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# Strong Absorption Enhancement in Si Nanorods

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**(5)** Supporting Information

**ABSTRACT:** We report two orders of magnitude stronger absorption in silicon nanorods relative to bulk in a wide energy range. The local field enhancement and dipole matrix element contributions were disentangled experimentally by single-dot absorption measurements on differently shaped particles as a function of excitation polarization and photon energy. Both factors substantially contribute to the observed effect as supported by simulations of the light-matter interaction and atomistic calculations of the transition matrix elements. The results indicate strong shape dependence of the quasidirect transitions in silicon nanocrystals, suggesting nanostructure shape engineering as an efficient tool for overcoming limitations of indirect band gap materials in optoelectronic applications, such as solar cells.



**KEYWORDS:** Absorption, nanocrystals, nanorods, atomistic theory, silicon

) ulk and thin film silicon are widely used in modern B photovoltaics, where the fundamental limit of efficiency in a single p-n junction cell (~29.5%) is largely defined by the bandgap energy.<sup>1</sup> Nanostructuring of silicon, for example, in the form of nanowires, was shown to be promising in shortening carrier collection length and suppressing reflection of the incident light.<sup>2</sup> At the limit of the smallest nanostructures, where the size approaches the exciton Bohr radius ( $\sim$ 5 nm), quantum confinement sets in, changing the basic material properties, such as bandgap and k-space structure.<sup>3</sup> This effect can push the efficiency limit higher by allowing a multijunction concept to be realized in the same material.<sup>4,5</sup> It can also provide new functionality for this ubiquitous material in photovoltaics and beyond, 6 where ordered 3D arrays of such nanoparticles<sup>7</sup> can form new energy bands suitable for the direct readout.8 Nanocrystals of silicon can also be used complementarily in solar cells for photon energy downshifting,<sup>9</sup> or photon multiplication by generating more low-energy photons than incoming high-energy quanta.<sup>10</sup> On the other hand, their enhanced photoluminescence<sup>11</sup> (PL) makes them attractive in several new applications, such as phosphors in white light-emitting diodes (LEDs),<sup>12</sup> or as biomarkers.<sup>13,14</sup> Because of strong absorption at high energies<sup>15</sup> these nanoparticles can also be considered as sensitizers for energy transfer to atomic or molecular species.<sup>16</sup>

In general, the electric field experienced by a nanoparticle under external illumination depends on its shape and dielectric contrast with the environment.<sup>17</sup> The incoming field for ablated particles may be locally enhanced or reduced through particle polarizability, depending on the electric field orientation relative to the particle major axis. As a result the absorption crosssection becomes slightly reduced for the perpendicular field orientation and substantially enhanced for the parallel one.<sup>18</sup> This effect was noticed previously for Si nanostructures as strong polarization dependence in nanowire and nanorod absorption.<sup>19–22</sup> Another important effect of the nanoparticle geometry on its interaction with light is the degeneracy lifting and relaxation of transition selection rules in an asymmetric particle.<sup>23</sup> The exact interplay between these effects depends on material properties as well as on the incoming photon energy and particle geometry. For silicon nanocrystals in particular, the energy-dependent quasidirect transitions<sup>15,24</sup> may also be nanoparticle shape-dependent. So for both fundamentals and applications an important question is what maximum absorption enhancement could be achieved by the nanoparticle shape control and under which conditions.

Here we investigate experimentally and theoretically both the local field enhancement and the exciton energy level structure effects on silicon nanoparticle absorption. We carried out photoluminescence and photoluminescence excitation measurements for single Si nanorods and close-to-spherical nanoparticles as a function of excitation polarization and energy. Indeed, the nanorods exhibit stronger absorption than spherical counterparts, which can reach as large as a factor of 50. The quantitative contributions of the local-field effect and intrinsic interband transitions in the observed enhancement were extracted from the experimental data with the help of numerical simulations of the wave-particle interaction. Atom-

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istic pseudopotential calculations show good agreement with the experimental results, clarifying the substantial contribution of the shape-dependent k-conservation rule breakdown to the nanorod absorption enhancement.

Oxide embedded nanocrystals were prepared by thermal oxidation of pre-etched silicon nanostructures. In this way Si nanorods (Figure 1, left) were formed from nanowall



**Figure 1.** (top) Schematics of the samples used in this study: (left) single nanorods embedded in nanowalls prepared by oxidation; (right) single Si nanodots randomly formed by oxidation of a thin SOI layer. (bottom) Corresponding PL images ( $\sim$ 50 × 50  $\mu$ m area). Individual bright spots correspond to single particles. Arrows indicate studied nanocrystals. (inset) SEM image of a nanowall (tilted view) of the sample with provided PL image. Bright part at the very top is a silicon nanowire breaking into nanorods as a result of oxidation (oxide is a darker part below). Scale bar is 100 nm.

structures<sup>21,25</sup> and close-to-spherical nanoparticles from thinned silicon-on-insulator (SOI) wafers<sup>26,27</sup> (Figure 1, right). Their shape was verified by cross-section (Figure S1, top) and top-view<sup>28</sup> HRTEM imaging. Both types of nanostructures have no significant strain as Fourier analysis reveals (Figure S1, bottom). Single-particle optical characterization was performed in a microphotoluminescence setup using a variable wavelength source or a polarized 405 nm laser diode for the excitation. The experimental results were compared to theoretical calculations, where Maxwell equations in 3D were solved numerically to evaluate the local field effect. We also performed atomistic calculations<sup>29,30</sup> of the nanoparticle electronic states with transition matrix elements<sup>6</sup> to account for the shape effect on absorption strength. Experimental and calculation details are provided in the Supporting Information.

Calculation of the Local Field Effect: At a Specific Polarization Angle the Local Field Effect Cancels Itself. The predicted local field effect using continuum calculations shows good agreement with polarization-dependent absorption measurements (Figure S3) that we reported previously for nanorods.<sup>21</sup> To obtain a more quantitative description of the local field effect for the case of Si nanocrystals in SiO<sub>2</sub> we calculated geometry and energy dependence of the absorption. Results for the same volume ellipsoids with varying long semiaxis *c* are shown in Figure 2, left. In the inset, the region of polarization degree angles at around  $\alpha = 75^{\circ}$  is enlarged. It is seen that in this range of excitation angles the geometry has little effect on absorption. Here the large field enhancement from the parallel field component compensates the small reduction from the perpendicular component (Figure S4). This effect appears to be valid across a wide spectral range, as shown in Figure 2, right. Here the absorption in a  $1.1 \times 1.1 \times 2.8$  nm semi-axes Si ellipsoid embedded in silica was evaluated under varying free-space excitation wavelength and compared with the same volume sphere. So at  $\alpha \approx 70^\circ$  the absorption in Si nanorods for all considered geometries and energies appears to be similar to a spherical particle of the same volume (3 nm diameter). Note that in these comparison calculations the difference in absorption strength between different shapes arises solely from the local field effect. Therefore, we conclude that under proper experimental conditions this geometryinduced local field effect can be suppressed.

Measured Absorption at This Specific Angle Still Reveals Difference between Nanorods and Nanodots. We measured absolute values of the absorption cross-section in nanorods and close-to-spherical nanoparticles at  $\alpha \approx 70^{\circ}$ (Figure 3, left). For that, we recorded luminescence decay and rise transients for several individual dots from each sample under 405 nm excitation.<sup>31</sup> The linear dependence of eq S1 with experimental data points is shown for one particular dot in the inset (the value at zero photon flux is the luminescence decay rate). Obtained from this slope absolute values of  $\sigma$ appear to be in the range  $0.8-1.9 \times 10^{-15}$  cm<sup>2</sup> for nanodots and  $0.7-1.4 \times 10^{-14}$  cm<sup>2</sup> for nanorods (Figure 3, left). Small variations in the absorption cross-section values for nanocrystals of similar emission energy can be attributed to small



**Figure 2.** Absorbed power of same volume ellipsoids calculated with the classical method. (left) Excitation polarization dependence for ellipsoids with different semiaxis *c* (the definition of angle  $\alpha$  is given on the right panel inset). For 70° <  $\alpha$  < 80°, the absorption depends very little on the nanoparticle shape, as the inset shows. (right) Spectral dependence for different excitation polarization angles  $\alpha$  in a Si ellipsoid with 1.1 × 1.1 × 2.8 nm semi-axes. The absorption at  $\alpha$  = 70° is nearly the same as in the same volume sphere (3 nm diameter, black) over the whole spectral range.



Figure 3. (left) Absolute values of the absorption cross-section under 405 nm excitation measured for different individual nanorods at  $\alpha \approx 70^{\circ}$  (blue squares) and SOI nanodots (red circles) as a function of emission peak position. The inset shows the dependence of the measured luminescence rise rate on the excitation photon flux for the nanorod with a 1.65 eV peak position. The slope defines the absorption cross-section value. For both samples, the error bars represent the standard deviation of the fittings. (right) Experimental excitation polarization dependence of the absorption cross-section for nanorods (blue squares) and spherical Si nanocrystals in nanowalls (red circles). At  $\alpha \approx 70^{\circ}$ , the absorption in nanorods is 6–7 times larger than what would be expected from the local field effect.

structural nonuniformities in a given sample.<sup>24</sup> The slightly different emission range for nanodots and nanorods cannot strongly affect the absorption cross-section. Indeed, for high-energy excitation used here the absorption cross-section for nanodots was shown to be only a factor of 2 lower at 1.9 eV than at 1.65 eV.<sup>32</sup> Here, instead, the measured difference reaches a factor of 20 between the lowest and the highest points in Figure 3, left. We can define the average value of the absorption cross-section at this excitation energy (3.06 eV) from the obtained data as  $\sigma_{ndot} \approx 1.5 \times 10^{-15}$  cm<sup>2</sup> and  $\sigma_{nrod} \approx 10^{-14}$  cm<sup>2</sup>. So on average there is a 6–7 times difference between these two geometries, while the local field effect predicts similar values under this excitation polarization angle (cf. Figure 2, left, inset).

Polarization and Energy Dependence of the Absorption Cross-Section for Nanorods and Nanodots. The obtained difference in absorption cross-section between nanorods and nanodots becomes clearer from the representation given in Figure 3, right. Here we compare polarization dependent data for a single nanorod (blue squares) with ensemble data for spherical nanocrystals (red dots) both emitting at ~1.65 eV and located on mesas of the same dimensions (Figure S2). The absolute value for each case is normalized to the measured absorption cross-section data at 405 nm excitation. As expected, spherical nanoparticles show no dependence on the excitation polarization, where the symmetry of valence and conduction bands in Si around  $\Gamma$ point ensures isotropic absorption in nanodots with cubic lattice.<sup>33</sup> It also confirms that nanowall mesas themselves do not affect absorption. On the other hand, the strong polarization dependence for nanorods translates the measured 6–7 times enhancement at  $\alpha \approx 70^{\circ}$  to a roughly 50-fold increase when the excitation is polarized along the nanorod long axis ( $\alpha = 0^{\circ}$ ).

The stronger absorption in nanorods at  $\alpha \approx 70^{\circ}$  polarization excitation persists over the whole spectral range as revealed by single-dot photoluminescence excitation measurements. In Figure 4, the nanorod and SOI nanodot absorption curves are shown for nanoparticles with the same emission energy (~1.75 eV), corresponding to a nanoparticle size of  $d \approx 3$  nm.<sup>6</sup> Strictly speaking, the same emission energy does not correspond to the same volume or number of atoms for different shape nanoparticles.<sup>37</sup> However, our calculations show



**Figure 4.** Absorption cross-section energy dependence measured for nanorods (for  $\alpha \approx 70^{\circ}$  excitation polarization at 405 nm excitation) and for SOI nanodots (blue and red curves) in comparison with some values from the literature.<sup>32,34–36</sup>

that the bandgap of a  $1.3 \times 1.3 \times 2$  nm Si nanorod and a  $1.5 \times 1.5 \times 1.5$  nm Si nanodot does not differ significantly: 1.82 and 1.88 eV respectively. So the emission energy can serve as an indicative parameter for comparing absorption in different nanodots and not too prolate nanorods.<sup>38</sup> One can see that while the SOI nanodot sample exhibits close to the previously reported values from the literature,<sup>32,34–36</sup> the nanorods have clearly higher absorption than any other sample of this emission energy. The structure of the absorption curve is also different, where for SOI nanodots four broad peaks can be distinguished,<sup>24</sup> while nanorods have a rather smooth curve.

A similar behavior for elongated particles was also observed in direct bandgap materials.<sup>18,39</sup> However, the enhancement value was not so large (2-3 times) and this effect was attributed primarily to the local field enhancement. Here for Si nanocrystals the local field effect has been minimized based on the choice of excitation polarization, while the enhancement factor appears to be larger in the range from 4 to 14 (the ratio is shown in Figure 5 as black points for two nanorod/nanodot pairs with different emission energies).

Atomistic Calculations of the Electronic States Explain the Absorption Enhancement. Consequently, there is obviously another effect responsible for the substantial increase in nanorod absorption. To explain this, we turn to



**Figure 5.** (top) Ratio of the measured absorption cross-section for nanorods (for  $\alpha \approx 70^{\circ}$  excitation polarization) to the one of SOI nanodots (black). Absorption enhancement as predicted from atomistic calculations (red). It results from shape-dependent k-conservation rule breakdown, enhancing the transition matrix elements for a  $1.3 \times 1.3 \times 2$  nm semi axes ellipsoid relative to the Si sphere of the same volume (3 nm diameter). (bottom) Absorption enhancement in nanorods versus bulk (per Si atom) for an ellipsoid oriented parallel to the incoming field.

atomistic pseudopotential calculations of the electronic states and transition matrix elements for Si nanocrystals of different shapes. We calculated absorption curves for  $1.3 \times 1.3 \times 2$  nm and  $1.1 \times 1.1 \times 2.8$  nm semi-axes Si ellipsoids and a spherical particle of the same volume from Fermi's golden rule, as described in the calculation methods in Supporting Information. Indeed, the absorption in the nanorod appears to be stronger (Figure S6), where the ratio to nanodot for these two nanorods as a function of energy is shown in Figure 5 as red lines. It exhibits very good quantitative agreement with experimental data for  $1.3 \times 1.3 \times 2$  nm nanorod at lower energies (<2.7 eV) and shows slightly lower values at higher energies. Qualitatively this effect can be attributed to the relaxation of the transition selection rules (momentum conservation breakdown) and degeneracy lifting for the electron and hole states due to the asymmetric geometry. The degeneracies in a Si NC are indeed high: for Se, Pe, De, Sh, and P<sub>h</sub> states they are 6, 12, 18, 3, and 6, respectively, without considering spin (S, P, and D are the electron and hole states with orbital angular momentum 0, 1, and 2).<sup>6</sup> The degeneracy lifting is experimentally observed here as the lack of structure in the absorption curve of nanorods in contrast to nanodots in which several distinguishable steps are seen (Figure 4).<sup>24</sup>

The difference between the calculated enhancement from the experimental values at high energies can be then explained by slight deviation of the probed nanocrystal shape from a perfect ellipsoid used for calculations. Another possible explanation would be a strain in nanorods, where 1-2% value of strain, which is within experimental error here (Figure S1, bottom), can induce an energy shift of at least 100–200 meV for the

direct optical gap of silicon.<sup>40</sup> Such a small strain would not affect the rest of the absorption spectrum, where the agreement between atomistic theory and experiment has been established (Figure 5, top). Also note that the average value of absorption enhancement (~6.5 times at 3.05 eV) was used to calibrate experimental curves in Figure 5, top. So the actual values can be slightly different for every two nanoparticles of the same emission energy.

Atomistic pseudopotential calculations reveal that the absorption enhancement does not simply scale with nanorod aspect ratio. Instead, at certain geometries this effect becomes more pronounced, such as for the  $1.3 \times 1.3 \times 2$  nm nanorod. A similar dependence featuring several resonances was shown previously for radiative<sup>41</sup> and Auger<sup>42,43</sup> rates in quantum dots. The exact effects of nanorod shape and crystallographic orientation on absorption will be investigated separately to identify these resonant conditions. With recent advances in shape-controlled synthesis of silicon nanoparticles,<sup>44</sup> large ensembles of such nanorods can potentially be synthesized.

Finally, we can evaluate the total absorption enhancement factor in silicon nanorods relative to bulk. We use previous results for nanodots, where the absorption was recalculated per Si atom for such a comparison.<sup>15</sup> Nanorods feature stronger dipole matrix elements than nanodots (Figure 5, top, 1.75 eV) and have stronger absorption for parallel polarization as a result of the local field effect (Figure 2, right,  $1.1 \times 1.1 \times 2.8$  nm semi-axes ellipse at  $\alpha = 0^{\circ}$ ). By combining all three effects, the total absorption enhancement factor in nanorods relative to bulk reaches 2 orders of magnitude in a wide spectral range (Figure 5, bottom).

Conclusions. We have measured polarization-dependent absorption in  $\sim$ 3 nm individual silicon nanorods and nanodots by photoluminescence and photoluminescence excitation techniques. The absorption in nanorods appeared to be strongly dependent on excitation polarization, while spherical particles exhibited no such dependence. Absolute values of the absorption cross section in nanorods turned out to be 5-50 times larger, depending on the excitation polarization and photon energy. This enhancement translates to up to 2 orders of magnitude increase in absorption relative to bulk material, when recalculated per silicon atom, for nanorods aligned to the excitation field. We reveal that both local field enhancement effect and dipole transition matrix elements make substantial contributions to the overall enhancement based on the combination of experimental results and theoretical calculations. This conclusion implies strong potential of nanostructuring for more efficient utilization of silicon material in photovoltaic applications. Elongated nanoparticles featuring stronger absorption may also be more favorable as fluorophores in bioimaging or as light-converting phosphors.

# ASSOCIATED CONTENT

# **Supporting Information**

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Experimental and calculation details provided (PDF)

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#### Notes

The authors declare no competing financial interest.

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