Modeling of Thermo-Optical Properties of Ferromagnetic Plasmon Nanocomposites for Laser Local Hyperthermia

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ABSTRACT

A theoretical study was made of the influence of the structure and optical properties of the components of ferromagnetic nanocomposites based on gold (GNS) and cobalt ferrite (CFO) nanospheres on the absorption spectrum upon irradiation with laser light. The application of such composites for local laser hyperthermia of biological tissues, including cancerous tumors, has been shown to be promising. Additional advantages are provided by the possibilities of implementing technologies for the targeted delivery of composites and the concentration of heat sources due to plasmonic field amplification. It is found that a continuous CFO layer leads to a 1.5-fold increase in the absorbed power of the composite and a simultaneous shift of the resonance from the point λ=526 nm to the point λ=600 nm. The form of the obtained spectral curve, in general, corresponds to the experimental results of measuring the suspension extinction. A non-trivial effect of the redistribution of absorbed power was also found, which consists in the fact that its value decreased in GNS and increased significantly in CFO.

The problem

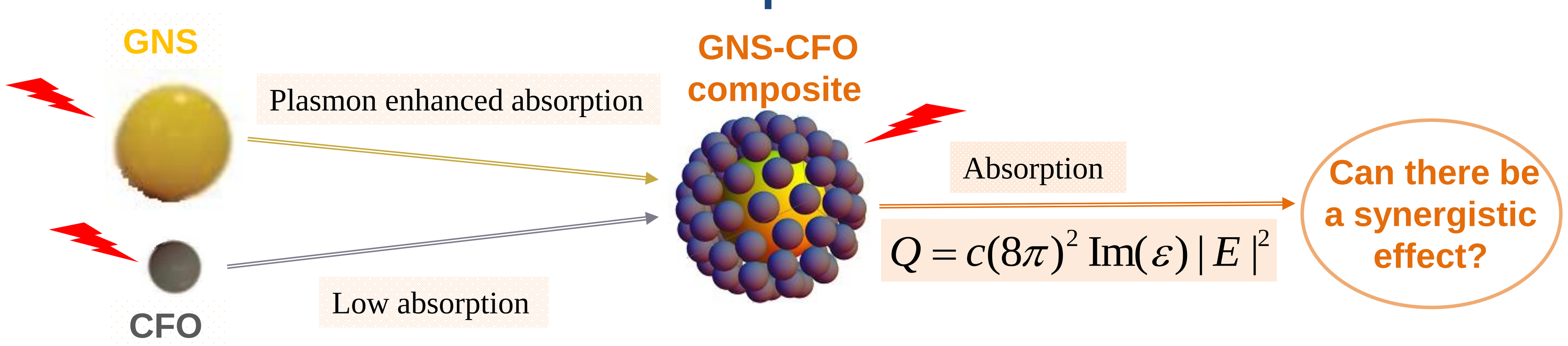

Figure 1. The objectives of the study.

Modeled structures options

Variant number	Structure	Sizes (diameter/ thickness), nm
1	Nanoparticle CFO	5
2	GNS	20
3	Composite GNS-1 CFO	20/5
4	Composite GNS-2 CFO	20/5
5	Composite GNS-layer CFO	20/5

Simulation results and discussion

The modeling of the thermo-optical properties of the structures [*Processes* **2021**, *9*, 2264, https://doi.org/10.3390/pr9122264] was carried out using the methods described in [*Sensors* **2021**, *21*, 1248, https://doi.org/10.3390/s21041248, *Sensors* **2022**, *22*, 4127, https://doi.org/10.3390/s22114127] in the COMSOL Multiphysics environment. First, the absorption spectra of solitary CFO and GNS nanoparticles were determined (options 1 and 2, respectively), then those of GNS-CFO composites with a small number of CFO nanoparticles (options 3 and 4). In the 5th variant, an approximation was considered with the replacement of the layer of magnetite nanoparticles (number N=80) with a continuous CFO layer of the same thickness.

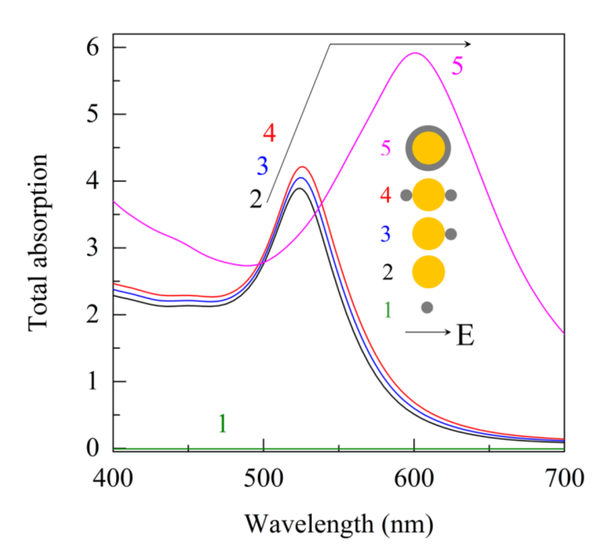

Figure 2. Absorption cross section of composite nanostructures.

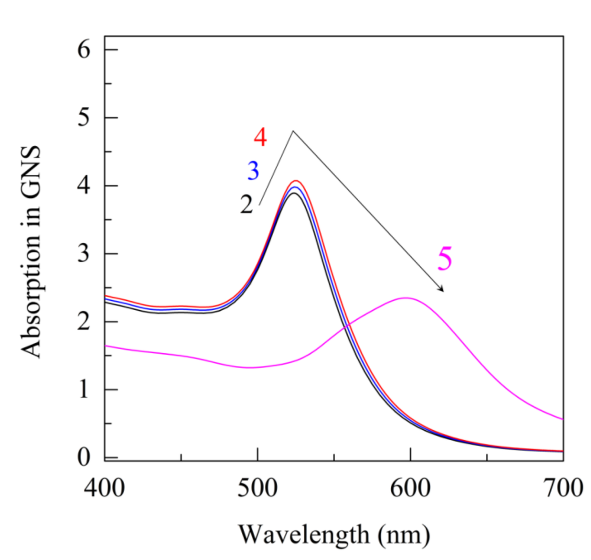

Figure 3. Absorption cross section of gold nanoparticles in the composite.

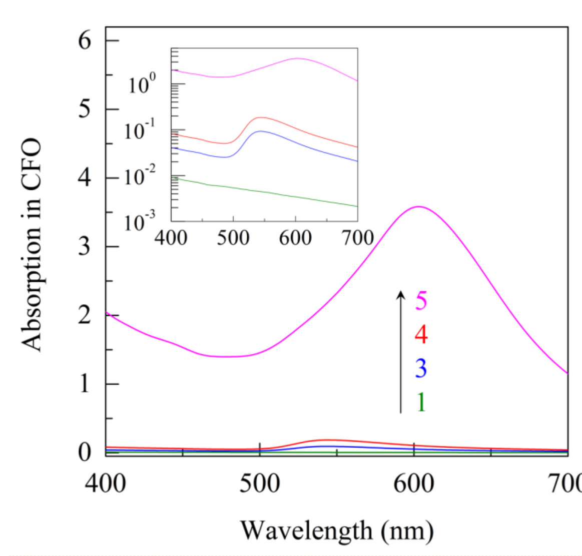

Figure 4. Absorption cross section of ferrite nanoparticles in the composite.

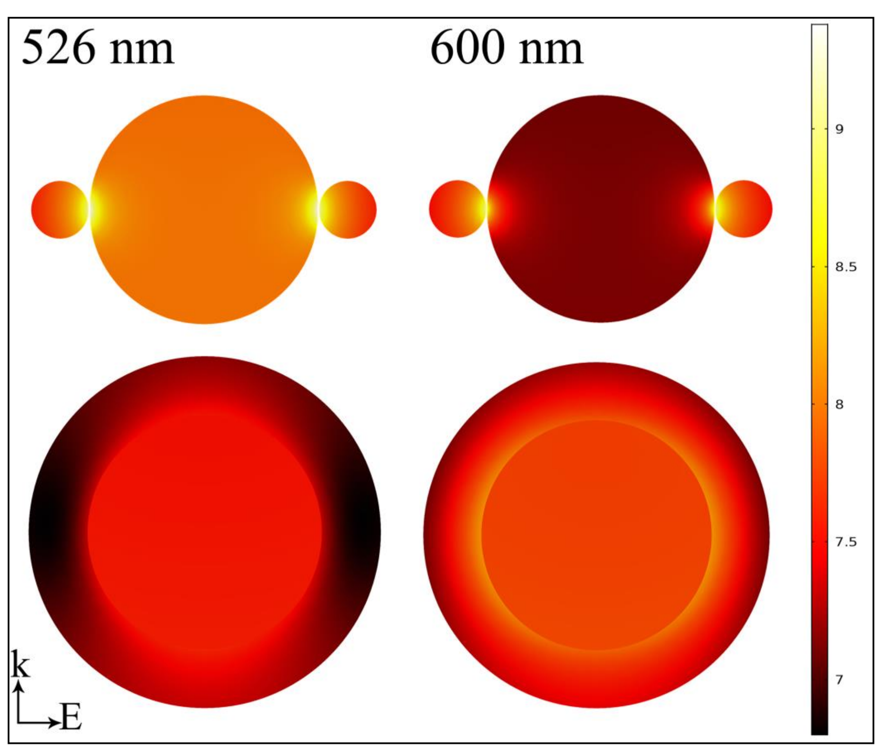

Figure 5. Topogram of distribution of specific volume absorption power in composites at wavelengths λ=526 nm (first column) and λ=600 nm (second column): option 4 – top row; option 5 - bottom row.

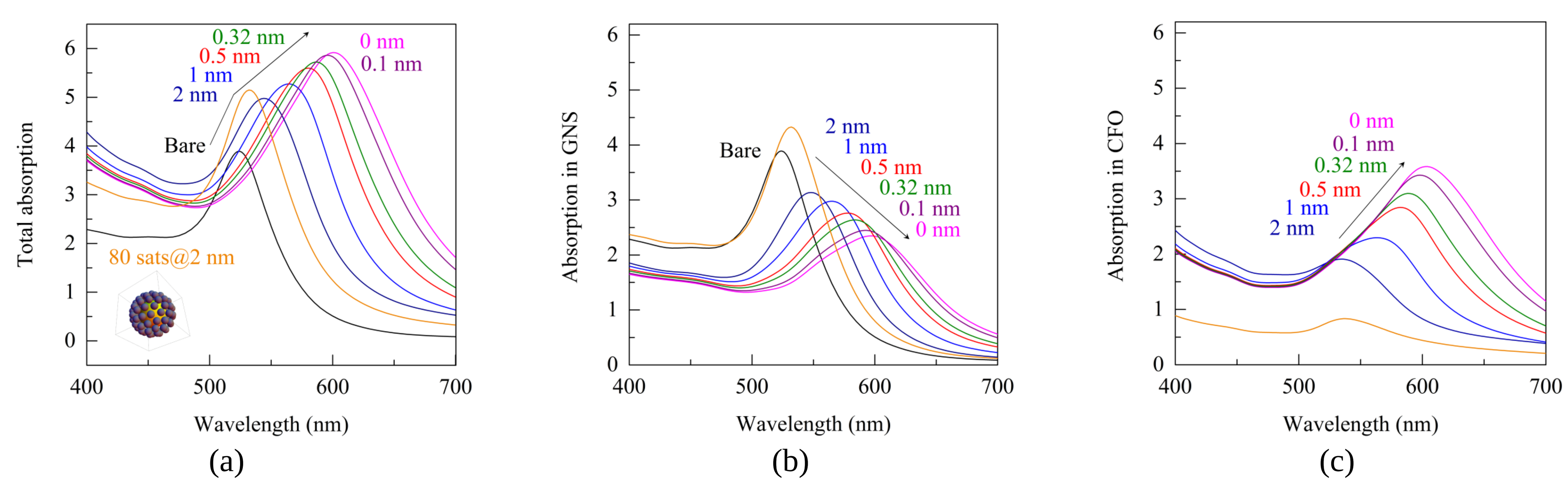

Figure 6. Dependence of the absorption cross section of the composite on the gap between the GNS and the CFO layer: (a) – total cross section; (b) - cross section of the GNS; (c) - cross section of the CFO layer. The results are also given for the structure GNS - a layer of 80 SFO nanoparticles (labeled as 80 sat@2 nm).

An analysis of the obtained numerical results leads to the nontrivial conclusion that the absorption cross section of nanoparticles near gold nanospheres can increase up to 10 times when irradiated with laser light at the plasmon resonance wavelength. In the case of a continuous layer of CFO, the absorption in it increases with a decrease in the gap between the CFO layer and surface of the GNS. These factors lead to the multiplication of the effect of photo hyperthermia when using the described composite structures.

CONCLUSIONS

1. **Suspension of CFO nanoparticles has no signs of plasmon resonance in the studied radiation range λ=400 -700 nm.**
2. **Interfacing GNS with individual CFO nanoparticles results in a 3% increase in thermo-optical conversion by the optical radiation composite at resonant wavelength in terms of each CFO nanoparticle.**
3. **A solid CFO layer results in a 1.5-fold increase in the absorbed power of the composite and simultaneous displacement of the resonance to the point of λ=600 nm.**
4. **The effect of enhancement of absorption in the composite, which is relevant for the further development of laser hyperthermia technology, is substantiated.**

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