Modeling of irradiation of plasmon nanoparticles with polarized light and investigation of localization features of electromagnetic and temperature fields

A.N. Yakunin[1], S.V. Zarkov[1], Yu.A. Avetisyan[1], G.G Akchurin[1,2], V.V. Tuchin[1,2,3]

[1] Institute of Precision Mechanics and Control, FRC "SRC of RAS", Saratov, Russia;

[2] Saratov State University , Saratov, Russia;

[3] Tomsk State University, Tomsk, Russia;

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ABSTRACT

The results of finite element modeling of localization processes of electromagnetic and temperature fields under irradiation of plasmon nanoparticles with polarized light are presented. Aspects of promising applications in biomedicine, engineering and electronics are discussed, in which the effects of concentration of the electromagnetic field and localization of the induced temperature field by plasmon nanoparticles are used.

1. INTRODUCTION

The entire variety of practical applications of the LSPR effect in technology, chemistry, and biomedicine can be reduced to two areas of using field enhancement: firstly, field enhancement inside plasmonic nanoparticles, and secondly, field enhancement outside the nanoparticles, in the vicinity of the outer surface. Therefore, the task of further development of traditional approaches in the study of field formation processes in terms of taking into account the influence of spectral properties of plasmonic materials and multifactorial nature of field concentration processes remains relevant.

2. Formulation of the problem

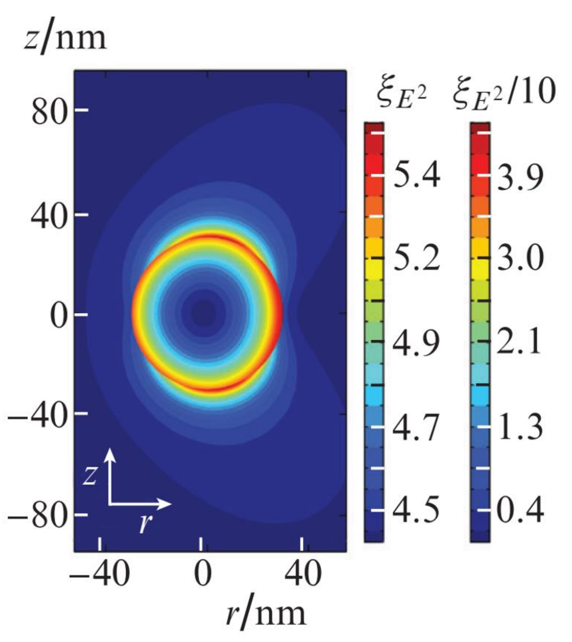

Figure 1. Field gain ξ_{E2} distribution topogram in the central sections of nanoparticle. The polarization vector is directed along the *z* axis, λ=532 nm, ***a***=30 nm.

To solve these two problems, we analyzed the spatial distributions of the complex vector of the electric field amplitude ***E***(***r***) induced by an irradiating plane monochromatic wave E_0 when it is scattered on a nanosphere of radius ***a*** in an aqueous environment.

3. Field enhancement outside NP

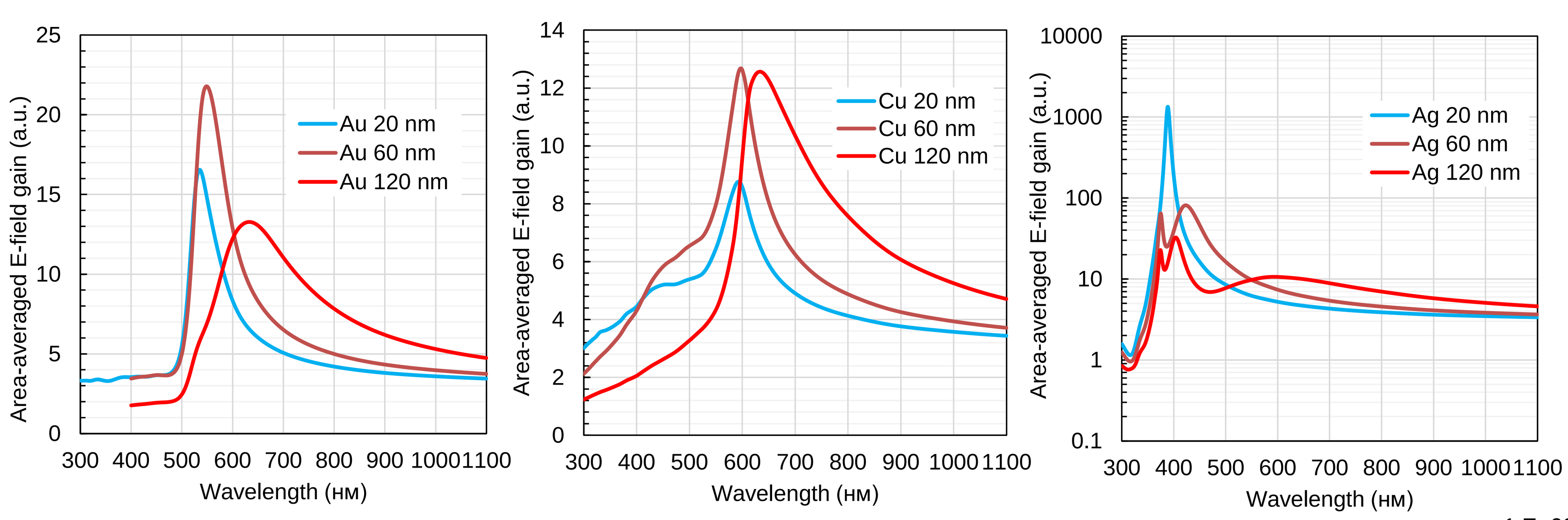

Figure 2. Spectral dependences of the field enhancement on the surface of **Au** (left fragment), **Cu** (middle fragment) and **Ag** (right fragment) nanoparticles of various diameters.

It can be seen that the general pattern is the following: the larger the diameter of the nanoparticles, the higher the field enhancement on the surface of nanoparticles in the long-wavelength part of the spectrum (to the right of the plasmon resonance wavelength); in the short-wave part of the range the trend is opposite.

The optimal diameter of a nanoparticle, from the point of view of achieving maximum field enhancement, depends on the dielectric properties of both the metal and the environment. In the case considered, the diameter of 60 nm is close to optimal for gold nanoparticles, 60 and 120 nm for copper nanoparticles, and 20 nm for silver nanoparticles. In general, silver nanoparticles provide a significant advantage in field enhancement compared to gold and copper ones.

Possible applications of the results of this area of research:
near-field scanning optical microscopy, SERS, enhanced fluorescence of plasmonic protein complexes, plasmon-enhanced photodynamics, catalysis and photovoltaics, high-speed photosensors, sources of photoinduced free electrons.

4. Field enhancement inside NP

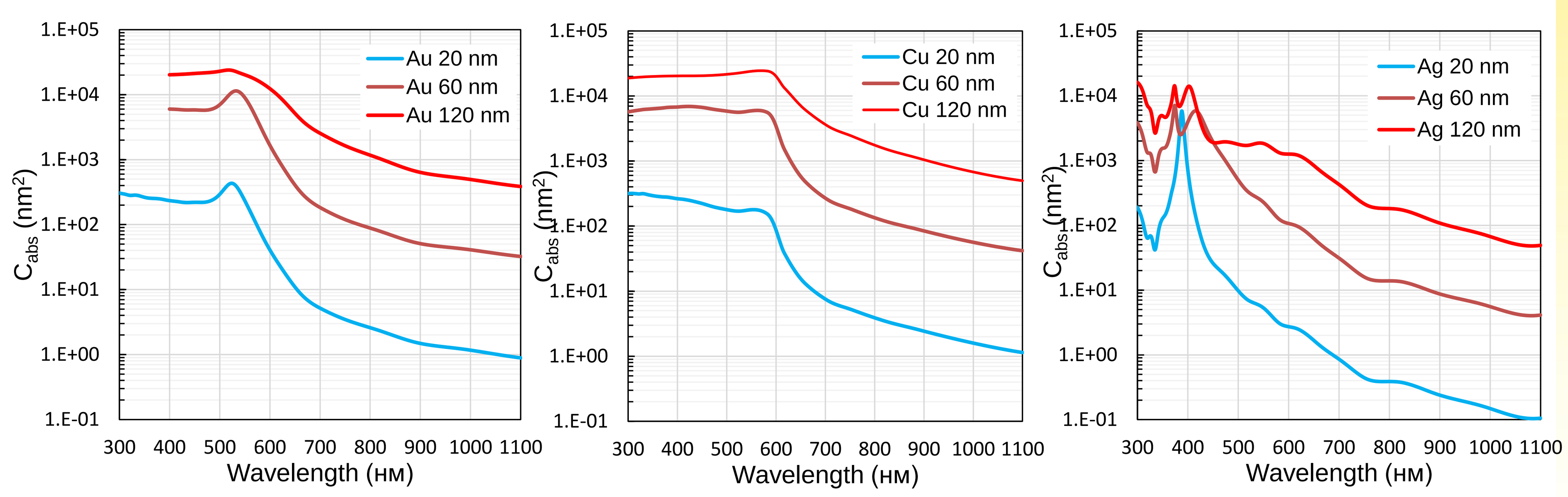

Figure 3. Spectral dependences of absorption cross section C_{abs} of **Au** (left fragment), **Cu** (middle fragment) and **Ag** (right fragment) nanoparticles of various diameter.

The absorption cross section of a nanoparticle is its fundamental integral characteristic, which determines the numerical fraction of the energy of electromagnetic radiation that is intercepted by the nanoparticle and converted into heat.

It should be noted that the parameters of gold and copper nanoparticles are very close in the plasmon resonance region (500-600 nm), which indicates the potential competitiveness of using copper nanoparticles along with gold nanoparticles to provide local heating of biological tissue (see Figure 3). The absorption of silver nanoparticles in the same wavelength range is significantly lower. This can be used to advantage in a number of special applications where thermal effects have a negative impact.

The results of solving the problem of a stationary temperature field of nanoparticles in a continuous irradiation mode show the existence of similar trends in the dependence of the spectra of the temperature increment of nanoparticles and the spectra of the absorption cross section (see the corresponding curves in Figure 3, Figure 4).

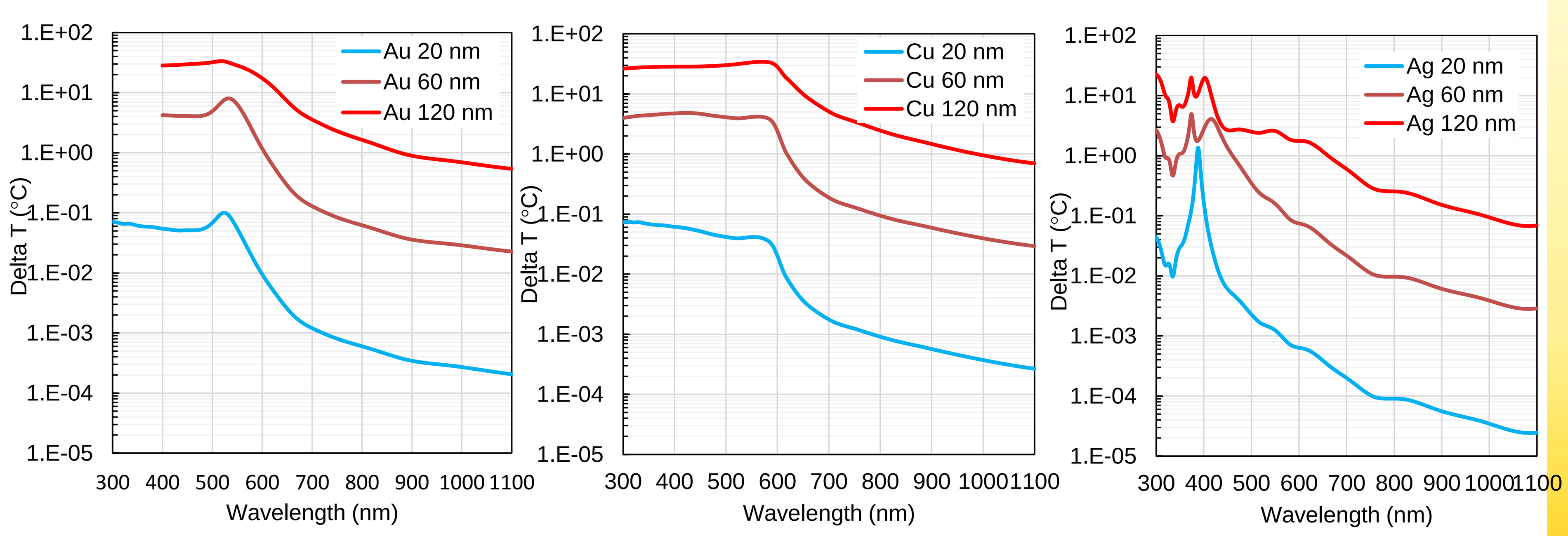

Figure 4. Spectral dependences of the stationary temperature increment Delta T of **Au** (left fragment), **Cu** (middle fragment) and **Ag** (right fragment) nanoparticles of various diameter under the influence of light of the same intensity.

Possible applications of the results of this area of research:
various types of concentrators of electromagnetic radiation power absorption localized in space - methods of hyperthermia, ablation, nano- and microsurgical effects on cells and biotissues, opening capsules with medicinal substances, increasing biotissue contrast, protein inactivation.

CONCLUSIONS

1. **The results of studies of the influence of the material properties of plasmonic nanoparticles and their sizes on the spectral dependences of field localization both inside and outside nanoparticles contribute to the targeted synthesis of effective functional structures for a wide range of biomedical and technical applications**.
2. **It has been shown that copper nanoparticles can, in some cases, be competitive with gold nanoparticles.**

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