Ray Tracing Derived From Wave-based Optics For Nanoscale Light Propagation Studies: A Theoretical Overview

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Abstract

As the application of nanoscale structures becomes increasingly commonplace in modern technologies, the comprehensive modelling of the subject has taken centre stage in its understanding. Take the modern application of nanoscale texturing for optical anti-reflectance as an example here; structures of such scale interact with light rather differently to their larger counterparts. The assumptions made by industry standard ray tracing (RT) methodologies do not hold true for structures comparable in size to that of the wavelength of light interacting with it. At this point, light does not simply view an approaching structure as smooth, but instead it sees deformation.

Electromagnetic wave optics (EMWO) was developed to address this problem, where, in lieu of the name, light is modelled as a wave with two or three dimensions rather than a ray with only one. The use of this form of modelling has several drawbacks; it is far more difficult to quantify light propagation direction for example. Furthermore, the computational demands of EMWO are considerably higher than those of RT methods.

We present, using the COMSOL Multiphysics® suite, a new method of combining both EMWO and RT methods to observe how nanoscale surface textures influence light propagation between air and a silicon (Si) substrate. Such studies are highly desirable and relatively unexplored in the areas of photonics, optics and photovoltaics. We take a black silicon (b-Si) surface coated with vertical protruding nanowires and complete an EMWO study to first identify how the waves of light are scattered by these structures. We then feed these wave fronts into a second RT study in order to render an optical path after the influence of this nanotextured surface. Applied here are the Wave Optics Module and Ray Tracing Module respectively. For the EMWO study, we configured incident light to be of both transverse electric (TE) and magnetic (TM) modes, simulated separately, and then averaged together to give transverse electromagnetic (TEM) incident radiation.

Focusing specifically on photovoltaic implications in this work, we can determine properties such as optical path length enhancement, radiation scattering patterns and broadband surface reflectance for microscale structures coated with nanoscale ones. Initial studies have presented us with incredibly detailed results, leading us on towards theorising tailor-made surfaces with very finely tuned properties appropriate for very high-performance solar cells. This is a first for b-Si solar technologies.

No models from the COMSOL Multiphysics® application library were used in this work. Simulations are currently ongoing and a full dataset will be ready for showcasing at the COMSOL® Conference 2020.

Figures used in the abstract

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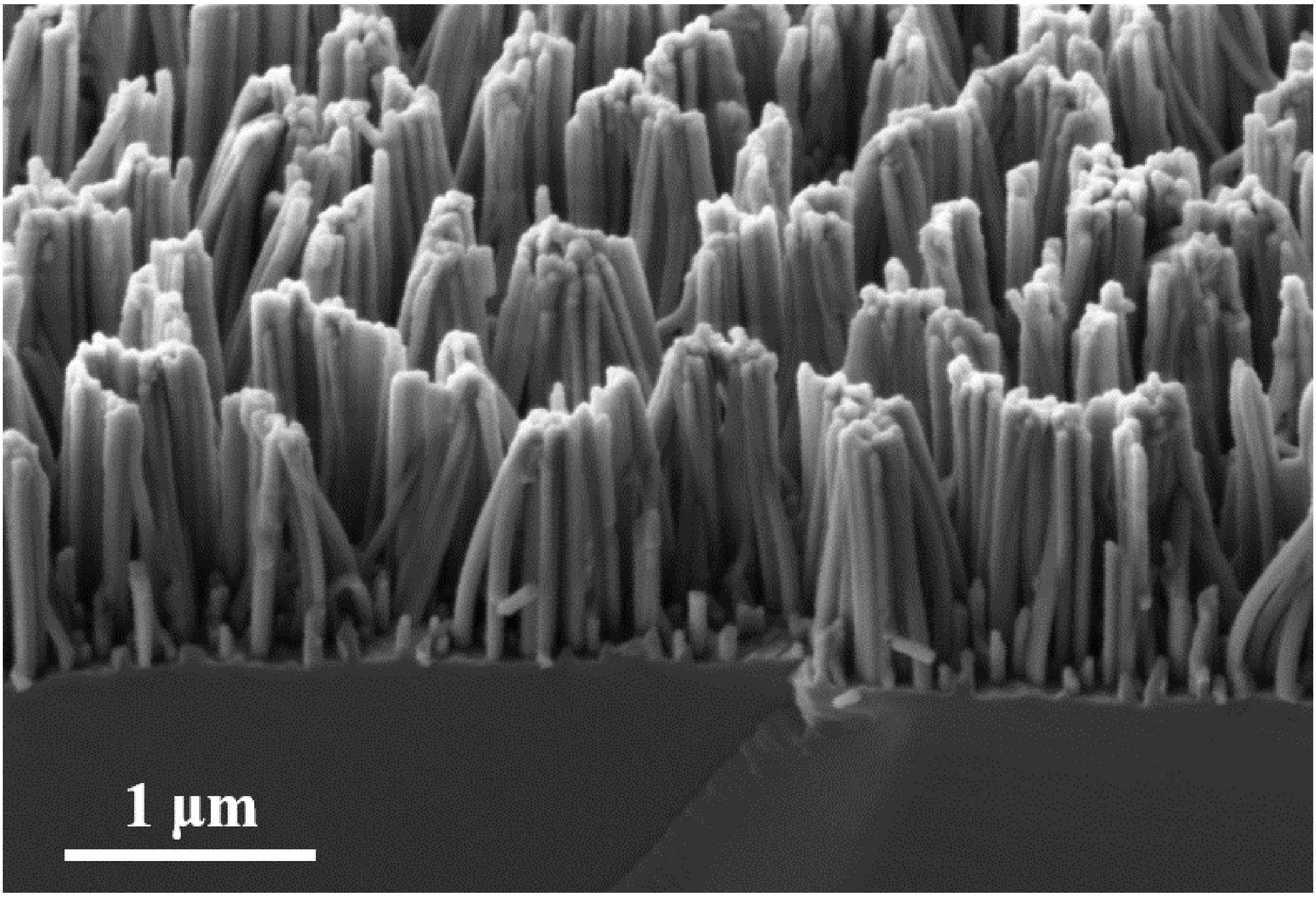

Figure 1 : An example of a real b-Si surface, textured using an Ag-MACE process.

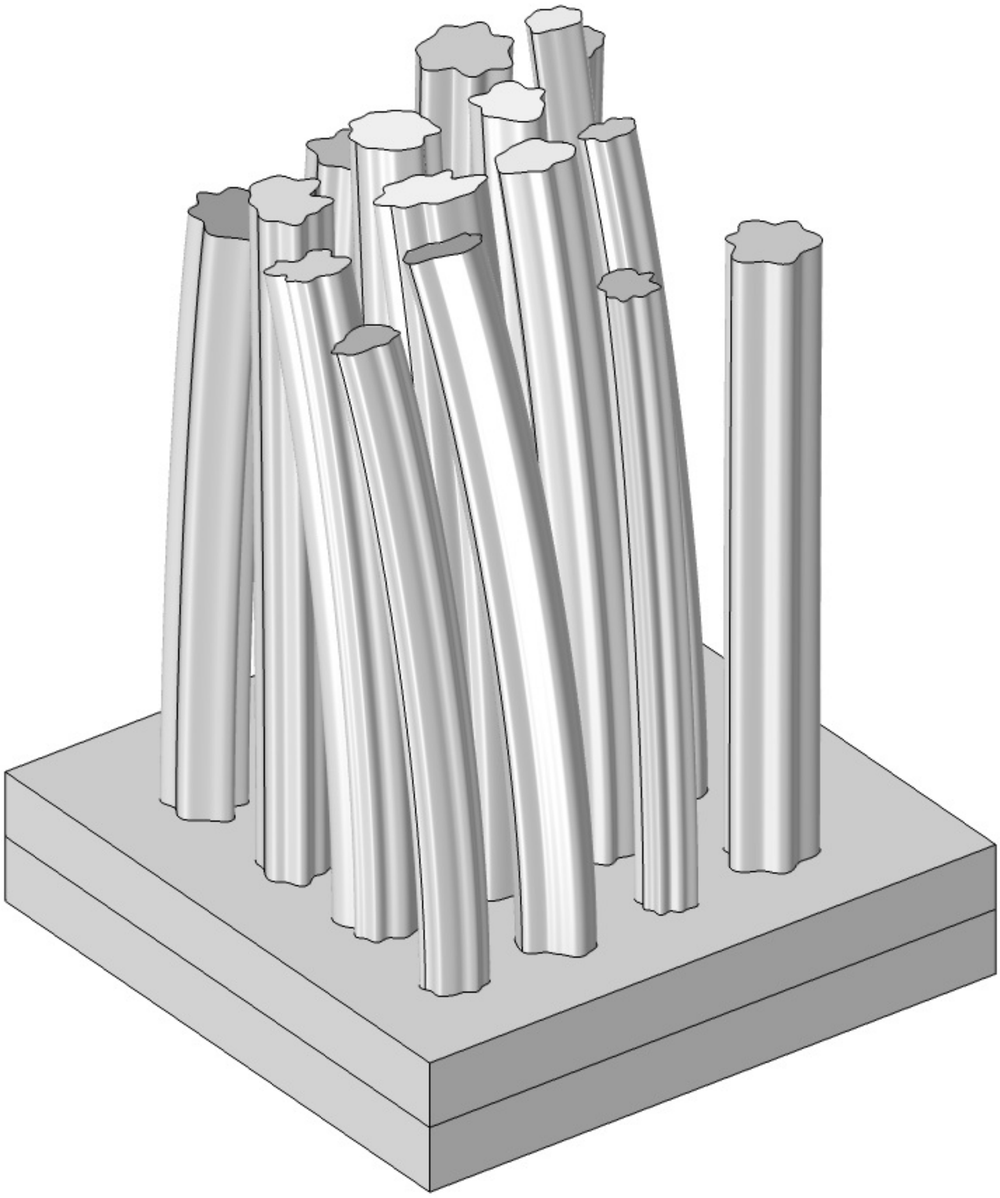

Figure 2 : An example of our pseudorandomised b-Si surface geometry as used here with the EMWO and RT methodologies.