ENHANCEMENT OF LOCAL FIELDS IN THE VICINITY OF BICONIC AND BIPYRAMIDAL METAL NANOPARTICLES

A.V. Korotun

National University Zaporizhzhia Politechnic, 64 Zhukovsky Str., Zaporizhzhia 69063, Ukraine

G.V. Kurdyumov Institute for Metal Physics of the NAS of Ukraine,36 Academician Vernadsky Blvd., Kyiv 03142, Ukraine

Abstract

Research in recent years [1] has shown that metal nanoparticles of biconical and bipyramidal shapes (Fig. 1) significantly enhance the signals of surface-enhanced Raman spectroscopy (SERS). In turn, high sensitivity to changes in dielectric constant, photothermal effect, and photothermal stability are related to the features of the geometry of these nanoparticles. Despite the above, the issue of field enhancement around biconic and bipyramidal nanoparticles remains unexplored, and therefore very relevant.

Statement of the problem and results of calculations

Due to the anisotropy of the shape of biconic and bipyramidal (we assume that the base of the bipyramid is a pentagon) nanoparticles, the amplification of local electric fields in their vicinity is a diagonal tensor of the second rank, the components of which are determined by the expressions

$$\mathcal{G}_{\perp(\parallel)} = \left| 1 + \left(1 - \mathcal{L}_{\perp(\parallel)}\right) \frac{\epsilon_{\perp(\parallel)}(\omega) - \epsilon_m}{\epsilon_m + \mathcal{L}_{\perp(\parallel)}\left[\epsilon_{\perp(\parallel)}(\omega) - \epsilon_m\right]} \right|^2 \qquad (1)$$

where $\mathcal{L}_{\perp(\parallel)}$ are depolarization factors; ϵ_m is the permeability of the surrounding dielectric medium, and the diagonal components of the dielectric tensor of the nanoparticle material are described by the Drude model

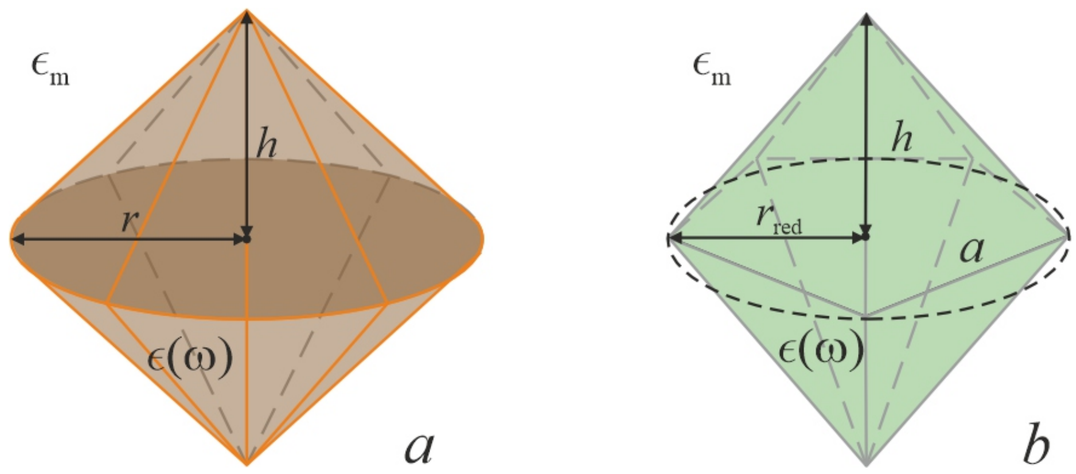
$$\epsilon_{\perp(\parallel)}(\omega) = \epsilon^{\infty} - \frac{\omega_p^2}{\omega\left(\omega + i\,\gamma_{\text{eff}}^{\perp(\parallel)}\right)} \qquad (2)$$

In formula (2) ϵ^{∞} is the contribution of the crystal lattice to the dielectric constant; ω_p is the plasma frequency, and $\gamma_{\text{eff}}^{\perp(\parallel)}$ is the effective rate of electron relaxation, which is the sum of volume and surface relaxation and radiation attenuation. It should be noted that it $\gamma_{\text{eff}}^{\perp(\parallel)}$ is calculated within the framework of the equivalent spheroid approach [2], and therefore $\mathcal{L}_{\perp(\parallel)}$ will have the same appearance as for elongated and flattened spheroids (depending on the ratio of the geometric parameters of the particles of the studied shapes:$h > 2r$ and $h < 2r$, where h is the height, r is the radius of the base of the bicone or the effective radius bases of the bipyramid).

Calculations were performed for biconic and bipyramidal elongated and flattened gold nanoparticles in Teflon.

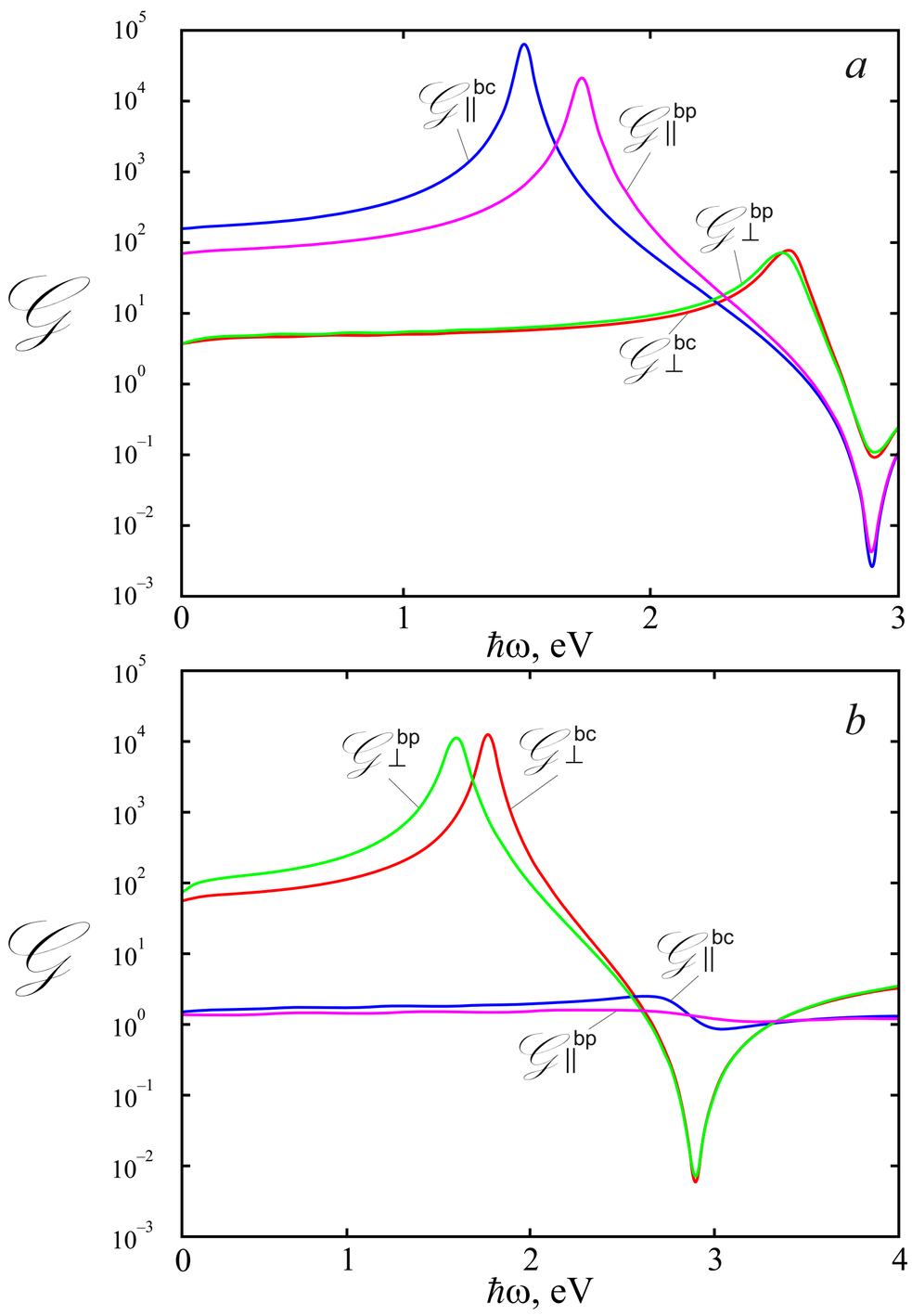
The results of calculations of the frequency dependences of the components of the gain tensor in the vicinity of nanosized Au bicones and bipyramids are shown in Fig. 2. It was established that the component of the amplification tensor in the direction corresponding to the larger particle size significantly (by 3-4 orders of magnitude) dominates the other component. In addition, the curves $\mathcal{G}_{\perp(\parallel)}(\omega)$ for bicones and bipyramids are qualitatively similar, and the quantitative results are close, which indicates the possibility of considering bipyramidal particles (which are most often obtained in the experiment) as biconical in the calculations.

Figure 1



Geometry of the problem: biconical (*a*) and bipyramidal (*b*) nanoparticles in the medium with permittivity ϵ_m

Figure 2



Frequency dependences of the components of the gain tensor in the vicinity of nanosized bicones and Au bipyramids from $h > 2r$ (*a*) and $h < 2r$ (*b*)

Conclusions

Within the framework of the equivalent spheroid approach and taking into account volume and surface relaxation and radiation attenuation, expressions for the diagonal components of the local electric field amplification tensor around biconical and bipyramidal metal nanoparticles were obtained. Calculations showed that the components of the local electric field amplification tensor, which correspond to the larger size of the investigated particles, reach significant values ($\sim 10^5$) at frequencies that fall into the biological window of transparency, and therefore such particles can be used in nanobiology and nanomedicine.

References

[1] S. Xu, L. Jiang, Y. Nie, J. Wang, H. Li, Y. Liu, W. Wang, G. Xu, and X. Luo. Gold nanobipyramids as dual-functional substrates for in situ “turn on” analyzing intracellular telomerase activity based on target-triggered plasmon enhanced fluorescence. ACS Appl. Mater. Inter. 10 (2018), 26851.

[2] A.V. Korotun. Plasmonic phenomena in biconical and bipyramidal metal nanoparticles. Ukr. J. Phys. 68 (2023) 695 – 704.