Optical heating of doped semiconductor nanocylinders supporting quasi-BIC modes

Daniil Ryabov, Olesia Pashina, George Zograf, Sergey Makarov and Mihail Petrov
The Department of Physics and Engineering ITMO University, Saint-Petersburg, Russia.
E-mail: daniil.ryabov@metalab.ifmo.ru

Abstract. In the recent years, semiconductor and dielectric nanophotonic structures attracted a lot of attention for their resonant optical properties finding applications in thermal tuning and optical heating. Exciting high quality optical modes of both electric and magnetic nature in nanoresonators of high-index materials, one can effectively enhance optical absorption in such structures. Another big advantage of semiconductor materials is the ability to finely control the level of optical losses in visible and near infrared (near-IR) range through varying the doping level. In this work, we show theoretically that by moderate carrier doping of silicon via donors from group V materials one can achieve effective heating of nanoresonators. We show that by tuning the doping level of crystalline silicon supporting high quality non-radiative modes based on quasi bound states in the continuum one can achieve strong heating in near-IR under continuous wave regime illumination. We believe that our finding will pave the way for an efficient semiconductor near-IR all-optical sensors and nanoheaters.

1. Introduction
The implementation of the concept of bound-states in the continuum (BIC) to photonics [1] attracted a lot of attention to a number of effects including harmonic generation [2, 3], lasing action [4] and many others. Although BIC requires infinite periodic structure for field localization, it was shown that single nanoresonators can support quasi-BIC mode through destructive interference of radiation in the far-field, manifested by the unprecedented increase of the quality factor of the optical mode [5]. Such prominent quality factor and field localization demonstrated record performance for SHG [6, 7] and the ability for fine-tuning of the scattering response [8] and many others. Such tight field localization inside a single nanoobject is very profitable for efficient light absorption, however many semiconductor materials posses ultralow losses in visible and near-infrared range which prevents them from being utilized for optical heating applications [9].

This comes into sharp contrast with thermoplasmonics where the ohmic losses are inevitable. In this work we show theoretically that moderate doping of crystalline silicon with donor concentration of \( n_d = 7.6 \cdot 10^{18} \text{cm}^{-3} \) leads to significant increase of heating efficiency in nanocylinders supporting quasi-BIC resonance. We provide engineering of the optimal geometry and material parameters for achieving maximal optical heating in the near-IR optical range which is very attractive for bio-related photothermal applications and thermosensing.

2. Results
We start our study from consideration of the eigenmodes of a single cylindrical nanoresonator made of crystalline silicon. At the first stage we neglect the non-radiative losses which can be extremely low in undoped silicon in near-IR. The radiative losses which are inevitably present in any open resonant system can be significantly reduced by engineering the resonant configurations of the nanoparticles which results in high radiative Q-factors of the investigated geometries. The quasi-BIC modes are formed of strongly coupled modes of a cylinder providing the destructive interference of light in the far-field zone and, hence, better localization of light inside of the particle [10, 11]. Such a regime allows...
for significant increase of the modes’ Q-factor, and opens a way for efficient heating of the particles with relatively low intensities of the incident field.

The high-Q quasi-BIC modes appeared in the nanodisk geometries posses cylindrical symmetry with zero azimuthal number \( m = 0 \) with respect to cylinder axis [6, 14, 15]. Figure 1 (a) shows the spectral positins and Q-factors of modes of a cylinder on top of glass substrate with \( m = 0 \). Red circle region highlights the anticrossing are where two modes of the same symmetry come into strong coupling regime (these modes branches are marked with thin black lines for the convenience).

High-Q mode branch in this region reveals the quasi-BIC configurations which are marked with red color dots. For the wavelength of 1400 nm declared quasi-BIC mode corresponds to the cylinder with radius \( \rho = 619 \) nm and height \( h = 885 \) nm. As shown in Fig.1(b) these mode can be accessed through a azimuthally polarized vector beam matching the symmetry of the mode.

At the next step, we simulate the heating of the above-mentioned nanostructures supporting high-Q quasi-BIC mode with the commercial software COMSOL Multiphysics by direct solving of the heat conduction equation for the stationary case:

\[
\nabla \cdot (\kappa(r) \nabla T(r)) + Q(r) = 0.
\]

Here, \( \kappa \) is the material coefficient of thermal conductivity; \( r \) is the spatial coordinate and \( T \) is the local temperature of the cylinder. In our calculations, the source of heating \( Q(r) \) corresponds to electromagnetic power absorbed by the resonant structure from azimuthally polarized beam. Optical losses in silicon in the infrared range are close to zero, hence the heating of the particle is negligible (\( \Delta T = 0 \)K).
all donors are ionized at 300 K. Thus, the concentration of charge carriers is completely determined by the concentration of the dopant \( n_d \) (see the inset of Fig. 2(a)). The temperature increase during heating is balanced by Ohmic and radiative losses [16]:

\[
P_{\text{abs}} \sim \frac{\gamma_{\text{ohm}}}{(\gamma_{\text{ohm}} + \gamma_{\text{rad}})^2}.
\]

In this formula \( \gamma_{\text{ohm}} \) and \( \gamma_{\text{rad}} \) are the material (Ohmic) and radiative losses respectively. In the case of fixed radiation losses, the maximum of this function is reached when the radiative and non-radiative losses are equal. Since we have already optimized the radiative losses in quasi-BIC regime, the maximum heating could be achieved with relatively low values of optical losses. We explicitly estimate the optimal value by simulating the temperature increase inside the nanostructure and obtain a maximal heating corresponding to the imaginary part of the complex refractive index \( k = 0.0031 \) (Fig. 2(a)). For further analysis of the quasi-BIC heating properties, we present the temperature increase dependence on the radius of the excited particles with the fixed height of 885 nm and optimal value of material losses (Fig. 2(b)). This graph confirms that resonant excitation of a high-Q mode leads to a drastic enhancement of the heating temperature reaching the value of 800 K for the intensity of 1 GW/m².

Finally, we estimate the donors concentration necessary to achieve the optimal value of optical losses in silicon. In accordance with Drude model the imaginary part of dielectric permittivity change could be expressed as:

\[
\Delta \text{Im} \varepsilon(n_d) = \frac{\omega_p^2(n_d) \tau_e}{\omega(1 + \omega^2 \tau_e^2)} = 2\tilde{n}k,
\]

where \( \omega \) is the incident light frequency; \( \tau_e = 1 \text{ fs} \) - electron relaxation time associated with the electron-electron interaction; \( \omega_p(n_d) = (n_de^2/\varepsilon_0 m_{\text{eff}})^{1/2} \); \( m_{\text{eff}} = 0.26m_e \) is the effective mass of electrons in the conduction band of c-Si; \( \varepsilon_0 \) is the permittivity of vacuum and \( e \) is the elementary charge. Supposing that the real part of the refractive index \( \bar{n} \) does not change significantly with the free carrier concentration increase, we immediately obtain donors concentration \( n_d = 7.6 \cdot 10^{18} \text{ cm}^{-3} \) corresponding to the optimal value of \( k = 0.0031 \).

3. Conclusion
We theoretically investigated the strong optical heating of silicon cylindrical nanoparticles. It resulted from the efficient coupling of the incident azimuthally polarized laser beam with the quasi-BIC mode.
and optimization of material optical losses via free carriers doping. The described approach provides both high quality factor due to the tight localization of light in structures supporting quasi-BIC modes and non-zero losses necessary for effective thermo-optic interaction between the laser radiation and the responding particles. We believe that our proposal will contribute to modern research on all-dielectric thermophotonics.

4. Acknowledgments

The work was supported by the Russian Science Foundation (project No. 18-72-10140).

References

[1] Hsu C W, Zhen B, Stone A D, Joannopoulos J D and Soljačić M 2016 Nature Reviews Materials 1 1–13
[2] Hu H G, Yang M, Yue P, Bai Y T, Wang W J and Liu S D 2020 J. Phys. D: Appl. Phys. 53 215101 ISSN 0022-3727
[3] Sautter J, Xu L, Miroshnichenko A E, Lysevych M, Volkovskaya I, Smirnova D A, Camacho-Morales R, Zangeneh Kamali K, Karouta F, Vora K, Tan H H, Kauranen M, Staude I, Jagadish C, Neshev D N and Rahman M 2019 Nano Lett. 19 3905–3911 ISSN 1530-6984
[4] Kogdala A, Lepetit T, Gu Q, Bahari B, Fainman Y and Kanté B 2017 Nature 541 196–199
[5] Rybin M V, Koshelev K L, Sadrieva Z F, Samusev K B, Bogdanov A A, Limonov M F and Kivshar Y S 2019 Phys. Rev. Lett. 119(24) 243901 URL https://link.aps.org/doi/10.1103/PhysRevLett.119.243901
[6] Koshelev K, Kruk S, Melik-Gaykazyan E, Choi J H, Bogdanov A, Park H G and Kivshar Y 2020 Science 367 288–292 ISSN 0036-8075
[7] Carletti L, Koshelev K, De Angelis C and Kivshar Y 2018 Phys. Rev. Lett. 121(3) 033903 URL https://link.aps.org/doi/10.1103/PhysRevLett.121.033903
[8] Tiguntseva E, Koshelev K, Frasovs P, Tonkaev P, Mikhailovskii V, Ushakova E V, Baranov D G, Shegai T, Zakhidov A A, Kivshar Y et al. 2020 ACS nano 14 8149–8156
[9] Mylnikov V, Ha S T, Pan Z, Valuckas V, Paniagua-Domínguez R, Demir H V and Kuznetsov A I 2020 ACS nano 14 7338–7346
[10] Koshelev K, Tang Y, Li K, Choi D Y, Li G and Kivshar Y 2019 ACS Photonics 6 1639–1644
[11] Melik-Gaykazyan E, Koshelev K, Choi J H, Kruk S S, Bogdanov A, Park H G and Kivshar Y 2021 Nano Letters 21 1765–1771
[12] Zograf G P, Petrov M I, Makarov S V and Kivshar Y S 2021 1–92 (Preprint 2104.01964) URL http://arxiv.org/abs/2104.01964
[13] Bogdanov A A, Koshelev K L, Kapitanova P V, Rybin M V, Gladyshev S A, Sadrieva Z F, Samusev K B, Kivshar Y S and Limonov M F 2019 Adv. Photonics 1 016001 ISSN 2577-5421
[14] Sadrieva Z, Frizyuk K, Petrov M, Kivshar Y and Bogdanov A 2019 Physical Review B 100 1–12 ISSN 24699969 (Preprint 1903.03039)
[15] Gladyshev S, Frizyuk K and Bogdanov A 2020 Physical Review B 102 75103 ISSN 24699969 URL https://doi.org/10.1103/PhysRevB.102.075103
[16] Zograf G P, Petrov M I, Zuev D A, Dmitriev P A, Milichko V A, Makarov S V and Belov P A 2017 Nano Lett. 17 2945–2952 ISSN 1530-6984