

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 absorptance 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 $d = 50\text{nm}$ and $d = 80\text{nm}$ with initial lattice constant $a = 100\text{nm}$ in a 500nm by 500nm super cell, as well as $d = 100, 130, 160\text{nm}$ with initial lattice constant $a = 200\text{nm}$ 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 $d = 160\text{nm}$ 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 $a = 650\text{nm}$ and $d = 520\text{nm}$ 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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