Thermoplasmonic optimization of nanostructured metals

A. Lalisse[1,3,*], G. Tessier[1], G.Baffou[2] and J. Plain[3]

[1]*Neurophotonics Laboratory, CNRS UMR 8250, University Paris Descartes, Sorbonne Paris Cité, 75006 Paris, France*

[2] *Institut Fresnel, CNRS, Aix Marseille Université, Centrale Marseille, UMR 7249, 13013 Marseille, France*

[3]*Laboratoire de Nanotechnologie et d'Instrumentation Optique (LNIO), Université de Technologie de Troyes, 12 rue Marie Curie, CS 42060, 10004 Troyes cedex, France*

[*]corresponding author: adrien.lalisse@parisdescartes.fr

Abstract-We investigate new materials for plasmonic metal nanostructures, to serve both as near-field enhancers and heat nanosources. Numerical simulations highlight the influence of morphology and composition on the nanoparticles absorption and temperature.

A metal nanostructure under illumination can lead to a resonant coupling of light and free electrons inducing enhanced light absorption and scattering. These resonances, called Localized Surface Plasmon (LSP), can be tuned from the visible to the near infrared frequency range for noble metals such as Gold (Au). However, in metals, this charge oscillation induces Joule heating. The enhanced heating at the nanostructure LSP resonance strongly depends on the material, morphology and dielectric environment, allowing a control of the nanostructure optical and thermal properties. This stimulates new research, with promising applications in photothermal therapeutics [1], photothermal imaging [2] or thermophotovoltaics [3].

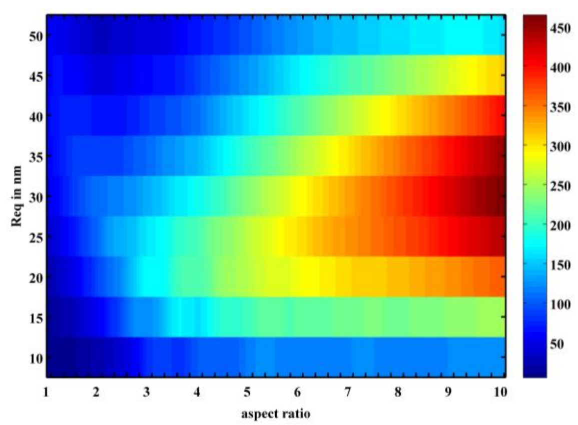

Figure 1- BEM-calculated temperature of gold ellipsoids in water, illuminated with a power density 1mW/µm^2 at the LSP resonance wavelength of each object. The temperatures (color) are plotted against the aspect ratios from 1 to 10, and the equivalent radius of the particle (i.e. the radius of the sphere having an equivalent volume).

For these applications, the ability to both enhance optical resonances and convert efficiently optical energy into heat is essential. Although noble metals exhibit high losses in the visible and near-infrared range, their low temperature sustainability in particular has motivated the quest for new plasmonic materials [4]. Following on the pioneering work of Shalaev et al [5] and research for plasmonics materials in the Ultraviolet (UV) range, we have assessed the performance of different NP plasmonic materals candidates including noble metals such as Gold (Au), Silver (Ag), Copper (Cu), Platinum (Pt) and Rhodium (Rh), and newer plasmonic materials like Aluminum (Al), Nickel (Ni), Mercury (Hg), Molybdenum (Mo), Tantalum (Ta), Tungsten (W), Titanium nitride (TiN) and Zirconium nitride (ZrN).

Using gold, which is the most commonly used plasmonic metal, simple geometries such as ellipsoids, disks and triangles in homogeneous media (see **Figure 1**) or glass substrates have been investigated. Two main features appear to compete in the determination of the temperature: the NP absorption cross-section and its geometry. We will present a numerical optimization of the thermal properties of these structures, showing that an optimal shape can minimize the achievable temperature for a given amount of gold on a substrate.

In addition, we examine the case of dipolar nanoparticles and determine simple universal dimensionless constants η_{out} and η_{in} to quantify the plasmonic and thermoplasmonic performance of spherical structures.

Based on the Boundary Element Method (BEM) , numerical simulations were carried out to compute the LSP resonance of the various materials discussed. Depending on the η_{out} and η_{in} parameters, we can then classify the various materials as either near-field enhancers or efficient heat nanosources.

To evaluate the influence of nanostructure morphology on the steady-state temperature, nano-ellipsoids of various compositions immersed in a homogeneous medium with a refractive index n=1.33 were modeled for several materials and geometries.

Although gold is an excellent thermoplasmonic material in many cases, we show that other materials should be preferred in specific geometries.

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