Tunable and selective resonant absorption in vertical nanowires

Baomin Wang and Paul W. Leu*

Department of Industrial Engineering, University of Pittsburgh, Pittsburgh, Pennsylvania 15261, USA
**Corresponding author: pleu@pitt.edu*

Received June 27, 2012; revised July 30, 2012; accepted July 30, 2012;
posted July 31, 2012 (Doc. ID 171234); published September 5, 2012

We demonstrate that vertical subwavelength diameter nanowires exhibit tunable and selective resonant absorption using numerical simulations and optical waveguide theory. Incident light on vertical nanowires only excites hybrid TM-dominant HE_{1m} leaky modes due to symmetry matching requirements. The transverse resonances associated with these hybrid modes result in strong absorption enhancements that may be adjusted by changing the nanowire diameter. In particular, the fundamental HE_{11} transverse resonance may be tuned across a wide range of wavelengths and is separated from that of the HE_{12} mode by a large spectral gap, which is advantageous for wavelength selectivity. Leaky longitudinal resonances result in weaker absorption peaks at larger wavelengths. We further study the effect of incident light angle on the absorption spectra.

OCIS codes: 040.5160, 040.6040, 250.0040.

Nanowires have been demonstrated as a promising new material for a variety of optoelectronic devices. The unique properties of nanowires, including light polarization sensitivity [1], absorption enhancement [2–5], high operation speed [6], low dark current [6,7], and large internal photoconductive gain [7] may offer advantages for photodetectors [7,8], lasers [9], and photovoltaics [3,10]. Most notably, recent demonstrations have shown that leaky mode resonances in horizontal semiconductor nanowires may be used to tune and enhance spectral absorption [11]. The nanowire acts as an optical antenna so when incident light couples to a leaky mode resonance, there is an enhanced electromagnetic field in the nanowire and increased absorption.

In this Letter, we demonstrate that vertical nanowires exhibit tunable resonant absorption features that may be useful for photodetectors or sensors where high absorption and high spectral selectivity are desired. While single horizontal nanowire photodetectors have been demonstrated to absorb light at several resonant wavelengths, the horizontal device geometry suffers from poor quantum efficiency and responsivity due to weak absorption [6]. Vertical nanowires may overcome the poor absorption in horizontal nanowires because the direction of incident light wave propagation is along the axis of the nanowire as opposed to in the radial direction. Vertical nanowires can be synthesized to long lengths to improve light absorption and high fill factors may be achieved by growing forests of these nanowires.

We demonstrate through simulations and symmetry arguments that incident light on vertical nanowires can only couple to HE_{vm} leaky modes where $v = 1$. By varying the diameter of the nanowires, the transverse resonance associated with the fundamental HE_{11} mode can be continuously tuned across a wide range of wavelengths. This resonance is separated from that of the HE_{12} mode by a large spectral gap, which may be used for wavelength selectivity. We use silicon as an example, but the spectral tuning of absorption in vertical nanowires may be extended to a range of other materials such as germanium or III–V semiconductors for applications such as wavelength division multiplexing in fiber optic communications [12] or temperature-sensitive infrared photodetectors [13].

To calculate the optical properties of nanowires, we utilized finite-difference, time-domain simulations. Figure 1(a) illustrates the square vertical nanowire arrays, which are defined by pitch a, diameter d, and length L. We considered vertical nanowires with length $L = 3800$ nm and pitch $a = 700$ nm. The results of our simulations, which were performed on square arrays, pertain to uniform diameter vertical nanowires in general–as long as the nanowires are not close enough to cause resonance modes on neighboring nanowires to couple to one another. This issue will be discussed in more detail later.

Figure 1(b) uses a contour plot to illustrate the dependence of optical absorption on the diameter of the silicon nanowires and the photon wavelength. Because of the subwavelength size of the nanowires, only a few leaky modes are supported. Leaky modes in step-index optical fibers satisfy the following dispersion relation [14]:

$$\left(n_1^2\frac{J_v'(u)}{uJ_v(u)}+n_0^2\frac{K_v'(w)}{wK_v(w)}\right)\times\left(\frac{J_v'(u)}{uJ_v(u)}+\frac{K_v'(w)}{wK_v(w)}\right)=\left(\frac{1}{u^2}+\frac{1}{w^2}\right)^2\left(\frac{\beta v}{k_0}\right)^2, \quad (1)$$

where u and w are the normalized transverse wave numbers inside and outside the cylinder and $u = \kappa\frac{d}{2} = \frac{d}{2}\sqrt{k_0^2n_1^2-\beta^2}$ and $w = \sigma\frac{d}{2} = \frac{d}{2}\sqrt{\beta^2-k_0^2n_0^2}$. In this case, n_1 and n_0 are the index of fraction inside and outside the cylinder, β is the propagation constant in the cylinder along the axis, and k_0 is the wavenumber in air. Generally, u, w, and β are complex, and J_v and K_v are the vth-order Bessel function of the first kind and modified Bessel function of the second kind and the prime denotes derivative with respect to its argument. In addition, $n_0 = 1$ for air and n_1 is a function of λ and complex for absorbing media. For silicon, the optical constants n_1 were taken from experimental results in Palik [15]. The leaky modes of optical fibers are generally hybrid with both H_z and E_z components. The solutions to Eq. (1) result in two

0146-9592/12/183756-03$15.00/0

classes of equations that are designated HE and EH for when the mode is TM and TE-dominant, respectively. Each mode is labeled with the integer subscripts v and m where v is the order and m is the mth root of the eigenvalue equation, which also corresponds to the radial mode number. The distinct peaks in the absorption spectra correspond to particular leaky mode resonances. We find that the strongest absorptions peaks in our simulations correspond to HE_{vm} transverse resonance modes with $v = 1$.

To understand why only HE_{1m} leaky modes result in absorption enhancements, we consider the symmetry of the different modes. For incident light polarized with the electric field in the x-direction, the electric field is antisymmetric under reflection about the yz plane. Only modes that are antisymmetric under mirror reflection about the yz plane can couple to this incident light. The electric fields must satisfy $\hat{O}_{M_x}\mathbf{E}(\mathbf{r}) = M_x\mathbf{E}(M_x\mathbf{r}) = -\mathbf{E}(\mathbf{r})$ [16], where $\hat{O}_{M_x}$ is a mirror reflection operator about the yz plane, which operates on a vector field by applying M_x to both the input and output vector. In this case, M_x flips the x-unit vector $\hat{\mathbf{x}}$ to $-\hat{\mathbf{x}}$, while leaving $\hat{\mathbf{y}}$ and $\hat{\mathbf{z}}$ alone. E_x must be symmetric about the yz plane or, equivalently, the mode must have no azimuthal symmetry. HE modes have azimuthal number $l = v - 1$, while EH modes have $l = v + 1$ [14]. Thus, the only modes with no azimuthal variation or the proper antisymmetry are the HE_{1m} modes. These are doubly degenerate modes that are antisymmetric about the yz or the xz plane, where one of the modes satisfies the required symmetry condition.

In Fig. 1(b), additional weaker resonant modes begin to appear for nanowires larger than 120 nm diameter for $\lambda > 670$ nm. These are longitudinal resonances associated with the HE_{1m} modes and the finite length of the nanowire. Hybrid leaky modes in nanowires are characterized by propagation constant β as defined by Eq. (1). Longitudinal resonances form when the guided wave picks up a round-trip phase change, $\beta_r = \frac{q\pi}{L}$ where β_r is the real part of β and q is a positive integer. At shorter wavelengths, the absorption length of silicon is small enough so the electromagnetic field intensity decays completely by the time it reaches the end of the nanowire. The long length of the nanowires is also why the absorption enhancement from these resonances are much weaker than the transverse resonances, since the light can make a fewer number of round trips before attenuating away. These longitudinal resonance modes can also couple to transverse resonance modes, leading to interference between the modal fields as can be seen in the absorption spectra at larger wavelengths.

The HE_{11} transverse resonance mode can be continuously tuned across the visible and near-infrared wavelengths and is separated from that of the HE_{12} mode by a large spectral gap. Three different nanowires indicated by the dashed white lines in Fig. 1(b) are highlighted in Fig. 1(c) to illustrate the tunability of the HE_{11} transverse resonance mode. The blue and green resonances at 470 and 530 nm are characterized by the Lorentzian function, but the red peak at 670 nm is characterized by some small additional peaks from longitudinal resonances. Due to the large spectral gap between the HE_{11} and HE_{12} transverse resonances, the nanowires also exhibit high wavelength selectivity. For example,

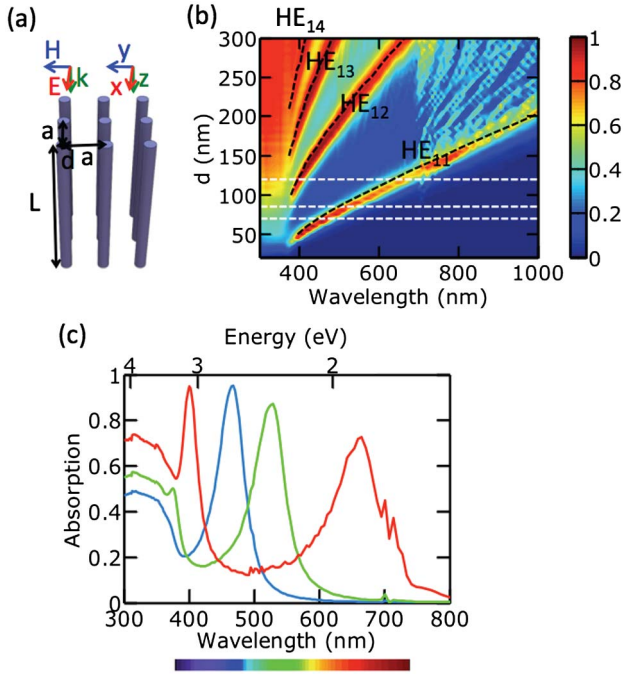

Fig. 1. (Color online) (a) Vertical nanowires array schematic. (b) Contour plot of absorption as a function of photon wavelength and nanowire diameter for vertical Si nanowire arrays. The dash-dotted white lines indicate nanowires illustrated in (c). (c) Absorption spectrum of nanowires with $d = 70$, 85, and 120 nm for blue, green, and red photodetectors.

the wavelength spacing between these two neighboring resonant peaks, called the free spectral range, is about 270 nm for the 120 nm diameter nanowires. The red, green, and blue photodetectors thus have minimal spectral cross talk.

In Fig. 2, we plot the electric field intensity $|\mathbf{E}(\mathbf{r})|^2$ for the 120 nm diameter vertical nm silicon nanowires at their tranverse resonant wavelengths. The HE_{1m} modes

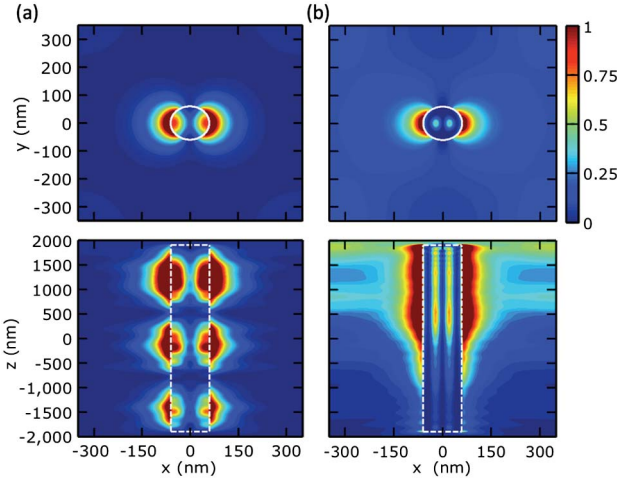

Fig. 2. (Color online) Electric field intensity plots of leaky mode resonances for $d = 120$ vertical nanowires at (a) $\lambda = 670$ and (b) 400 nm which correspond to the HE_{11} and HE_{12} modes, respectively. The top row illustrates the top view of $|\mathbf{E}(\mathbf{r})|^2$ at $z = 0$ nm, while the bottom row shows a side view at $y = 0$. White lines indicate the edges of the nanowires.

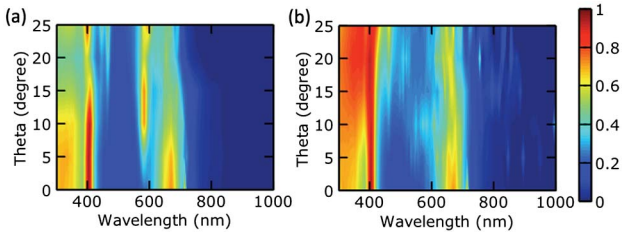

Fig. 3. (Color online) Angular dependence of absorption for (a) TE-polarized light and (b) TM-polarized light.

are dipole-like and primarily dominated by the E_x component. The HE_{11} mode shown here has distinct maxima along the length of the nanowires. On the other hand, for the HE_{12} state, the absorption length for silicon at $\lambda = 400$ nm is only about 80 nm such that the guided wave attenuates rapidly and does not reach the bottom of the nanowires. While we have simulated square arrays of nanowires of a particular pitch, the HE_{11} and HE_{12} leaky modes are concentrated in and around the nanowires and thus should not be affected by the order or position of vertical nanowires, as long as the nanowires are not too close together. When the nanowires are close, the modes couple together and the absorption peaks begin to broaden. We found that down to pitch $a \approx 500$ nm, the absorption resonances do not shift or split much. This is approximately the radial extent of the HE_{11} and HE_{12} guided resonance modes.

We plot the angular dependence of the 120 nm diameter vertical nanowires for both TE-polarized and TM-polarized light for incident angle θ from 0 to 25° in Fig. 3. For $\theta \le 5°$, the nanowires still primarily couple to the HE_{1m} leaky modes. However, for $\theta > 5°$, other absorption peaks can be seen for both polarizations of incident light. Additional leaky modes with azimuthal mode number $l > 0$ in addition to the $l = 0$ modes are excited and the absorption spectra no longer has a large free spectral range. We recently also demonstrated that tapering vertical nanowires breaks their symmetry, resulting in more broadband absorption, which is advantageous for photovoltaics [17].

We have used waveguide theory to explain the spectral tunability and selectivity of absorption resonances in vertical nanowires. In particular, incident light can only couple into HE_{vm} modes where $v = 1$, resulting in distinct absorption peaks separated by a large spectral gap. This demonstrates the use of leaky mode resonances and their symmetry for engineering spectral selectivity in vertical nanowires. These mechanisms may be useful for a variety of optoelectronic applications such as, photodiodes, photodetectors, phototransistors, optical modulators, optical amplifiers, light-emitting diodes, and lasers.

The authors acknowledge support from a grant from Mascaro Center for Sustainable Innovation at the University of Pittsburgh. Paul W. Leu also acknowledges the support of an Oak Ridge Ralph E. Powe Junior Faculty Enhancement Award.

References

1. J. Wang, M. S. Gudiksen, X. Duan, Y. Cui, and C. M. Lieber, Science **293**, 1455 (2001).
2. C. Lin and M. L. Povinelli, Opt. Express **17**, 19371 (2009).
3. E. Garnett and P. Yang, Nano Lett. **10**, 1082 (2010).
4. H. Bao and X. Ruan, Opt. Lett. **35**, 3378 (2010).
5. Q. G. Du, C. H. Kam, H. V. Demir, H. Y. Yu, and X. W. Sun, Opt. Lett. **36**, 1884 (2011).
6. L. Cao, J. Park, P. Fan, B. Clemens, and M. L. Brongersma, Nano Lett. **10**, 1229 (2010).
7. A. Zhang, S. You, C. Soci, Y. Liu, D. Wang, and Y. Lo, Appl. Phys. Lett. **93**, 121110 (2008).
8. Y. Ahn, J. Dunning, and J. Park, Nano Lett. **5**, 1367 (2005).
9. C. F. Zhang, Z. W. Dong, G. J. You, S. X. Qian, and H. Deng, Opt. Lett. **31**, 3345 (2006).
10. J.-Y. Jung, K. Zhou, H.-D. Um, Z. Guo, S.-W. Jee, K.-T. Park, and J.-H. Lee, Opt. Lett. **36**, 2677 (2011).
11. L. Cao, J. S. White, J. Park, J. A. Schuller, B. M. Clemens, and M. L. Brongersma, Nat. Mater. **8**, 643 (2009).
12. C. Brackett, IEEE J. Sel. Areas Commun. **8**, 948 (1990).
13. H. Pettersson, J. Trägårdh, A. I. Persson, L. Landin, D. Hessman, and L. Samuelson, Nano Lett. **6**, 229 (2006).
14. A. W. Snyder and J. Love, *Optical Waveguide Theory*, 1st ed. (Springer, 1983).
15. D. E. Palik, *Handbook of Optical Constants of Solids*, Vol. 1 (Academic, 1997).
16. J. D. Joannopoulos, S. G. Johnson, J. N. Winn, and R. D. Meade, *Photonic Crystals: Molding the Flow of Light*, 2nd ed. (Princeton University, 2008).
17. B. Wang and P. W. Leu, Nanotechnology **23**, 194003 (2012).