Criteria for evaluating the effectiveness of plasmonic nanoparticles for biomedical and technical applications

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ABSTRACT

The paper deals with the peculiarities of synthesis of quality criteria for plasmonic nanoparticles intended for biomedical and technical applications. Particular attention is paid to the differences in the structure of criteria for assessing their efficiency of the optical parameters of nanoparticles proper. The ultimate goal of the study is to develop tools for quantitative evaluation of synthesized nanoparticles to ensure precise dosed effects, increase the sensitivity of plasmonic complexes during local laser hyperthermia of biological tissues and cells; cell transfection; formation of effective fluorescent complexes; nanocomplexes for photodynamic therapy; photoemission structures.
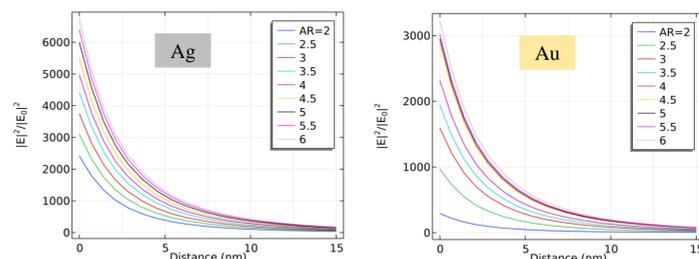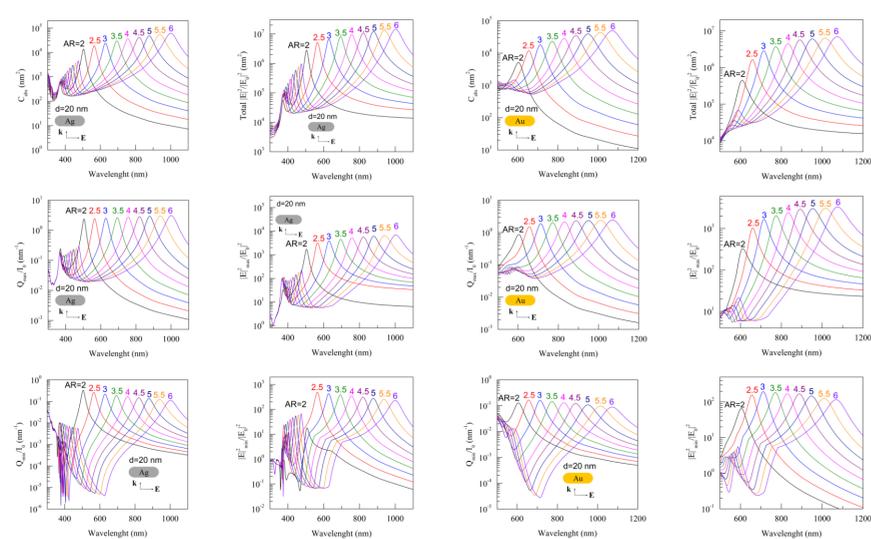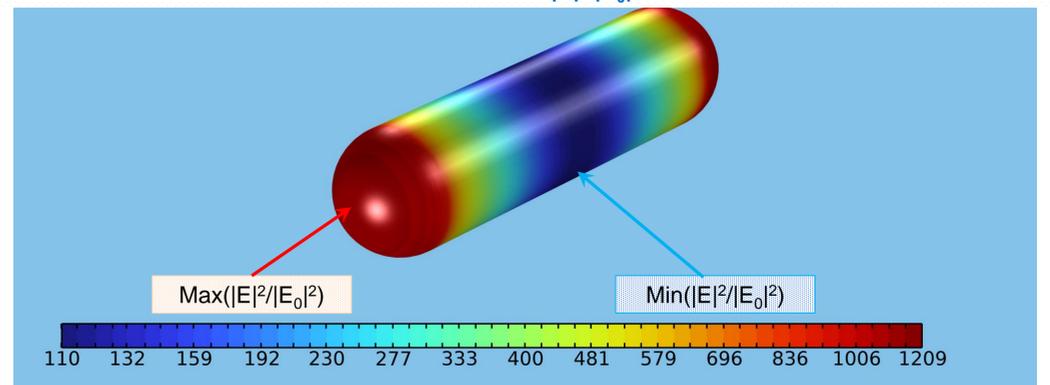
Formulation of the problem

For a reasonable assessment of the efficiency of practical application of plasmonic nanoparticles, it is necessary to use the following system of significant parameters:

laser hyperthermia (continuous irradiation mode, long pulses) — absorption cross-section C_{abs};

cell transfection (irradiation mode with femto- and picosecond pulses) — localization of maxima Q_{max} and minima Q_{min} of absorbed thermal power;

photodynamic therapy — enhancement of field intensity $|E|^2/|E_0|^2$ (integral, as well as localization of extrema) on the surface of nanoparticles;

fluorescent complexes — enhancement of field intensity $|E|^2/|E_0|^2$ in the near zone;

photoemission structures — distribution of the squared modulus of the normal field component on the surface of a nanoparticle.

Simulation results of and discussion

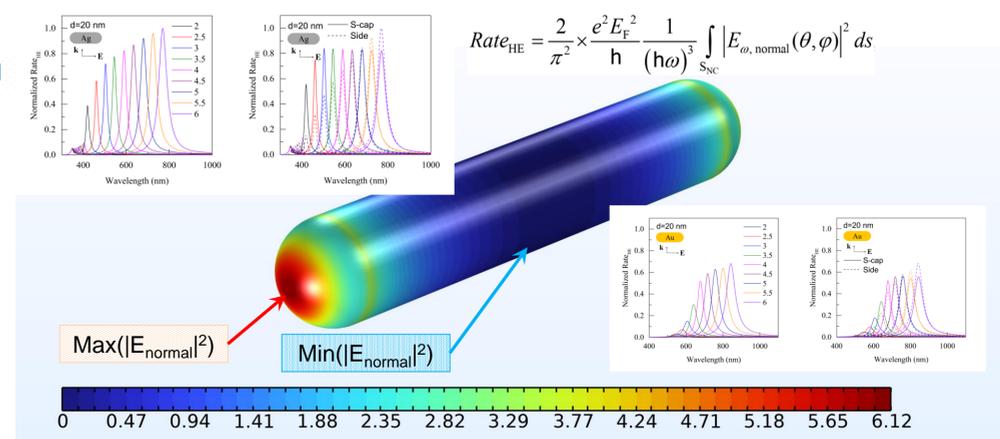### Distribution of specific volumetric power of heat sources Q inside a nanorod

Min Q   Max Q

0.07   0.29   0.5   0.71   0.92   1.13   1.34
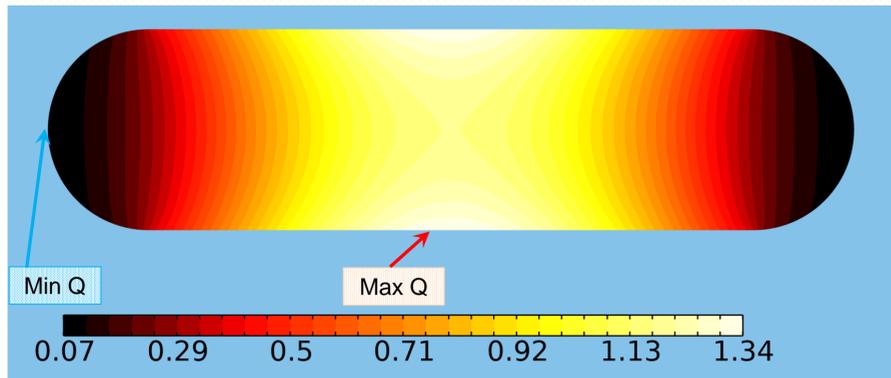
Distribution of the field enhancement coefficient $|E|^2/|E_0|^2$ on the outer surface of the nanorod

Max($|E|^2/|E_0|^2$)   Min($|E|^2/|E_0|^2$)

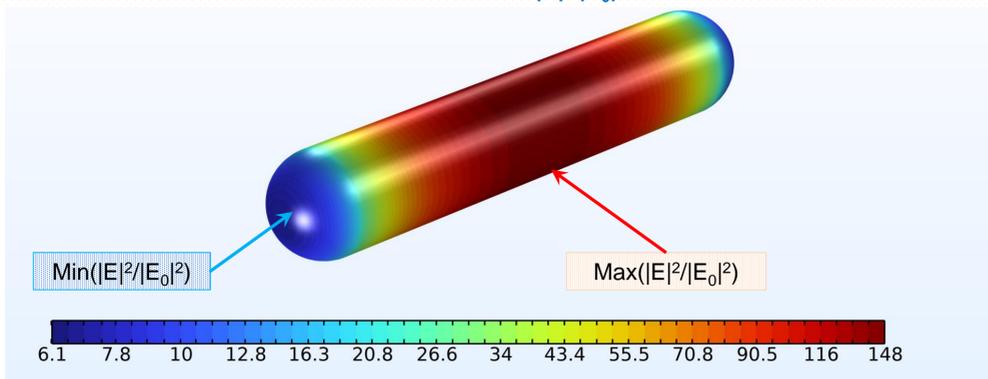110   132   159   192   230   277   333   400   481   579   696   836   1006   1209

The presented results of modeling the distributions of significant parameters of physical fields in nanoparticles contain information necessary for tuning the wavelength of plasmon resonance. Based on its analysis, a choice is made of optimal materials and sizes of nanoparticles that ensure the efficiency of use in various biomedical and technical applications.

Distribution of the field enhancement coefficient $|E|^2/|E_0|^2$ on the inner surface of the nanorod

Min($|E|^2/|E_0|^2$)   Max($|E|^2/|E_0|^2$)

6.1   7.8   10   12.8   16.3   20.8   26.6   34   43.4   55.5   70.8   90.5   116   148

Tuning a nanorod tuned to generate hot high-energy electrons under λ=808 nm irradiation

$$Rate_{HE} = \frac{2}{\pi^2} \times \frac{e^2 E_F^2}{h} \frac{1}{(h\omega)^3} \frac{1}{S_{NC}} \int_{S_{NC}} \left| E_{\omega,\,normal}(\theta,\varphi) \right|^2 ds$$

Max($|E_{normal}|^2$)   Min($|E_{normal}|^2$)

0   0.47   0.94   1.41   1.88   2.35   2.82   3.29   3.77   4.24   4.71   5.18   5.65   6.12

CONCLUSIONS

1. The concept of determining the parameters of effective plasmonic nanoparticles with various integral and differential characteristics of the electromagnetic field and thermal source distribution as quality criteria is discussed and illustrated by numerical simulation results.
2. The advantage of silver nanorods over gold nanorods as effective photoactivation enhancement agents for nanocomplexes designed for biomedical and technical applications has been quantitatively evaluated.

SARATOV FALL MEETING SFM '24
September 23 - 27, 2024