Enabling Solar Cells

VIRTUAL PROTOTYPING OF NANOSTRUCTURES

Solar panels offer the possibility of harvesting the almost limitless electromagnetic energy radiated from the sun. However, widespread commercial deployment requires that greater conversion efficiencies can be attained at cheaper costs than that available with current solar cell technologies. New nanophotonic materials and technologies coupled with advanced simulation software based on the finite-difference time-domain (FDTD) technique offer great promise to overcome these challenges.

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While the price of solar electricity has been steadily decreasing, more than halving in each of the past two decades, it is still several times more expensive than that produced by other methods for today's electricity grid. However, solar cells do have the potential to make a significant contribution to the world's future energy requirements as technological innovations continue to improve both their efficiency and cost.

Currently, crystalline silicon cells are the most widely deployed and have efficiencies typically between 13 and 22 percent. These solar cells account for more than 90 per cent of the photovoltaic market, but as the market is experiencing rapid growth, the landscape is changing rapidly. In fact, solar applications now account for more than half the usage of silicon wafers, surpassing the semiconductor industry since 2006 for wafers consumed worldwide.

Thin film solar cells are an innovative competitor and are attractive because of their lower production costs, but the trade off is slightly lower efficiencies (between 8 and 18 percent). These cells are typically multi-layer designs, consisting of different materials deposited onto glass or metallic substrates. The desire to reduce costs and increase efficiency is leading researchers to investigate a number of new nanophotonic technologies which may provide part of the answer. Anyone who has looked at a polished silicon wafer will have noticed that it acts like a mirror. In fact, almost half of the incident light is reflected back. Anti-reflection coatings are thus routinely used to reduce this reflection. Ideally, one would like to use a broadband antireflection coating to reduce the reflection across the entire solar spectrum.

Moth eye pattern versus thin films

However, traditional designs for such a broadband antireflection coating would require multiple layers of special materials to be deposited, which would add significantly to the cost of the solar cell. Thus typically in practice, a single thin layer of SiN$_x$ (or

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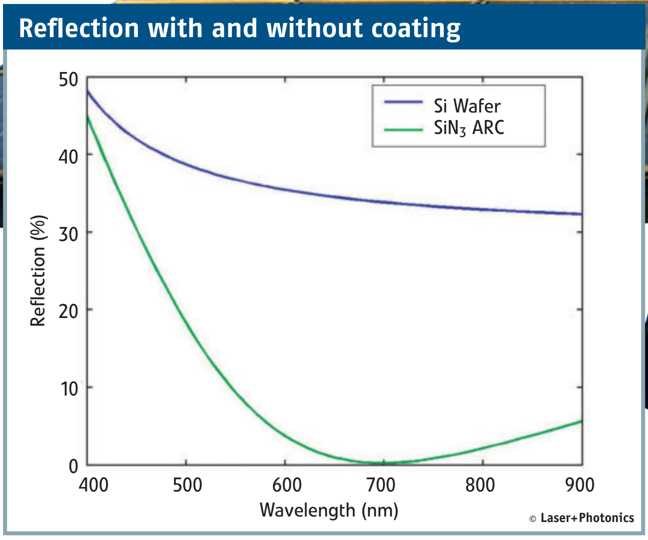


1 Reflection from silicon wafer with and without anti-reflection coating (ARC)

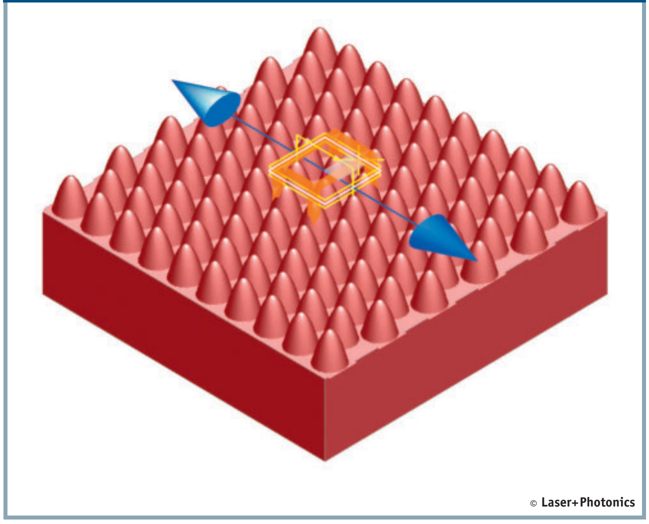
TiO_2) is deposited on to the Si solar cell effectively reducing the reflection at wavelengths around 600 to 800 nm as illustrated in **Figure 1**, but leaving a residual reflection at other wavelengths and consequently a corresponding loss in efficiency.

One possible nanophotonic solution for a low cost, broadband antireflection coating is based on sub-wavelength patterning that mimics a moth-eye, as depicted in **Figure 2**. Some night-active moths have such patterns on the surface of their eyes to efficiently suppress light reflection. While moths use this effect for camouflage, it is useful for solar cells because it increases the absorption inside the silicon and therefore the yield of charge carriers. Such wafer-scale sub-wavelength patterns can be etched into silicon wafers using spin-coated silica colloidal monolayers as etch-masks [1]. The reflection properties of such structures can be accurately modeled using the FDTD technique.

The whole spectrum in one simulation

The finite-difference time-domain (FDTD) technique has become the industry standard for accurate simulation of nanophotonic structures and devices. Based on the seminal work by Yee [2], the numerical FDTD technique iterates the Maxwell's curl equations in time on a discrete mesh in space. The advantages of the technique are its accuracy as no approximations are made apart from the discreteness of the mesh, and its flexibility as complicated heterogeneous structures comprised of arbitrary optical materials may be simulated. Furthermore, as computational power continues to rapidly increase with a simultaneous decrease in cost, what was only a few years ago considered an intractable simulation problem can routinely be solved on current desktop workstations or even laptops. The laptop currently being used to facilitate writing this has the computational speed to place it in the Top 500 of the world's fastest super computers from 1995. This is one reason for the growing popularity of the FDTD method in industrial research and development.

Moth eye structure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2 **The moth-eye structure is etched to the surface of a silicon wafer**

The moth-eye pattern in **Figure 2** consists of a silicon substrate on top of which is a triangular array of period 510 nm, comprised of paraboloid-shaped bumps 800 nm high with a base diameter of 470 nm. The basic principle behind the design for such a broadband antireflection coating is to effectively create a graded refractive index layer. If one considers a slice of the patterned layer, the in-plane fraction that is comprised of silicon is given by

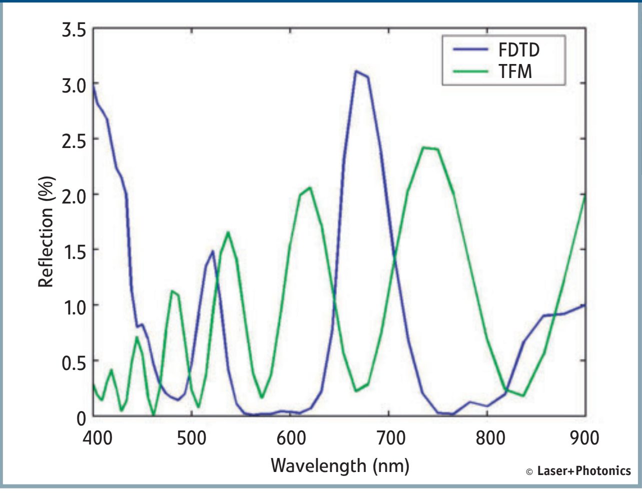
$$f(z) = 2\pi\, r(z)^2 / (a^2 \sqrt{3})$$

where r(z) is the radius in the silicon bump. Thus, as r(z) increases through the patterned layer, so does the fill fraction of the silicon. In the framework of the effective me-dium approximation in [1], the refractive index varies with height as

$$n(z) = \left[f(z) n_{Si}^{\,q} + (1 - f(z)) n_{air}^{\,q} \right]^{1/q}$$

where q = 2/3 , n_{Si} is the complex refractive index of silicon – itself a strongly dispersive function of frequency – and n_{air} is the refractive index of the surrounding air. Using the effective refractive index above in a standard thin film multi-layer model in which the moth-eye pattern is sub-divided into a large number of slices in z allows one to estimate the reflection from the moth-eye pattern as shown by the green line in **Figure 3**. However, because the refractive index contrast between silicon and air is quite large, the effective medium approximation is not valid strictly speaking. Qualitatively, however, this approximation predicts a noticeable reduction of reflection – an interesting result, which can be quantitatively re-examined using the FDTD method.

FDTD versus thin film model



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3 **Calculated reflection from silicon wafer etched with a moth-eye pattern as calculated by FDTD Solutions (blue line) and an effective medium thin film model (green line)**

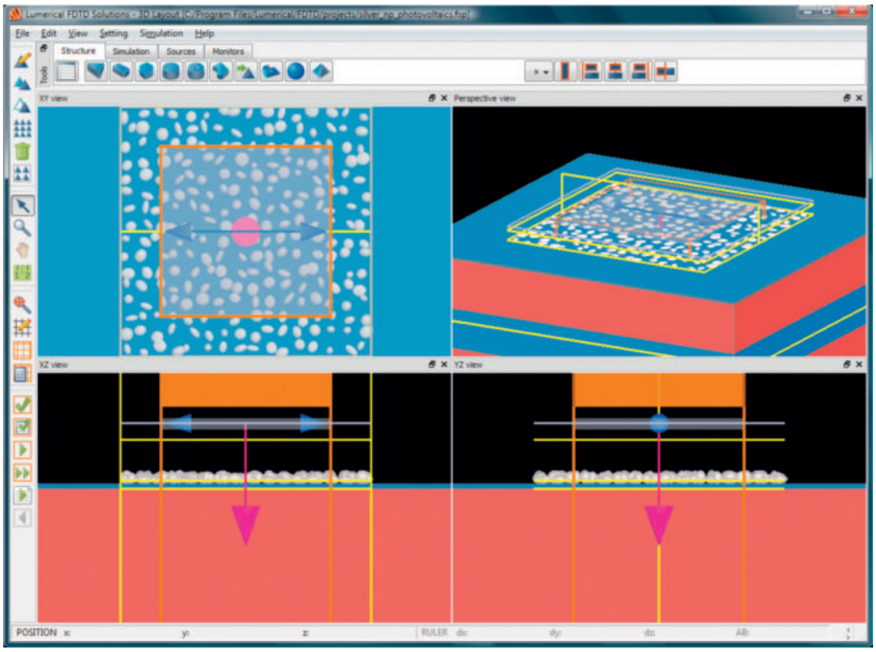
fotolia (2)

For the simulations we use the commercial software FDTD Solutions by Lumerical, assuming normal incidence of the sunlight. Using the built-in dispersive material model for silicon allows one to calcu-

▶

late the entire reflection spectrum in one simulation. The result is shown in **Figure 3** and one sees a marked difference between the correct reflection spectrum as calculated using the FDTD method and that from the approximate effective medium technique. Clearly, the latter is inadequate for a quantitative analysis, whereas the FDTD simulations produce reliable results.

Another advantage of using FDTD simulation for these types of calculations is that the reflection properties of different patterns with other periods, varying etch depths, or other bump shapes may be simulated so that the desired design may be optimized, without having to manufacture each possible combination. In addition, the effect of surface roughness or other structural imperfections may also be simulated.



4 **Silver nanoparticles on an SOI wafer**

Silver as a light trap

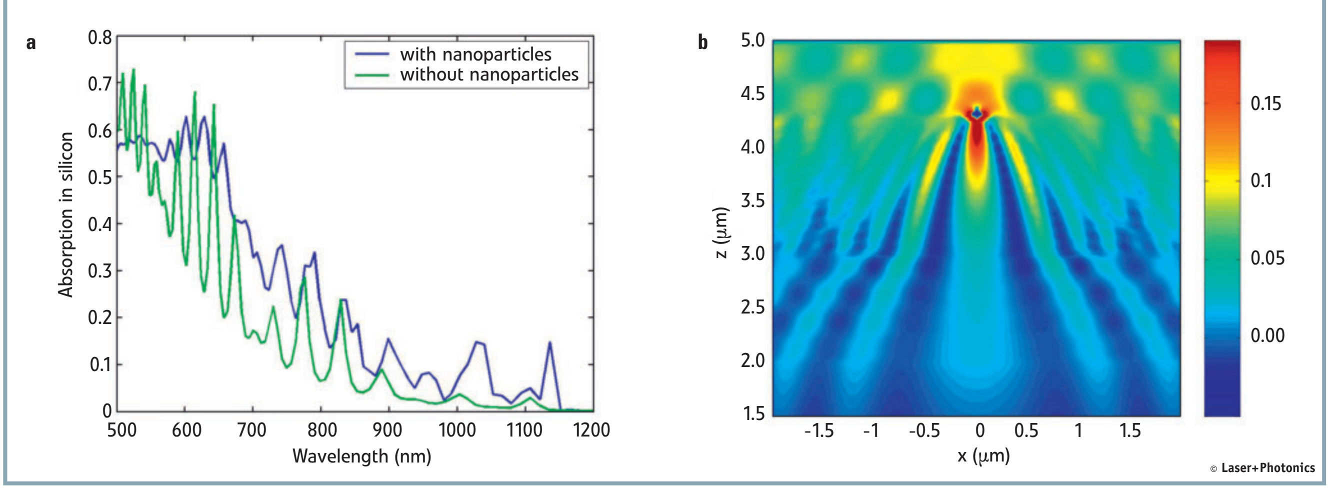
A large fraction of the cost of solar modules is the cost of the ›thick‹ silicon wafers. While thin film technologies can be more cost effective, they are, in general, less efficient than their bulk counterparts because of relatively poor light absorption and carrier loss due to surface recombination. Thus, innovative techniques to trap light in the thin film absorbing layer are being investigated.

One such technique uses the addition of metallic nanoparticles to couple light into the underlying silicon layer [4] as depicted in **Figure 4**. Here the silver nanoparticles are created by a thermal evaporation process compatible with the solar cell production in which an annealing process causes the nanoparticles to coalesce. The resulting random assortment of silver nanoparticles have an average diameter of 100 nm and are situated on top of a dielectric coating, itself on top of the silicon-on-insulator (SOI) wafer. By judicious choice of the dielectric material, the surface plasmon resonance may be tuned to optimize the design of an efficient light-trapping layer.

In **Figure 4**, a SOI wafer structure is shown drawn up in the ›Layout Editor‹ of FDTD Solutions. The top silicon layer is 1250 nm thick and is covered with 30 nm of native oxide (SiO_2); the buried oxide layer is 1000 nm thick.

The incident sunlight is modeled as a broadband planewave source incident on a 3 x 3 micron section of the surface. Power monitors (shown as yellow rectangles in **Figure 4**) are used to calculate the power reflected from the device and the power transmitted into the bottom silicon layer. An additional power monitor is used to determine the flow of power from the native oxide layer into the top silicon layer. Conservation of energy, then, allows one to de-

Calculated absorption in the top silicon layer / energy flux density



5 **a) absorption with nanoparticles (blue line) and without (green line); b) Energy flux density (modulus of Poynting vector) near a silver nanoparticle on top of the SOI structure. The figure clearly shows how much light the particle scatters into the silicon layer, finally leading to an enhanced light absorption**

termine the absorption in both the nanoparticle layer and the top silicon layer.

FDTD Solutions rigorously and automatically includes all optical effects without approximation including: the surface plasmon resonances in the nanoparticles; the multiple scattering between layers of the SOI wafer and the nanoparticles; and coupling to waveguide modes. The absorption in the silicon layer is shown in the plot in **Figure 5** below for the SOI wafer both with and without the nanoparticles. Significant enhancement is shown for the device with the nanoparticles, particularly at longer wavelengths.

The photocurrent enhancement as a function of wavelength can be determined from the ratio of the two curves in the above plot and by integrating the curves over wavelength; an overall efficiency enhancement of 24 percent is predicted. This result is somewhat counterintuitive, because naively one would expect that a solar cell with a silver coating would reflect more light and not less. But this only shows to what extent the properties of nanoparticles differ from those of thin films and how unreliable intuition may be for such nanophotonic systems. ■

Summary: Lowering costs for solar power

Nanophotonic materials and technologies offer the possibility to lower costs and improve efficiencies in next generation solar cells. Simulation enables designers to virtually prototype ideas and, as computation speed increases and while computer costs continue to decrease, accurate simulation in solar cell design will continue to play an ever increasing role. With the use of advanced simulation software based on the FDTD technique allowing researchers to investigate the use of nanophotonic technologies to confront the current challenges, the future looks bright for the solar cell industry.

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