Doping of resonant silicon nanodisks for efficient optical heating in the near-infrared range

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Abstract. All-dielectric nanophotonics attracted high interest during last years in the field of thermal applications and optical heating mainly due to the ability of electromagnetic field localization inside the nanostructures due to different resonant modes excitation. However, most conventional dielectrics and semiconductors (e.g. silicon, germanium etc.) are transparent in the near-IR, and, thus, optical heating in this region becomes a challenging task. In this work, we reveal that carrier doping can significantly increase optical heating of a resonant silicon nanodisk, without changing its optical properties dramatically. In addition, semiconductor nanostructures support high-Q thermally responsive Raman signal, which can be used as the temperature sensor at the nanoscale. We believe, that such approach might be very effective for numbers of applications, including bio-medical ones, by working in the ‘biological tissue window’.

1. Introduction

All-dielectric resonant nanostructures and nanoparticles attracted a lot of attention in the last decade [1], owing to the presence of electric- and magnetic-type optical modes in the visible and near-infrared ranges, allowing to effectively control radiation pattern [2], excite non-radiating states [3], high-Q optical modes [4] and their strong nonlinear optical response [5]. Such ability to maintain resonances and to control radiation efficiency lead to the implementation of resonant semiconductor nanoparticles as a versatile nanoscale optical heater and thermometer [6, 7]. These structures one may find even more beneficial in comparison with conventional plasmonic ones in optical heating applications [8], owing to strong inherent temperature sensitive Raman response [9]. However, the ability to tune into near-IR localized surface plasmon resonance (LSPR) by elongating to an elliptical shape a single metal nanoparticle remains a problem for all-dielectric structures, since the materials inherent losses (Si, Ge) become negligibly low for optical heating. Indeed, as it was revealed in the work [6], the absorbed power $P$ by the nanoparticle is following:

$$ P \sim \sigma F^2 V_{\text{eff}} , $$

where $\sigma$ is the conductivity, $F$ is the field enhancement factor and $V_{\text{eff}}$ is the effective mode volume. Therefore, by exciting high-Q resonances in the near-IR [10], one can achieve near unity absorption in broad range. However, heat generation would remain low due to very low conductivity $\sigma$ in semiconductors in this range. Thus, we believe that our approach based on doping of semiconductor resonant nanostructures will dramatically enhance optical heating efficiency and will pave the way for a variety of applications.
2. Results

Doping of a single conventional semiconductor nanoparticles is still quite a challenging task except some nanostructures based on hybrid halide perovskites, where one can achieve a drastic change in the optical and conductive properties by in-situ nanoparticles doping [11]. In this regard, for the doping one should consider the films which subsequently would be reshaped by lithography techniques into mesasurfaces and nanoparticles. Thus, a resonant silicon nanodisk is a reasonable structure for consideration.

To start with, it is necessary to estimate the affection of doping on optical and conductive properties of the material, since it impacts significantly on optical properties [12]. The free carrier contribution to the semiconductors permittivity is described by a Drude model [13]:

\[ \varepsilon' = \varepsilon_\infty \left(1 - \frac{\omega_p^2 \tau^2}{\omega^2 + \omega_p^2 \tau^2}\right) \]
\[ \varepsilon'' = \frac{\varepsilon_\infty \omega_p^2 \tau}{\omega(1 + \omega^2 \tau^2)} \]

where the plasma frequency \( \omega_p \) and scattering time \( \tau \) are defined as \( \omega_p = \sqrt{\frac{N e^2}{m^* \varepsilon_0 \varepsilon_\infty}} \) and \( \tau = \frac{m^*}{e \mu} \), where \( N \) is the free carrier concentration, \( e \) is the electron charge, \( m^* \) is the conductivity effective mass and for n-type doping of silicon \( m^* = 0.26 \cdot m_e \), \( m_e \) is the electron mass, \( \varepsilon_0 \) and \( \varepsilon_\infty \) are the permittivity of free space and the high frequency permittivity, respectively, and \( \mu \) is the free carrier mobility.

![Figure 1](image.png)

**Figure 1:** A) Electron mobility in silicon from phosphorous doping level (carriers concentration) B) Real (x-axis) and imaginary (y-axis) parts of silicon permittivity at a wavelength \( \lambda \) of 1.3 \( \mu m \) for different doping level concentrations (from red to blue: \( 10^{18}, 5 \times 10^{18}, 10^{19}, 5 \times 10^{19}, 2 \times 10^{20} \) cm\(^{-3} \)). Inset depicts schematic of the optical heating calculation model. Normal incident plane wave excitation of a single silicon nanodisk of 220 nm height. C) Calculated temperature increase in logarithmic scale for single nanodisk with different doping levels.

The electron mobility and hole mobility have a similar doping dependence: for low doping concentrations the mobility is almost constant and is primarily limited by phonon scattering. At higher doping concentrations, the mobility decreases due to ionized impurity scattering with the ionized doping atoms. The actual mobility also depends on the type of dopant.

The mobility at a particular doping density is obtained from the following empiric expression (see Fig. 1(A)):

\[ \mu = \mu_{\text{min}} + \mu_{\text{max}} - \mu_{\text{min}} \frac{N}{N_r}^{\alpha} \]

where fitting parameters for phosphorous doping of silicon \( \mu_{\text{min}} = 68.5 \) cm\(^2\)/V \cdot s, \( \mu_{\text{max}} = 1414 \) cm\(^2\)/V \cdot s, \( N_r = 9.2 \cdot 10^{16} \) cm\(^{-3} \), and \( \alpha = 0.711 \).
The mobility of the carriers and concentration affects the permittivity of the material according to the Eq. 2. Fig. 1(B) depicts the alteration of permittivity for different doping levels. Slight change of the real part of permittivity affects the spectral position and quality factor of the resonance as one can see from Fig. 1(C). The imaginary part of permittivity defines the absorption and, therefore, optical heating.

In order to study optical heating performance of a doped silicon nanodisk, numerical model in commercial software COMSOL was created. Continuous wave illumination with normal incidence and $I_0 = 2 \text{ mW/}\mu\text{m}^2$, wavelength $\lambda = 1.3 \mu\text{m}$ and nanodisk with various radii and 220 nm height. Fig. 1(C) shows temperature increase of a single silicon nanodisk on a glass substrate for a different doping level. One can see that increase of doping level leads to a dramatic enhancement of optical heating by more than 3 orders of magnitude at a wavelength $\lambda$ of 1.3 $\mu\text{m}$.

3. conclusion
In summary, we have demonstrated the model of optical heating of doped silicon nanodisks in the near-IR. It was revealed that the maximum temperature can be increased by more than 3 orders with higher free carriers concentration. We believe that such approach will pave the way for implementation of all-dielectric nanophotonics in thermal applications in the near-IR.

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