Journal of Physical and Theoretical Chemistry
of Islamic Azad University of Iran, 19 (3) 69-75: Fall 2022
(J. Phys. Theor. Chem. IAU Iran)
ISSN 1735-2126

Investigation of Silicon Nanowires Roles in Solar Cells

Ali Mahmoudloo [1]*, Seyyed Sadegh Gholami [2]

[1] Department of Physics Education, Farhangian University, P.O. Box 14665-889, Tehran, Iran
[2] Department of Mathematics Education, Farhangian University, P.O. Box 14665-889, Tehran, Iran

Received February 2023; Accepted March 2023

ABSTRACT

This paper will discuss the science of nanowire technology in the field of solar energy. It will elaborate on how this recent innovation improves upon the current methods in efficiency, cost, and durability. The value of this technology to its field, and its ability to make solar power a viable worldwide option will also be discussed. It is estimated that the world's supply of fossil fuels will be reduced to a bare minimum during this century. Renewable energy sources such as wind and solar energy have yet to become major contributors to our energy supply due to their cost and efficiency. Presently, nanotechnology is being introduced into the field of solar energy to combat this fault and improve both efficiency and cost. Nanowire solar cells that have already been developed are mostly based on hybrid organic-inorganic materials or are made of semiconductors. Presently the efficiency produced by the traditional crystalline silicon based solar cells is approximately 6.5% [1]. These first attempts at using nanowires in solar cells have increased this efficiency up to 8.5%. New technologies are looking into all-inorganic solar cells based on silicon nanowires. The silicon nanowires are relatively easy to synthesize and can be used with low cost substrate technologies like glass and metal foil. These low cost substrates will allow the nanowires to be not only durable but also much easier to produce than current silicon base solar cells [2]. Overall the continued developments in fields such as this are crucial if we as a nation are committed to securing the stability of our economy.

Keywords: Nanotechnology; Nanowires; Photovoltaic cells; Renewable resources; Solar cells; Solar energy.

INTRODUCTION

Solar cells, also known as photovoltaic cells, create energy by converting sunlight into electricity and have been used since the late 1950s. The early stages of solar cells were used almost exclusively in space due to much more cost effective energy sources available on earth's surface. Solar cells had a relatively slow start until the

---

*Corresponding author: a.mahmoodlou@cfu.ac.ir

1970s energy crisis. Since then, the field of solar energy has seen rapid growth [3]. Solar energy has also seen a growth in the variety of technology that uses it. Solar cells can now be seen on houses, calculators, and cars.

Traditional Photovoltaic (PV) cells are made using semiconductors like silicon [4]. Silicon has only four electrons in its outer energy shell causing it to bond with four nearby atoms. Because of this pure silicon is a poor conductor of electricity because it has no free electrons. To combat this issue impurities are added in a process called doping [4]. Silicon can be doped with elements that have three electrons in their outer shell to create silicon with free openings and carry a positive charge, or silicon can be doped with elements that have five electrons in their outer shell to create silicon with free electrons and carry a negative charge [4]. A silicon PV cell is composed of a thin N-type wafer, which is silicon doped with an electron rich compound, and a thicker P-type wafer, which is silicon doped with an electron deficient compound. A typical PV cell consists of a thin layer of phosphorus doped silicon (N-type wafer) on a much thicker layer of boron doped silicon (P-type wafer) [5]. These cells are then electrically connected in a grid of parallel circuits to form a module. Connecting cells into a module allows for higher voltages to be produced. Multiple modules are then assembled together to for a panel. Then multiple panels are connected to form the complete power generating unit called an array [5].

PV cells generate an electrical towards the top of the cell where the wafers come in contact, known as the P-N junction. Sunlight then contacts the surface of the PV cells where the electrical field provides direction and momentum to the light-stimulated electrons. These light stimulated electrons result in a flow of direct current. This process can be seen in Figure 1.

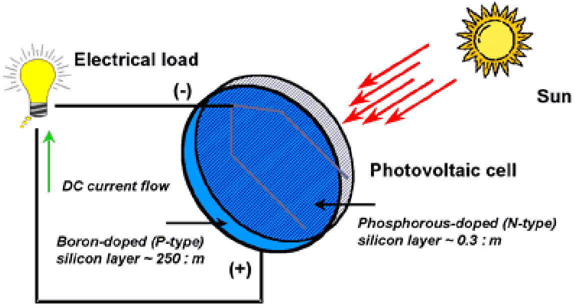

Fig. 1. Converting sunlight into energy [5].

NANOWIRES IN SOLAR CELLS

Scientists are now researching new ways to use silicon in solar cells because rising costs of the high purity silicon required by tradition solar cells, along with the complex and energy demanding process. One of these emerging technologies is using silicon to make small nanowires. The efficiency of nanowires is currently lower than that of conventional wafer cells; however the benefit of these new nanowires is they use a reduced quantity and quality of silicon compared to tradition silicon wafers. As of now the benefits of nanowires are outweighed by their lower efficiency.

Our simulation model is based on first-principles quantum mechanics (QM) calculations combined with Marcus-Hush theory, which we have validated by predicting anisotropic hole mobilities of several typical p-type organic compounds. Using the hopping mechanism for an organic crystal at room temperature, the nonadiabatic electronic hopping rate (W) is given by Marcus-Hush equation:

$$W = \frac{V^2}{\hbar}\left(\frac{\pi}{\lambda\, k_B T}\right)^{1/2} \exp\left(-\frac{\lambda}{4k_B T}\right) \qquad (1)$$

where V is the electronic coupling between neighboring molecules in the organic single-crystal, λ is the reorganization energy, T is the temperature, and k_B is the Boltzmann constant.

Assuming no correlation between hopping events, the hopping rate between neighboring molecules in the organic single-crystal leads to the diffusion coefficient

$$D = \frac{1}{2n}\sum_i r_i^2 W_i P_i \qquad (2)$$

where n is the spatial dimensionality and *i* represents a specific hopping pathway with hopping distance r_i (the intermolecular center-to-center distance of different dimer types). P is the hopping probability which is calculated as

$$P_i = \frac{W_i}{\sum_i W_i} \qquad (3)$$

The diffusive mobility from charge hopping μ is then evaluated from the Einstein relation, leading to the bulk (isotropic) mobility of the material:

$$\mu = \frac{e}{k_B T} D \qquad (4)$$

The magnitude of the field-effect mobility in a particular transistor channel depends on the specific surface of the organic crystal. We analyze the mobility of components for each surface in terms of angles (γ_i) between the charge hopping pathways and the plane of interest ($W_i \cdot r_i \cdot \cos\gamma_i$). In most instances, unsubstituted π-conjugated molecules crystallize into a layered herringbone packing, which gives rise to a 2D transport within the basal stacked organic layers while transport between layers is less efficient. For the hopping paths in the basal stacked layers, the γ_i are 0 degrees.

Using the basal plane as the reference, Φ is the orientation angle of the transistor channel relative to the reference axis (such as the crystallographic axes *a, b* or *c*) and $\{\theta_i\}$ are the angles of the projected hopping paths of different dimer types relative to the reference axis. Thus the angles between the hopping paths and the conducting channel are $\theta_i - \Phi$ (see Figures 1a and 1c). We then project the hopping paths onto the different transistor channels ($W_i \cdot r_i \cdot \cos\gamma_i \cdot \cos(\theta_i - \Phi)$). In the typical layered herringbone packing, neighboring molecules in the same layers can be characterized as transverse dimers T and parallel dimers P as illustrated in Figures 1a and 1c. For crystals with structural disorder, we use distribution functions to describe the probability density of dimer types. For the ideal high-purity crystals without disorder, the orientations of the surrounding molecules are identical, so that equations 2-4 lead to the orientation function describing the mobility in a specific conducting direction on a specific surface in the organic crystal:

$$\mu_\Phi = \frac{e}{2k_B T}\sum_i W_i r_i^2 P_i \cos^2\gamma_i \cos^2(\theta_i - \Phi) \quad (5)$$

Here $P_i \cdot \cos^2\gamma_i \cdot \cos^2(\theta_i - \Phi)$ describes the relative hopping probability of various dimer types to the specific transistor channel, while r_i, γ_i and θ_i are determined by the molecular packing architecture in the organic crystal; other terms are defined as above. In eq (5), we suggest that the mobility in a special conducting direction is determined by all related hopping pathways and it is a combined effect of electronic couplings (*V*) from different hopping pathways in organic materials. In eq (5), a specific Φ corresponds to a specific conducting direction, which means that it is a one-dimensional model. Thus, the spatial dimensionality n in eq (2) is taken to be 1 for the derivation of eq (5).

Equation (5) provides an analytic function to determine the angular-resolved anisotropic mobilities for any type of organic semiconductors by relating the crystal packing and electron coupling *V* to the angle Φ. We describe the mobility as a function of the orientation angle of the transistor channel in a plane, taking $\mu'(\Phi) = 0$ while $\mu''(\Phi) > 0$ defines the direction for the conducting channels with the highest mobility in the plane and μ'' (Φ)< 0 defines the direction for the conducting channels having the lowest mobility in the plane. Taking μ' (Φ) = 0, leads to:

$$\Phi_{extrema} = \frac{n\pi}{2} + \frac{1}{2}\arctan\left(\frac{\sum_i P_i V_i^2 r_i^2 \cos^2 \gamma_i \sin 2\theta_i}{\sum_i P_i V_i^2 r_i^2 \cos^2 \gamma_i \cos 2\theta_i} \right), n = 0, \pm 1, \pm 2, \pm 3, \cdots \quad (6).$$

When the orientation angle of the transistor channel equals to $\Phi_{extrema}$, the highest/lowest mobility in the plane could be calculated by substitution of the $\Phi_{extrema}$ values into equation (5). We have validated equations (5) and (6) for some of the highest performing p-type organic semiconductors, such as ruberene, pentacene, tetracene, 5,11-dichlorotetracene (DCT) and hexathiapentacene (HTP), by comparing the calculated results with the available experimental data.[13]

Just two parameters, electron coupling V and reorganization energy λ, determine the relations in equations (1) - (6) and both of which can be derived from first principle calculations. We use the adiabatic potential-energy surfaces method to calculate λ. The geometries for the isolated molecules in the neutral and cationic/anionic states are optimized using DFT with the B3LYP functional and with the 6-311G** basis set. For the neutral monomer A, the reorganization energies for hole transport and electron transport are as follows:

$$\lambda_{hole} = \lambda_0 + \lambda_+ = \left(E_0^{A^*} - E_0^A\right) + \left(E_+^{A^*} - E_+^A\right) \quad (7)$$

$$\lambda_{electron} = \lambda_0 + \lambda_- = \left(E_0^{A^*} - E_0^A\right) + \left(E_-^{A^*} - E_-^A\right) \quad (8)$$

where E_0^A and E_+^A / E_-^A denote the energies of neutral and cation/anion monomers in their respective optimized geometries, and $E_0^{A^*}$ and $E_+^{A^*} / E_-^{A^*}$ denote the energies of neutral and cation/anion monomers with the cation/anion and neutral geometries, respectively.

How Nanowires are made

There are two main techniques used to synthesize nanowires: chemical vapor deposition and patterned chemical etching. In chemical vapor deposition, nanowires are synthesized by flowing chemical precursor vapors into the hot zone of a furnace to react on a substrate, often with the assistance of a metal catalyst nanoparticle [6].The precursor vapors are then transported to the substrate with an inert carrier gas, often combined with other reactant gases along the way [6]. The substrate is placed in the deposition one of the furnace, where chemical decomposition is favorable. Multiple mechanisms then promote nanowire growth instead of thin-film deposition. “The most common mechanism for this is the vapor-liquid-solid mechanism. This mechanism uses a metal catalyst that forms a liquid eutectic with the desired nanowire material. Upon chemical decomposition and dissolution into the liquid eutectic droplet, the solution becomes supersaturated and overcomes the nucleation barrier to begin precipitation” [6].

Patterned chemical etching is a top-down or hybrid top-down/bottom-up approach [6]. First n-type silicon is dipped into a silica bead solution to form the patterned substrate. Then patterned substrate is dissolved with a directional, substrate-selective etch like deep reactive-ion etching or metal-assisted chemical etching to begin to form nanowires. Then the silica beads are removed in hydrofluoric acid and diffusion dope to form radial p-n junctions as seen in Figure 2[6].

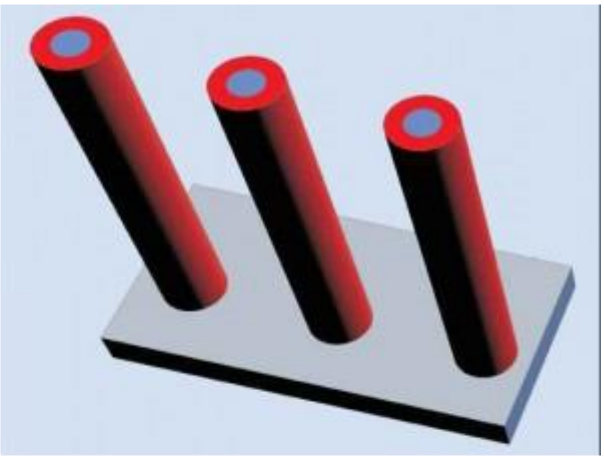

Fig. 2. This shows a layer of n-type silicon forming a shell around a p-type silicon core [8].

Absorption

The amount of sunlight a PV cell absorbs depends on two this: reflection, in which not all light enters the semiconductor, and transmission, in which the sample is to thin or does not have enough light-trapping schemes to quench all the photons [6].

Reflection is caused by a difference in refractive indexes between two media [6]. Without an antireflection coating semiconductors will reflect much of the suns energy, drastically reducing the amount of power it generates. To reduce reflection one or more coatings are added that have a refractive index intermediate between that of the semiconductor and that of air [6]. Another way to reduce reflection is to construct nanowires into a cone-shaped array with the tip much smaller than the wavelength of light. Nanowires made from certain materials can greatly reduce reflection when arranged in this cone-shaped array [6].

Charge Separation and Carrier Collection

Nanowires provide an opportunity to use new change separation mechanisms. The new mechanisms would not require the solar cells to be made with doped material. This would lower recombination rates, which is a prevalent limiting factor in high-efficiency solar cells.

Nanowires also display much higher carrier collection efficiency due to faster band conduction rather than a trap-limited diffusion transport mechanism [6]. This works because nanowires can be grown directly on a substrate, there is much less series resistance because the distance the current travels through the silicon to the metal is much less.

Benefits of Nanowires

While current nanowire based solar cell have not yet reached the efficiency of the traditional planar silicon wafer cells, they have many other benefits. Nanowires using a radial junction require a much lower quality and quantity of materials. Because of this there is a potential to make solar cells with performance close to that of tradition cells, but made of a small quantity of abundant, nontoxic, low-cost materials [7].

Future of Nanowires in Solar Cells

For nanowires to become a better candidate for large scale development a 10 percent or better conversion efficiency must be obtained. To achieve this research is being done into the different geometries of nanowire arrays. For instance, nanowires grown in an ordered array show much more potential in light trapping than nanowires grown in a random array. Also, nanowires grown vertical have increase light-trapping by a factor of 73 compared to those grown horizontally [6]. Another benefit of nanowires is that they can be grown on many inexpensive substrates like tin foil. This reduces the need for costly lattice-matched substrates used in silicon wafer cells.

With a decrease in cost seen with the use of nanowires, solar cells will soon be incorporated into many new technologies. Right now solar power is only practical in certain situations, but once efficiency and cost are improved the potential for solar cells to be incorporated into current technology is huge. For example, It could be used in things like hybrid cars as another source of electricity to reduce the amount of fuel consumed.

IMPORTANCE OF SOLAR ENERGY

For many centuries our society has used fossil fuels for lighting, cooking, heat, and electricity. Because of their abundance and effectiveness we have not needed to significantly branch out energy sources. But now, our society is too dependent on fossil fuels. With the threat of global warming, conflict over the supply of fossil fuels, and their inevitable depletion, there is an increased pressure to invest more into renewable resources. If we do not branch out our energy sources, then we will not be able to maintain our energy consumption once fossil fuels run out. Switching to renewable energy resources like solar power not only gives us an everlasting source of energy, but one without the pollution of burning fossil fuels [8].

"Solar radiation represents the largest energy flow entering the terrestrial ecosystem."[9] With the enormous amount of free solar energy flowing through our atmosphere the potential for solar energy to become a major part of society's sustainable energy providers is very real. An increase in solar energy would also drastically reduce pollution because of the reduction of need for fossil fuels. However, for this potential to be achieved solar energy must improve its cost and efficiency. That is why research into new solar technologies like the use of nanowires is so important our future.

REFERENCES

[1] Tsakalakos, L., J. Balch, J. Fronheiser, and B. A. Korevaar. "Silicon Nanowire Solar Cells."Http://bg.bilkent.edu.tr. APPLIED PHYSICS LETTERS, 07 Dec. 2007. Web. 30 Jan. 2012. <http://bg.bilkent.edu.tr/jc/topics/Photovoltaic%20Overview/papers/Silicon%20nanowire%20solar%20cells.pdf>.

[2] Hamilton, Tyler. "Flexible, Nanowire Solar Cells." Technology Review: The Authority on the Future of Technology. 6 Feb. 2008. Web. 23 Jan. 2012. http://www.technologyreview.com/Nanotech/20163/.

[3] "Solar Power." Wikipedia. Wikimedia Foundation, 29 Feb. 2012. Web. 01 Mar. 2012. http://en.wikipedia.org/wiki/Solar_power

[4] Toothman, Jessika, and Scott Aldous. "How Solar Cells Work." HowStuffWorks. Web. 01 Mar. 2012. <http://science.howstuffworks.com/environmental/energy/solar-cell.htm>

[5] "How PV Cells Work." Florida Solar Energy Center. Web. 01 Mar. 2012. http://www.fsec.ucf.edu/en/consumer/solar_electricity/basics/how_pv_cells_work.htm

[6] Garnett, Erik C., Mark L. Brongersma, Yi Cui, and Michael D. McGehee. "Nanowire Solar Cells." *Www.stanford.edu*. Stanford University, 23 Mar. 2011. Web. 27 Feb. 2012. <http://www.stanford.edu/group/mcgehee/publications/ARMS2011.pdf>.

[7] Yarris, Lynn. "Trapping Sunlight with Silicon Nanowires « Berkeley Lab News Center."Berkeley Lab News Center. University of California, 3 Mar. 2010. Web. 13 Feb. 2012. <http://newscenter.lbl.gov/feature-stories/2010/03/03/trapping-sunlight/>.

[8] Ethics of Solar Power and Global Warming." http://greenplanetethics.com. Web. 23 Jan. 2012.

<http://greenplanetethics.com/wordpress/ethics-of-solar-power-and-global-warming/>.
[9] An Assessment of Solar Energy Conversion Technologies and Research Opportunities."Global Climate and Energy Project. Stanford University. Web. 26 Feb. 2012.

مجله شیمی فیزیک و شیمی نظری
دانشگاه آزاد اسلامی واحد علوم و تحقیقات
جلد ۱۹، شماره ۳، پاییز ۱۴۰۱
ISSN ۱۷۳۵-۲۱۲۶

بررسی نقش نانوسیم‌های سیلیکونی در سلول‌های خورشیدی

علی محمودلو*[1]، سید صادق غلامی[2]

[1] گروه آموزش فیزیک، دانشگاه فرهنگیان، صندوق پستی ۸۸۸ -٥٦٤٤١ تهران، ایران
[2] گروه آموزش ریاضی، دانشگاه فرهنگیان، صندوق پستی ۸۸۸ -٥٦٤٤١ تهران، ایران

چکیده

در این مقاله علم فناوری نانوسیم در زمینه انرژی خورشیدی مورد بحث قرار خواهد گرفت. در مورد چگونگی بهبود این نوآوری اخیر بر روش های فعلی در کارایی، هزینه و دوام توضیح داده خواهد شد. ارزش این فناوری در زمینه خود و توانایی آن در تبدیل انرژی خورشیدی به یک گزینه قابل دوام در سراسر جهان نیز مورد بحث قرار خواهد گرفت. تخمین زده می شود که عرضه سوخت های فسیلی در جهان در طول این قرن به حداقل ممکن کاهش یابد. منابع انرژی تجدیدپذیر مانند انرژی باد و خورشید به دلیل هزینه و کارایی که دارند هنوز به سهم عمده ای در تامین انرژی ما تبدیل نشده اند. در حال حاضر، فناوری نانو برای مقابله با این عیب و بهبود کارایی و هزینه، در حوزه انرژی خورشیدی معرفی شده است. سلول‌های خورشیدی نانوسیمی که قبلاً توسعه یافته‌اند، بیشتر بر اساس مواد آلی–غیر آلی ترکیبی هستند یا از نیمه‌رساناها ساخته شده‌اند. در حال حاضر راندمان تولید شده توسط سلول های خورشیدی مبتنی بر سیلیکون کریستالی سنتی تقریباً ٦,٥٪ است [۱]. اولین تلاش‌ها برای استفاده از نانوسیم‌ها در سلول‌های خورشیدی، این راندمان را تا ۸,۵ درصد افزایش داده است. فناوری‌های جدید به دنبال سلول‌های خورشیدی غیرآلی بر پایه نانوسیم‌های سیلیکونی هستند. سنتز نانوسیم‌های سیلیکونی نسبتاً آسان است و می‌توان آن‌ها را با فناوری‌های زیرلایه کم‌هزینه مانند شیشه و فویل فلزی استفاده کرد. این بسترهای کم هزینه به نانوسیم‌ها اجازه می‌دهند که نه تنها بادوام باشند، بلکه تولید آنها بسیار آسان‌تر از سلول‌های خورشیدی پایه سیلیکونی فعلی است [۲]. به طور کلی، اگر ما به عنوان یک ملت متعهد به تضمین ثبات اقتصاد خود باشیم، ادامه تحولات در زمینه هایی مانند این بسیار مهم است.

کلید واژه‌ها: فناوری نانو؛ نانوسیم؛ سلول های فتوولتائیک؛ منابع تجدیدپذیر؛ سلول های خورشیدی؛ انرژی خورشیدی

---

[*] مسئول مکاتبات: a.mahmoodlou@cfu.ac.ir