Optimal design of aperiodic, vertical silicon nanowire structures for photovoltaics

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Abstract: We design a partially aperiodic, vertically-aligned silicon nanowire array that maximizes photovoltaic absorption. The optimal structure is obtained using a random walk algorithm with transfer matrix method based electromagnetic forward solver. The optimal, aperiodic structure exhibits a 2.35 times enhancement in ultimate efficiency compared to its periodic counterpart. The spectral behavior mimics that of a periodic array with larger lattice constant. For our system, we find that randomly-selected, aperiodic structures invariably outperform the periodic array.

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References and links

There is growing interest in how nano- and microstructured materials can be used to achieve high absorption within small material volumes [1–3]. This area of structural absorption engineering has the ultimate goal of making cheaper, more efficient solar cells. Photovoltaic cells based on silicon nanowire arrays are one important system [2,3]. While silicon nanowire arrays offer potentially advantageous electrical and optical properties [4–10], the highest experimentally measured efficiencies are currently ~5% [10]. Theoretical studies of optical absorption [11–13] are critical for maximizing the achievable efficiency and guiding device design. Interestingly, previous results have shown that a nanowire array can have higher broadband absorption than a solid film, given proper design parameters [14–17]. Yet, previous work has largely been limited to periodic structures. Expanding the parameter space to include complex, aperiodic structures can offer huge, potential gains in performance. Here, we study the case in which the nanowire array is the absorber itself. We use large-scale simulations and machine-based optimization techniques [18–25] to design optimal, aperiodic nanowire structures with greater than 100% increase in photovoltaic efficiency compared to their periodic counterparts.

Our work exploits in-plane resonances of aperiodic nanowire structures, localized modes that can be excited by normally incident light. The modes provide resonant absorption enhancement, trapping light of particular wavelengths within the absorptive, silicon material. This mechanism allows high absorption, even within thicknesses shorter than the optical absorption length. Achieving high absorption within a small material volume is particularly important between the wavelengths of 800nm and 1100nm, which contain a large fraction of the solar spectrum, yet are poorly absorbed by crystalline silicon [26]. In contrast to previous work on structural randomness [27], we deliberately exploit aperiodicity to optimize photovoltaic performance. Other previous work has experimentally demonstrated the use of aperiodic silicon nanotip arrays as anti-reflection coatings [28]. In contrast, we study the case in which the nanowire array itself is used as a thin film absorptive layer.

The broadband absorption of a solar cell is characterized by the ultimate efficiency [29]:

$$\eta = \frac{\int_{310\text{nm}}^{1000\text{nm}} I(\lambda)A(\lambda) \frac{2}{\lambda_g} d\lambda}{\int_{310\text{nm}}^{1000\text{nm}} I(\lambda)d\lambda}$$
where \( \lambda \) is the wavelength, \( I(\lambda) \) is the spectral irradiance (power density) of the ASTM AM1.5 direct normal and circumsolar spectrum \([30]\), and \( A(\lambda) \) is the absorptance of the structure. For a silicon-based solar cell, the relevant wavelength range is from 310nm, where the solar irradiance becomes negligible, to \( \lambda_g = 1127\)nm, the wavelength corresponding to the band gap of crystalline silicon. The calculation assumes that each photon with energy greater than the band gap produces one electron-hole pair at the energy of the gap, and that all carriers are collected to produce current. In an actual solar cell, collection will be limited by factors including surface recombination \([31]\). The ultimate efficiency thus provides an upper bound on the efficiency of the solar cell.

We used the ISU-TMM package \([32]\), an implementation of the generalized transfer matrix method, to calculate optical properties of nanowire arrays. Absorptance was calculated as \( A(\lambda) = 1 - R(\lambda) - T(\lambda) \), where \( R(\lambda) \) and \( T(\lambda) \) are the reflection and transmission. We used the optical constants for intrinsic crystalline silicon listed in Ref. \(31\), neglecting the effect of doping on the optical properties. The integrals were evaluated using the trapezoid rule with 915 sampling points.

Figure 1 shows schematics of the nanowire structures we study. We will consider the optical absorption within the nanowire. This model is appropriate to photovoltaic cells in which the nanowires serve as the photoactive material, for example, due to incorporation of radial p-n junction in nanowires \([5,17]\).

![Fig. 1. Schematics of periodic (a) and aperiodic (b) silicon nanowire structures.](image)

Figure 2(a) illustrates the top view of a periodic, vertically-aligned silicon nanowire array. Incident light propagates in the \( z \)-direction with the electric field polarized in the \( x \)-direction. The nanowire diameter \( d \) is 65nm. The nanowires are arranged in a square lattice with lattice constant \( a = 100\)nm and are surrounded by air. Each nanowire has a height of 2.33\( \mu \)m in the \( z \)-direction. Calculations were performed using a 500nm by 500nm super cell, containing 25 nanowires. The size of the super cell was limited by computational feasibility. The boundary conditions are periodic in \( x \) and \( y \).

Starting from the periodic configuration, we adjusted the positions of the nanowires within the super cell one at a time to maximize the ultimate efficiency. An iterative random walk algorithm was used for the optimization. At each iteration, a nanowire in the super cell was randomly selected and moved to a new position. The new position was drawn from a uniform distribution around its original position over the whole super cell, under the constraint that the selected wire will not overlap with any other wire in the super cell after the move. The ultimate efficiency of the new structure was then calculated by TMM. If the ultimate efficiency was higher than that before the move, the new position of the selected wire was accepted and stored. Otherwise, the move was rejected and the selected wire was moved back to its original position. The procedure was iterated for 1000 times. The resulting structures, such as the one shown in Fig. 2(b), are partially aperiodic. Within the super cell, the rods are arranged aperiodically. From super cell to super cell, the aperiodic arrangement repeats.
We calculated the ultimate efficiency of the periodic structure of Fig. 2(a) to be 8.70%. The efficiency is lower than that of a solid, silicon thin film with the same thickness (13.83%). Aperiodicity provides dramatic absorption enhancement. The optimal, aperiodic structure in Fig. 2(b) has an ultimate efficiency of 20.44%, 2.35 times higher than the periodic array. Its efficiency is higher than a solid, thin film and also slightly higher than a solid, thin film with a Si$_3$N$_4$ antireflective coating (20.34% for optimized coating thickness of 63nm). The fact that the aperiodic structure is more absorptive than the thin film is notable, given that the volume of absorbing material is three times less.

We plot the absorptance spectrum for the periodic structure in Fig. 3(a). The absorptance spectrum for the thin film is plotted for reference. The absorptance of the periodic array is higher than the thin film in the high-energy range, which can be attributed to reduced reflection from the top surface. However, the absorptance is lower in the low energy range, which contains a large proportion of solar photon flux. As a result, the ultimate efficiency of the periodic array is lower than that of the thin film.

The absorptance spectrum of the optimally-designed, aperiodic array is also shown in Fig. 3(a). In the high energy range, the absorptance is similar to that of the periodic array and higher than that of the thin film. This is also due to the significantly reduced reflection from the top surface. More importantly, it exhibits an overall shift towards the lower energy range compared to the periodic array. In addition, numerous absorption enhancement peaks appear at lower energies. From previous work, we know that these two spectral features are also characteristic of periodic arrays with larger lattice constants (for example, $a\sim500$nm and $d\sim300$nm) [14]. In Ref.14, we attributed the features to (1) an increase in field concentration inside the nanowire, and (2) the excitation of guided resonance modes. In a sense, the aperiodic array can thus be said to mimic a periodic array with larger lattice constant. An absorption enhancement peak of the optimal aperiodic array is shown in Fig. 3(b). Strong absorption corresponds to high reflectance and low transmittance, as observed previously for guided resonances in periodic arrays [14].
In Fig. 4, we plot the power loss rate (or absorption profile) inside the periodic (Fig. 4(a)) and the optimal aperiodic (Fig. 4(b)) structures, normalized to the maximal power loss rate inside the periodic array. The incident wavelength is $\lambda = 992.3\text{nm}$, corresponding to a resonant absorption enhancement peak inside the aperiodic array as shown in Fig. 3(b). The power loss rate is calculated as $\frac{1}{2} \omega \varepsilon'' |E|^2$, where $\omega$ is the frequency of the incident light, $\varepsilon''$ is the imaginary part of the dielectric constant, and $|E|^2$ is the local electric field intensity. The power loss rate is only non-zero inside the silicon nanowires. The evaluation plane was located 0.233$\mu$m beneath the top surface of the nanowire array. Figure 4(b) shows several localized, strongly enhanced absorption regions in the optimal aperiodic array, consistent with the peak in the absorption spectrum.

For periodic structures, guided resonances result from the coupling of normally incident light to a superposition of modes propagating in the plane of the array. This mechanism decreases the fraction of light escaping the structure (either through reflection or transmission) and increases absorption. For the aperiodic structure, normally incident light excites localized resonances of the aperiodic array. Such resonances could be viewed as resulting from “multiple reflection” or “multiple scattering” between nanowires. This mechanism serves a similar function of resonant absorption enhancement.
We next investigated whether aperiodic structures outperform the periodic array in general. The ultimate efficiency was calculated for 1000 randomly selected aperiodic structures. Figure 5 shows the histogram of the calculation results. Interestingly, all of the aperiodic structures we investigated had a higher ultimate efficiency than their periodic counterpart. For the randomly selected structures, the ultimate efficiency has a mean value of 14.51% and a standard deviation of 1.60%. The mean value is higher than the ultimate efficiency of a silicon thin film of the same thickness (13.83%). Examination of the solar absorptance spectra revealed that the two prominent spectral features of the optimal aperiodic array, an overall shift towards low energies and the appearance of absorption enhancement peaks, were generally observed.
In summary, we have demonstrated the optimal design of aperiodic, vertically-aligned silicon nanowire structures for photovoltaic applications. An optimization procedure based on the random walk algorithm enhanced the ultimate efficiency by 2.35 as compared to the periodic array. The solar absorbance spectrum of the optimal aperiodic array was found to resemble that of a periodic array with larger lattice constant and higher ultimate efficiency. In our study, the super cell size was restricted to make the optimization computationally feasible. We have verified that broadband absorption enhancement is also observed for super cells with sizes from 300nm-700nm.

For the diameter and filling fraction used here, randomly selected, aperiodic structures all had higher ultimate efficiencies than the periodic array. We have also performed calculations on other wire sizes, including $d = 50$nm and $d = 80$nm with initial lattice constant $a = 100$nm in a 500nm by 500nm super cell, as well as $d = 100, 130, 160$nm with initial lattice constant $a = 200$nm in an 800nm by 800nm super cell. In all of these cases, all aperiodic structures had higher ultimate efficiencies than their periodic counterparts. Interestingly, for certain large enough rod sizes, the aperiodic structure can have a higher ultimate efficiency than the optimum periodic array. More specifically, we simulated rods with $d = 160$nm and an initial spacing of 200nm in an 800nm by 800nm super cell and calculated the ultimate efficiency of 100 randomly-selected configurations. The highest ultimate efficiency found in this set was 25.69%. In comparison, previous work identified $a = 650$nm and $d = 520$nm as the approximate optimal values for periodic structures, yielding an ultimate efficiency of 24.28% [15].

While the random walk algorithm used in this work is relatively easy to implement, it is not guaranteed to reach the global optimum. Future work will employ adaptive optimization algorithms, such as simulated annealing or genetic algorithms, to help avoid getting stuck in local optima while insuring fast convergence [33]. Further, the identification of “robust” optima [34], or configurations of nanowires that exhibit both high ultimate efficiency and low sensitivity to perturbations in the design parameters, is a challenging optimization problem for future research.

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