OVERHEATING OF METALLIC NANOPARTICLES UNDER EXCITATION OF PLASMONIC RESONANCES ON THEIR SURFACE

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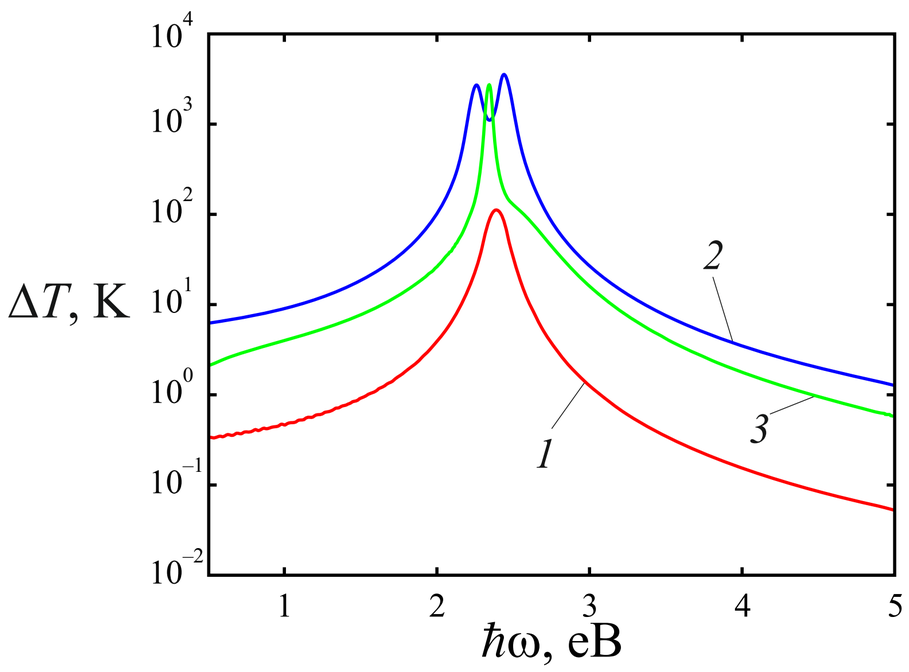
Abstract

In recent years, thermoplasmonic phenomena in metallic nanoparticles of the different shapes and compositions have been actively investigated. This is associated with such practical applications of thermonanoplasmonics as photothermal therapy of malignant tumors, acceleration of some physical reactions, thermoplasmonic sensing of phase transformations taking place in nanoscale systems. Let us point out that the physical cause of the overheating is the rapid conversion of electromagnetic energy into thermal energy when light is absorbed. However, the studies of the overheating of nanoparticles of different geometry under the excitation of surface plasmonic resonances have hardly been carried out and are, therefore, actual.

Figure 1



Frequency range of overheating of metal nanoparticles of different geometries:
1 – spherical particles (R = 50 nm);
2 – cylindrical particles ($2r$ = 66.67 nm, l = 150 nm);
3 – disk particles (D = 163.3 nm, H = 25 nm)

Statement of the problem and results of calculations

Let us assume that plasmonic nanoparticle of arbitrary shape is located in the dielectric medium with the given dielectric permittivity. The overheating of nanoparticles, the value of which is determined by the expression [1], takes place under the excitation of surface plasmonic resonances

$$\Delta T = \frac{C_{\text{abs}}\, I_0}{4\pi\kappa\beta R_{\text{eq}}}\ , \qquad (1)$$

where I_0 is the intensity of light incident on the nanoparticle; κ is environmental thermal conductivity coefficient; C_{abs} is absorption cross-section; β and R_{eq} are shape parameter and the equivalent radius of nanoparticle, R is the radius of sphere, d is diameter of cylinder / disk, l is the length of cylinder, h is the height of disk (table. 1).

The calculations have been performed for spherical, cylindrical and disk-shaped nanoparticles of gold.

In fig. 1 shows the frequency distribution curve for overheating of gold nanocules, cylinders and disks. Due to the fact that $\Delta T \sim C_{\text{abs}}$ the curves $\Delta T(\omega)$ and $C_{\text{abs}}(\omega)$ shape have a new appearance, and the overheating of cylindrical and disk nanoparticles is always greater than for spherical ones. The result is that in practice, the required slight overheating completely distorts spherical particles, rather than cylindrical or disk ones.

Table 1. Geometric parameters of nanoparticles

Parameter	Shape		
	Sphere	Cylinder	Disk
R_{eq}	R	$\frac{1}{2}\sqrt[3]{\frac{3}{2}d^2 l}$	$\frac{1}{2}\sqrt[3]{\frac{3}{2}d^2 h}$
β	1	$1+0.96587\ln^2\left(\frac{l}{d}\right)$	$\exp\left\{0.040-0.0124\ln\left(\frac{h}{d}\right)+0.0677\ln^2\left(\frac{h}{d}\right)-0.00457\ln^3\left(\frac{h}{d}\right)\right\}$

Conclusions

It has been found that the maximum overheating (at the frequency of surface plasmonic resonance) increases by approximately one order of magnitude under the variation of the shape of nanoparticles in the row “sphere→cylinder→disk”. The above fact indicates the feasibility of using spherical nanoparticles for photothermal therapy, since the overheating is minimal for them. At the same time, it is reasonable to use disk particles in photocatalysis because the reaction rate increases with increasing temperature, according to Arrhenius law.

1. G. Baffou, Thermoplasmonics: Heating Metal Nanoparticles Using Light (Cambridge University Press 2017).