Van Duyne R P 2008 Surface-Enhanced Raman Spectroscopy Annual Review of Anal. Chem. 1 601–626
[4] Lakowicz J R et al. 2008 Plasmon-controlled fluorescence: a new paradigm in fluorescence spectroscopy Analyst 133 1308–1346
[5] Valev V K et al. 2010 Asymmetric Optical Second-Harmonic Generation from Chiral G-Shaped Gold Nanostructures Physical Review Letters 104 127401
[6] Atwater H A & Polman A 2010 Plasmonics for improved photovoltaic devices Nature Materials 9 205–213
[7] Tian Y & Tatsuma T J 2005 Mechanisms and Applications of Plasmon-Induced Charge Separation at TiO2 Films Loaded with Gold Nanoparticles J. Am. Chem. Soc. 127 7632–7637
[8] Ordal M A, Bell R J, Alexander R W, Long L L, Querry M R 1985 Optical properties of fourteen metals in the infrared and far infrared: Al, Co, Cu, Au, Fe, Pb, Ni, Pd, Pt, Ag, Ti, and W Applied Physics Lett 24 (24) 4493-4499
[9] Pendry J B, Martin-Moreno L and Garcia-Vidal F J 2004 Mimicking Surface Plasmons with Structured Surfaces Science 305 847-848
[10] Pors A, Moreno E, Martin-Moreno L, Pendry J B & Garcia-Vidal F 2012 Localized spoof plasmons arise while textured closed surfaces Phys. Rev. Lett. 108 223905.
[11] Jeon T-I and Grischkowsky D 2006 THz Zenneck surface wave (THz surface plasmon) propagation on a metal sheet Appl. Phys. Lett. 88 061113
[12] Liao Z, Shen X, Pan B C, Zhao J, Luo Yu and Cui Tie Jun 2015 Combined System for Efficient Excitation and Capture of LSP Resonances and Flexible Control of SPP Transmissions ACS Photonics 2 (6) 738-743
[13] Chen L, Wei Y M, Zang X F, Zhu Y M and Zhuang S L 2016 Excitation of dark multipolar plasmonic resonances at terahertz frequencies Scientific Reports 6 1-11
[14] Bulgakova V, Gerasimov V, Lemzyakov A and Milekhin Ilya A 2018 Infrared localized surface plasmon resonances on subwavelength corrugated metal disks Proceedings of 43-th International conference IRMMW-THz Nagoya, Japan 9-14 Sept.We-POS-51,
[15] Gao Z, Wu L, Gao F, Luo Y and Zhang B 2018 Spoof Plasmonics: From Metamaterial Concept to Topological Description Advance Materials 30 1706683
[16] Liao Z, Fernández-Domínguez A I, Zhang J, Maier S A, Cui T J and Luo Yu 2016 Homogenous Metamaterial Description of Localized Spoof Plasmons in Spiral Geometries ACS Photonics 3 1768–1775
[17] Handbook of optical constants of solids, E. D. Palik, ed. (Academic Press, 1998).

Acknowledgments
The work was supported by the Russian Science Foundation (grant No. 18-72-00112).