Infrared localized surface plasmon dark multipole modes generated on subwavelength corrugated metal disks

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Abstract. Terahertz (THz) radiation is very promising for chemical and biological sensing. One of the ways to realize a THz sensor is exciting multipole localized surface plasmon resonances (LSPRs) on subwavelength corrugated metal disks. In this paper, numerical modeling and analysis of LSPRs on a periodic array of such structures were made. At normal incidence of the incoming wave, only dipole resonances can be excited. An additional C-shaped resonator placed in the vicinity of the disk produces dark multipole modes (quadrupole, hexapole, octupole, and decapole ones) due to hybridization of these modes with the bright dipole mode of the C resonator. Besides, multipole modes can be excited at oblique illumination of the structure. With increase in the incident angle, the multipole resonances become stronger. The high Q-factor resonance modes observed for PEC disks are wider or disappeared in case of Drude gold permittivity.

1. Introduction
Surface plasmons (SPs) is a combination of an evanescent electromagnetic TM wave and a wave of free charge density, propagating along a metal-dielectric interface [1]. In the visible and near-infrared frequency regions, SPs have been studied completely and found wide applications [2]. For example, SPs are used in the surface enhanced Raman spectroscopy (SERS) technique. Unlike other methods, biosensors based on the SERS are the most sensitive and enable structural diagnostics of component under investigation without special preparation of sample. The enhancing of the sensitivity is due to using localized surface plasmon resonances (LSPRs) (collective oscillations of conductive electrons in subwavelength structures) excited on surface roughness or metal particles attached to the surface [3]. The middle- and far infrared (terahertz (THz)) ranges cover the frequency domains from 10 to 120 THz and from 0.3 to 10 THz, respectively. This radiation is of great importance for spectroscopy because it is nonionizing, and rotational and vibrational modes of complex intra- and extra-molecule bonds of biological substances lie in this region. However, the long-wavelength surface plasmons have been studied insufficiently, because of their special characteristics. Due to the large free electron density, metals weakly support SPs in the far IR range [1]. Besides, no localized surface plasmon resonances can be exited on metallic nanoparticles, particularly in the THz range, because the plasma frequency is two orders higher than the THz frequencies. To overcome these limitations, Pendry and his colleagues suggested making periodic modulation of flat surface, which leads to formation of bound surface states [4].
In this work, we studied theoretically the localized surface plasmon resonances exited on spiral disks by an incident THz beam. Besides dipole modes, we consider higher multipole modes of LSPRs (called dark modes [5]). Multipole modes can have great potential for sensing as they are more sensitive to the presence of dielectric on the structure and enable realization of the multiple biosensing on one sample structure.

In paper [6] it was shown that multipole resonance modes can be exited selectively by using a vortex beam. The order of resonance depended on the orbital angular momentum of the beam. This effect can be applied for exciting stronger multipole resonances by vortex beam, which is promising for sensing applications.

2. Numerical simulation results
The scheme of the disk geometry is presented in figure 1. The disks were simulated as gold layers 0.3 µm thick with Drude conductivity, patterned on a silicon substrate 0.4 µm thick with the dielectric permittivity \( \varepsilon = 11.77 \cdot (1 - j \cdot 0.58 \cdot 10^{-4}) \) [7]. Basing on study of similar structures in the microwave region [5], we took parameters of spiral disk, rescaled to the THz region: the inner radius of the metallic disk \( r = 9 \) µm; the outer radius \( R = 22 \) µm; the number of grooves \( N = 36 \); the period \( d = 2\pi R/N \) (4 µm); the groove width \( a = 0.4d \) (1.5 µm). The lateral periodicity of the disks in the \( x \) and \( y \) directions was chosen to be \( p = 60 \) µm, in which case fields from adjacent disks do not affect each other (no “hybridization effect”). An additional “C-shaped” gold resonator was placed near the structure. A strong dipole resonance could be excited on it, which could produce multipole resonances in a corrugated disk due to the hybridization effect [5]. The angle of the C resonator was \( \alpha = 60^\circ \); the inner radius \( R_c = 24.6 \) µm; the width \( w = 2.9 \) µm.

![Figure 1. Scheme of subwavelength corrugated metal disk with C resonator.](image)

The transmission spectra (figure 2) of periodic array of corrugated disks (with and without C resonator) at normal incidence of the incoming wave in the range of 0.04–6 THz were simulated using CST Microwave studio Suite, in which the regime of Floquet ports and periodic open boundary conditions applied to the structure’s unit cell were employed.

At normal incidence for corrugated disks without C resonator, only dipole resonances can be excited (white gray line in figure 2), as was shown in literature [5]. The spectra for \( E_x \) and \( E_y \) polarization are the same due to the 2D symmetry of the structure. When asymmetry in the form of C resonator is added, an \( E_x \)-polarized wave excites a strong dipole resonance on the C resonator at 4.23 THz, which produces dark multipole modes at 2.36, 2.75, 3.08, 3.35, and 3.44 THz. 2D \( E_z \) field distributions at the silicon substrate surface for such frequencies (see the right inset in figure 2) correspond to quadrupole, hexapole, octupole, and decapole resonances. When the incoming wave is \( E_y \)-polarized, the C dipole
and corresponding multipole modes cannot be excited, and the spectrum is the same as for symmetric structure without C resonator (black line in figure 2). The transmission spectra of Drude gold structure have plasmon resonances, which are little wider than those of perfect electric conductor (PEC) (see figure 3) and shifted toward lower frequencies. At the spectral region from 3.30 to 3.52 THz there are several high Q-factor resonances for PEC disks, which are disappeared for Drude conductivity due to Joule losses in the real metal. Thus it is necessary to account for the Drude metal permittivity in simulations.

![Figure 2](image2.png)

**Figure 2.** Transmission spectra of corrugated gold disks for normally incident EM wave with vectors $E_x$ and $E_y$ (white gray line); corrugated gold disk with C-shaped resonator for $E_y$ (black line) and $E_x$ (red line) EM wave. Right inset: $E_z$ field distribution for corrugated disk with C resonator at silicon substrate surface ($E_x$ polarization).

![Figure 3](image3.png)

**Figure 3.** Spectra of transmission of normally incident $E_y$ - wave through corrugated disks with PEC and Drude gold conductivity. In the right inset – zoom area from 3.30 to 3.52 THz.

Oblique illumination of structures to examine is simulated in the regime of Floquet ports by specifying the polar angle $\theta$, which describes the angle between the wave vector of the incoming wave and $Z$ axis. The example of transmission spectra of corrugated disks with a C resonator at $\theta = 0$, 20, and 40° calculated for the Drude gold conductivity are shown in figure 4. At oblique illumination, the dark
multipole mode at 2.97 THz is produced. We found, that with increase in the angle $\theta$, the multipole resonances become stronger.

![Figure 4. Spectra of transmission through periodic array of corrugated gold disks at oblique illumination: $\theta = 0$, 20 and 40° (Drude gold conductivity).](image)

3. Conclusion

The transmission spectra of the periodic array of corrugated disks in the range of 0.04–6 THz were simulated. At the normal incidence of incoming wave onto a symmetric structure, only dipole surface plasmon resonances can be excited. An additional C-shaped resonator placed in the vicinity of disk produces dark multipole modes (quadrupole, hexapole, octapole, and decapole ones) due to hybridization of these modes with the bright dipole mode of the C resonator. Also multipole modes can be excited at oblique illumination of the structure. With increase in the angle $\theta$, the multipole resonances become stronger. The high Q-factor resonance modes observed for PEC disks are wider or disappeared in case of Drude gold structures.

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