

## Wavelength Dependent Optical Characteristics: Intensity Distribution in Flat Silicon and Silicon Nanowire Used as Absorber in Solar Cell

Mohammad K. Hossain<sup>1,\*</sup>, Billel Salhi<sup>1</sup> and Ayman W. Mukhaimer<sup>2</sup>

<sup>1</sup> Center of Research Excellence in Renewable Energy (CoRERE), King Fahd University of Petroleum and Minerals (KFUPM), Dhahran 31261, Dhahran (Kingdom of Saudi Arabia)

<sup>2</sup> Department of Mechanical Engineering, King Fahd University of Petroleum and Minerals (KFUPM), Dhahran 31261, Dhahran (Kingdom of Saudi Arabia)

\*Correspondence to: kamalhossain@kfupm.edu.sa

### Abstract

Solar cells utilize a small portion of solar spectrum depending on the technology while solar radiation being a full of UV-VIS-IR wavelengths does not leave absorbing and other layers unaffected. Only the photon energy that matches with absorber layer contributes to effective power generation of solar cell. Higher and lower energy wavelengths induce thermalization and absorption losses which in turn introduce several consequences including heating and degradation in the cell level. Therefore engineered absorbing layer such as nanowire based solar cell holds huge potential. Here in this work, we have investigated and simulated four deterministic characteristics, viz, absorption depth profile, electromagnetic field, Poynting vector and exciton generation rate distribution at different incidents. Flat silicon and silicon nanowire were considered as examples along with a comparative outlook. Such predictive studies facilitate the choice of technology and how to improve the cell efficiency using light trapping technique.

*Key-words: Optical characteristics, Silicon nanowire, FDTD simulation, Optical confinement.*

---

### 1. Introduction

Solar radiation per second (i.e.  $1.74 \times 10^5$  TW) is more than sufficient to provide all the energy demands needed to facilitate entire world population in a year. Unfortunately it has been impractical because of technological challenges. Silicon (Si)-based solar panel is the most popular one in this regard and holds more than 90% of current photovoltaic (PV) market

(Sachs 2011). Although Si is abundant and superior in stability and non-toxicity, the Shockley and Queisser efficiency limit (i.e. ~31%) for a single band gap Si-based solar cell has become an issue and a matter of challenge for current research community. A small portion of solar spectrum contribute to solar cells performances, whereas solar radiation being a full of other wavelengths does not leave the associate layers unaffected. The photon energy that matches with absorber layer contributes to effective power generation of solar cell. Higher and lower energy wavelengths induce thermalization and absorption losses respectively which in turn introduce several subsequent problems including heating and degradation in the cell level. These additional consequences add up extra cost whereas current technology is already facing various challenges to limit the cost below 1¢ per kWh. Therefore, it is important to increase the cell efficiency at low cost to bring this technology within afford and reach.

Si nanowires (Si-NWs) have been considered potential to face the efficiency constrain because of nanometric features led unique properties (Kelzenberg et al. 2010; Polman and Atwater 2012; Zhao at al. 2004; Krogstrup et al. 2013; Yu et al. 2014). Si-NWs have strong optical absorption compared to that of flat silicon along with many other electrical characteristics that lead to reduced production cost (Salhi et al. 2016). The efficiency can be further improved by optimizing and tuning incident solar spectrum that is useful in efficient solar cell system. A predictive analysis of inherent optical characteristics of such nanowire based system indeed facilitates to determine and improve other associate layers of the solar cell. Previously we have reported absorption profile, energy flow, EM field distribution and exciton generation rate at 740 nm in addition to spectral analysis of absorption depth profile for Si-NW system (Hossain 2016a, 2016b). Nevertheless, further correlated spectral analysis on absorption profile, energy flow, EM field distribution and exciton generation rate distributions is indispensable.

Two key challenges, low cost materials as well as higher efficiency, are immensely needed at this moment to accelerate mass-production and utilization of PV technology. PV solar cell based on nanometric Si-NW-based possess huge potential in this regard. Apart from optical characteristics, short collection length for charge carriers in Si-NWs boosts up efficiency and allows to use down grade absorbing materials. First ever PIN configured solar cells based on Si-NWs was presented by Tian group in 2007 (Tian et al., 2007). The Si-NWs were grown by vapor-liquid-vapor process. Since then, a variety of methods have been reported to obtain Si-NW such as high temperature evaporation of silicon powder in furnace (Cui et al., 2001,

2000; Wu et al., 2004), vapor-liquid-solid process (Wang et al., 1999; Westwater, et al 1997), laser ablation (Zhang et al., 1999), liquid solution solid process (Davidson et al., 2004), solid liquid solid process (Yan et al., 2000), metal catalyst assisted electroless etching (Peng et al., 2009, 2006a, 2006b, 2005, 2002), etc. There are huge and extensive studies on conventional flat panel, although 3<sup>rd</sup> generation solar cell especially nanostructured materials based photovoltaic solar cell is not well understood. Numerical studies always support to implement the proof-of-concept into prototype that ultimately ends up with a suitable product. The studies also open up new avenue and in-depth understanding of the technology. Therefore, an correlated and simulative study, such as absorption profile, electromagnetic (EM) field, Poynting vector, excitation generation rate distribution, etc. are inevitable.

Here in this work, we have investigated and simulated four deterministic characteristics, *viz.*, spectral absorption depth profile, electromagnetic field, Poynting vector and exciton generation rate distribution. Two Si-based absorbing layers generally used in thin film solar cell, such as flat silicon and silicon nanowire, were considered as examples. A comparative study has been carried out to illustrate how an efficient light management can be obtained in silicon nanowire based solar cell.

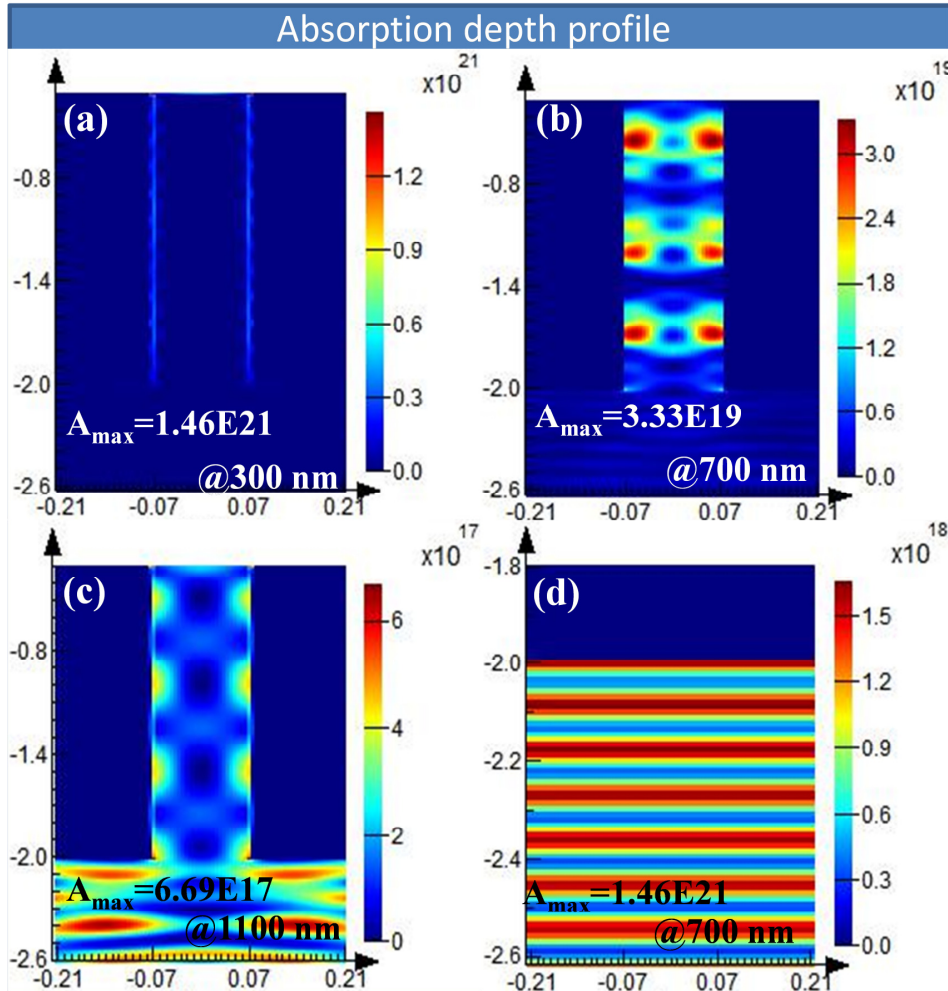
## **2. Method and materials**

c-Si slab and Si-NW on c-Si wafer were modeled in FDTD package of Lumerical Solution (ver 8.6) and a three-dimensional (3D) analysis was carried out to obtain and compare optical characteristics of such systems. The model geometry was selected in such a way so that the parameters can be as close as of those reported previously (Hossain et al. 2016). Absorption profile, Poynting vector, EM field distribution, and generation rate distributions at different wavelengths ranging from UV to NIR region were extracted. Unpolarized plane wave as illumination source was set as incident to the vertically modelled Si-NW. The characteristics of Si-NW system were compared with that of c-Si slab only. Intensities of absorption profile, Poynting vector, EM field and exciton generation rate distributions were obtained slice by slice at different incident wavelengths.

## **3. Results and discussion**

Solar cell internal quantum efficiency is known to be directly related to the photon absorption profile of the absorbing layer. Such photon absorption can be confined and enhanced depending on the geometry of absorbing layer in solar cell. Absorption profile, EM field distribution, Poynting energy and excitation generation rate distribution are inter-related and

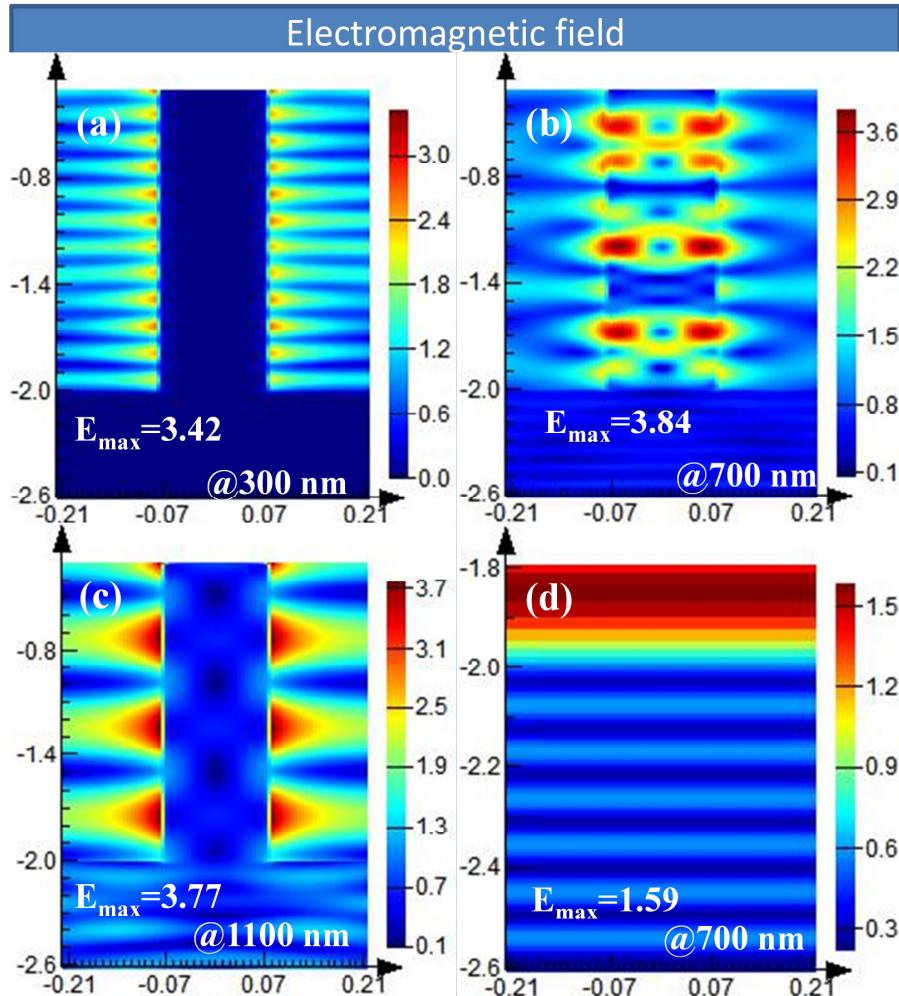
deterministic factor to efficient solar cell. We have extracted aforementioned characteristics at different wavelength ranging from UV to NIR region (i.e. at 300, 500, 700, 900, and 1100 nm). Figure 1a–c and Fig. 2a–c show absorption profiles and electromagnetic field distribution



**Fig. 1: (a)-(c) Spectral absorption depth profile of Si-NW model system at 300, 700 and 1100 nm wavelengths respectively, and (d) that of flat c-Si slab at 700 nm wavelength.**

of nanowire model system at 300, 700, and 1100 nm wavelength respectively. Absorption profile and electromagnetic field distribution of c-Si slab only at 700 nm wavelength of solar spectrum was shown in Fig. 1.d and Fig. 2d respectively as references. For shorter wavelength with higher energy, such as at 300 nm, almost no absorption and EM field distribution was observed. On the other hand, for longer wavelengths, such as at 1100 nm, slight distribution was observed near the edge and started to reduce within the absorbing layer. At 700 nm wavelength of solar spectrum, the intensity distribution was confined within

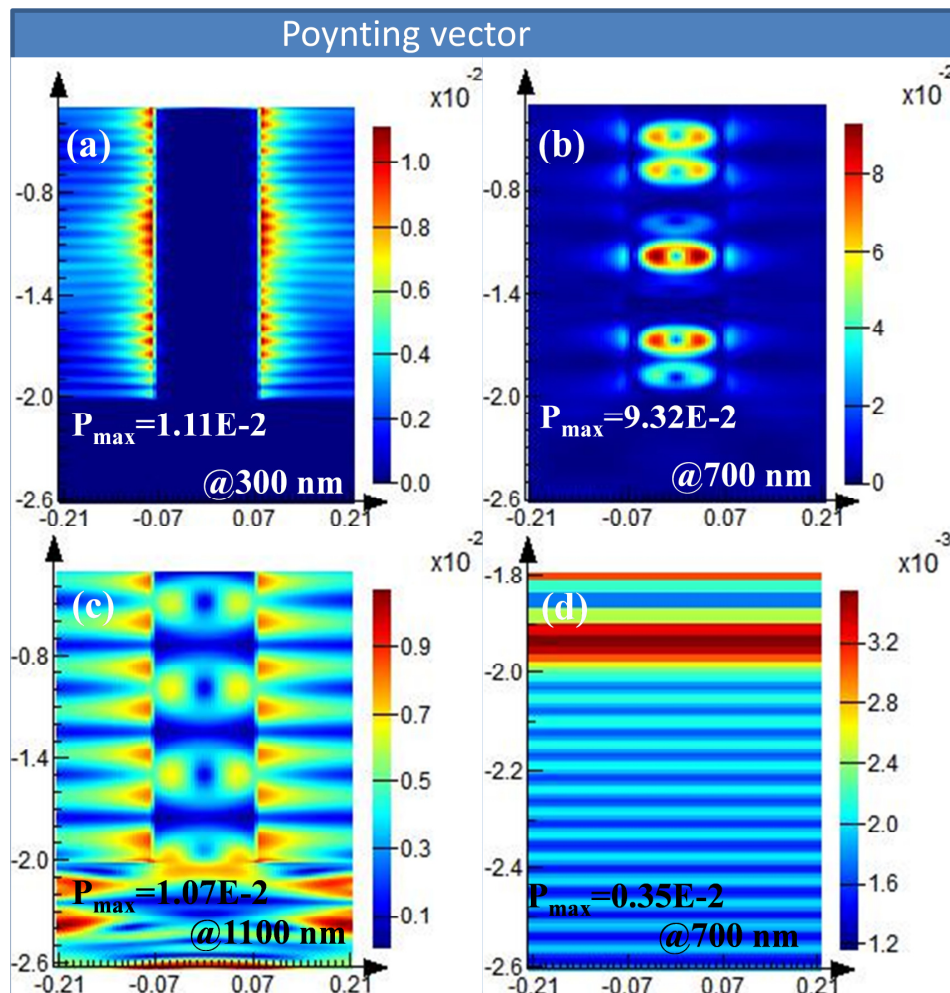
the nanowire model system. For conventional flat panel Si-based solar cell, single band gap material ( $E_g = 1.8$  eV or 700 nm) utilizes the solar spectrum at around 700 nm.



**Fig. 2:** (a)-(c) spectral EM field distribution for Si-NW model system at 300, 700 and 1100 nm wavelengths respectively and (d) that of flat c-Si slab at 700 nm wavelength.

In photovoltaics, excitation generation rate defines how many of excess excitons (i.e., excited electrons and holes) are available to collect. Number of useful excitons per incident photon is very crucial in designing efficient solar cell. Current (i.e. rate of charge flow) in solar cell depends on the concentration of such excitons. Therefore, generation rate is calculated by taking divergence of Poynting vector considering a zero recombination loss. Therefore, understanding of spectral distribution of Poynting vector and excitation generation rate within flat silicon as well as Si-NW system is very important. Energy flow distribution throughout a

single Si-NW from top to the bottom are shown in Fig. 3a–c at different wavelength such as 300, 700, and 1100 nm wavelength respectively. At shorter wavelength, such as at 300 nm, distributions were found intense near the edge and there was almost no distribution within the nanowire model system. For longer wavelengths with lower energy, such as at 1100 nm, there was slight confined distribution but that started to reduce within the absorbing layer. At 700 nm wavelength of solar spectrum, the intensity distribution was observed to be confine and well distributed. Confined energy flow distribution was observed within the nanowire model system. Figure 3d shows the Poynting vector profile obtained in flat c-Si slab at 700 nm wavelength as reference.

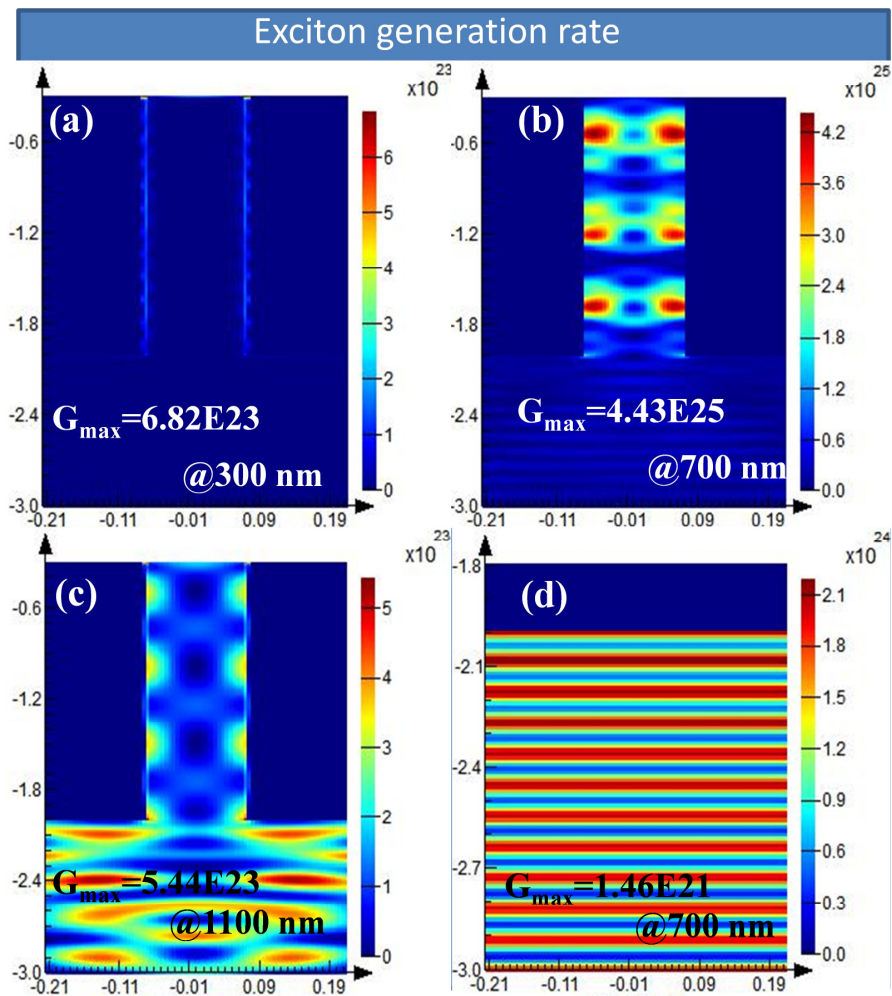


**Fig. 3:** (a)–(c) Spectral Poynting vector profile of Si-NW model system at 300, 700 and 1100 nm wavelengths respectively, and (d) that of flat c-Si slab at 700 nm wavelength.

Figure 4a–c show excitation generation rate distribution of nanowire model at 300, 700, and



1100 nm wavelength, respectively. At shorter wavelength with higher energy, no excitation generation rate distribution was observed. For longer wavelengths, such as at 1100 nm, slight distribution near the edge was observed. At 700 nm wavelength of solar spectrum, most of the exciton generation rate distribution was confined within the nanowire model system and the intensity distribution was well distributed. Excitation generation rate distribution of c-Si slab only at 700 nm wavelength of solar spectrum was shown in Fig. 4d as references.



**Fig. 4:** (a)-(c) spectral exciton generation rate distribution for Si-NW model system at 300, 700 and 1100 nm wavelengths respectively and (d) that of flat c-Si slab at 700 nm wavelength.

#### 4. Conclusion

Absorption depth profile, electromagnetic field, Poynting vector, and excitation generation rate distribution of two typical model systems, flat silicon and nanowire model systems, were observed at different wavelengths. At around 700 nm (band gap,  $E_g = 1.8$  eV), intensity distributions were found confined and well distributed within the Si-NW model system with reference to those obtained at other wavelengths. Exciton generation rate was available and well distributed all the way down to the bottom of the wire. Lower wavelength with higher energy solar spectrum was not found to be efficient for Si-NW model system.

#### 5. Acknowledgment

Authors like to thank Center of Research Excellence in Renewable Energy (CoRERE), King Fahd University of Petroleum and Minerals (KFUPM) for the support in this work.

#### 6. References

- Kelzenberg, M.D., Boettcher S.W., Petykiewicz J.A., Turner-Evans D.B., Putnam M.C., Warren E.L., Spurgeon J.M., Briggs R.M., Lewis N.S., Atwater H.A., 2010. Enhanced absorption and carrier collection in Si wire arrays for photovoltaic applications. *Nat Mater.* 9, 239–244.
- Polman A., Atwater H.A., 2012. Photonic design principles for ultrahigh-efficiency photovoltaics. *Nat Mater.* 11, 174–177.
- Yu L.W., Misra S., Wang J.Z., Qian S.Y., Foldyna M., Xu J., Shi Y., Johnson E., Cabarrocas P.R., 2014. Understanding light harvesting in radial junction amorphous silicon thin film solar cells. *Sci Rep.* 4, 4357–4363.
- Krogstrup P., Jorgensen H.I., Heiss M., Demichel O., Holm J.V., Aagesen M., Nygard J., Morral A.F., 2013. Single-nanowire solar cells beyond the Shockley-Queisser limit. *Nat Photonics.* 7, 306–310.
- Salhi B., Hossain M.K., Mukhaimer, A.W., AlSulaiman, F.A., 2016. Nanowires: A New Pathway to Nanotechnology-based Applications. *J Electrocer.* 37, 34–49.
- Hossain M.K., Salhi B., Mukhaimer A.W., 2016. Optical confinements in correlated spectral characteristics of vertically aligned silicon nanometric wires followed by a facile fabrication thereof. *Plasmonics.* 1–8 (10.1007/s11468-016-0387-y).
- Hossain M.K., Salhi B., Mukhaimer A.W., Al-Sulaiman F.A., 2016. Fabrication and optical



simulation of vertically aligned silicon nanowires. *Appl Nanosci.* 6, 1031–1036.

Tian, B., Zheng, X., Kempa, T.J., Fang, Y., Yu, N., Yu, G., Huang, J., Lieber, C.M., 2007. Coaxial silicon nanowires as solar cells and nanoelectronic power sources. *Nature*, 449, 885–889.

Cui, Y., Duan, X., Hu, J., Lieber, C.M., 2000. Doping and Electrical Transport in Silicon Nanowires. *J. Phys. Chem. B.* 104, 5213–5216.

Cui, Y., Lauhon, L.J., Gudiksen, M.S., Wang, J.F., Lieber, C.M., 2001. Diameter-controlled synthesis of single-crystal silicon nanowires. *Appl. Phys. Lett.* 78, 2214–2216.

Wu, Y., Cui, Y., Huynh, L., Barrelet, C.J., Bell, D.C., Lieber, C.M., 2004. Controlled growth and structures of molecular-scale silicon nanowires. *Nano Lett.* 4, 433–436.

Wang, N., Tang, Y.H., Zhang, Y.F., Lee, C.S., Bello, I., Lee, S.T., 1999. Si nanowires grown from silicon oxide. *Chem. Phys. Lett.* 299, 237–242.

Westwater, J., Gosain, D.P., Usui, S., 1997. Control of the size and position of silicon nanowires grown via the vapor-liquid-solid technique. *Japanese J. Appl. Phys. Part 1-Regular Pap. Short Notes Rev. Pap.* 36, 6204–6209.

Zhang, Y.F., Tang, Y.H., Peng, H.Y., Wang, N., Lee, C.S., Bello, I., Lee, S.T., 1999. Diameter modification of silicon nanowires by ambient gas. *Appl. Phys. Lett.* 75, 1842.

Davidson, F.M., Schrickler, A.D., Wiacek, R.J., Korgel, B. a, 2004. Supercritical fluid-liquid-solid synthesis of gallium arsenide nanowires seeded by alkanethiol-stabilized gold nanocrystals. *Adv. Mater. (Weinheim, Ger.)* 16, 646–649. doi:10.1002/adma.200306284.

Yan, H., Xing, Y., Hang, Q., Yu, D., Wang, Y., Xu, J., Xi, Z., Feng, S., 2000. Growth of amorphous silicon nanowires via a solid-liquid-solid mechanism. *Chem. Phys. Lett.* 323, 224–228. d

Peng, K., Fang, H., Hu, J., Wu, Y., Zhu, J., Yan, Y., Lee, S., 2006a. Metal-particle-induced, highly localized site-specific etching of Si and formation of single-crystalline Si nanowires in aqueous fluoride solution. *Chem. Eur. J.* 12, 7942–7947.

Peng, K., Hu, J., Yan, Y., Wu, Y., Fang, H., Xu, Y., Lee, S., Zhu, J., 2006b. Fabrication of single-crystalline silicon nanowires by scratching a silicon surface with catalytic metal particles. *Adv. Funct. Mater.* 16, 387–394.

Peng, K., Xu, Y., Wu, Y., Yan, Y., Lee, S.T., Zhu, J., 2005. Aligned single-crystalline Si

nanowire arrays for photovoltaic applications. *Small* 1, 1062–1067.

Peng, K.-Q., Wang, X., Wu, X., Lee, S.-T., 2009. Fabrication and photovoltaic property of ordered macroporous silicon. *Appl. Phys. Lett.* 95, 143119.

Peng, K.-Q., Yan, Y.-J., Gao, S.-P., Zhu, J., 2002. Synthesis of Large-Area Silicon Nanowire Arrays. *Adv. Mater.* 14, 1164–1167.