Ray Tracing Derived from Wave-based Optics for Nanoscale Light Propagation Studies: A Theoretical Overview

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INRODUCTION: We present, using the COMSOL Multiphysics®† suite, a new theoretical modelling methodology, whereby combining both EMWO and RT methods allow us to observe how nanoscale surface textures influence light propagation between air and a silicon (Si) substrate coated with a nanoscale texture. 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.

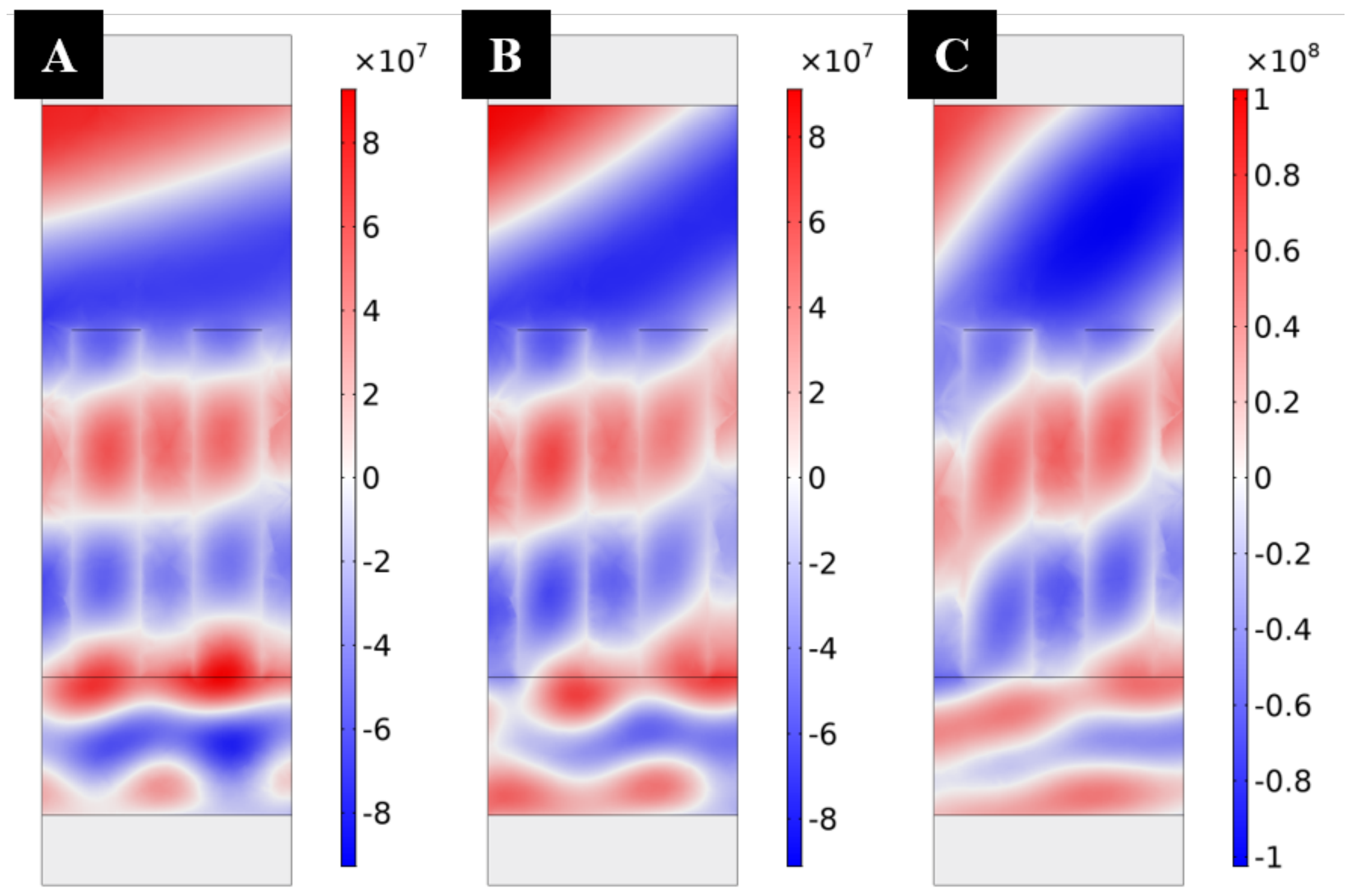

Figure 1. Showing how the EM wave propagation is distorted by the presence of SiNWs for 15 (a), 30 (b), and 45 (c) degree angles of incidence.

COMPUTATIONAL METHODS: We have first taken our silicon nanowire (SiNW) model, as shown in previous work [1-3], and reconfigured the study to show us the EM wave propagation. The EM wave is configured to have be directed along the *z*-axis from the upper perfectly matched layer (PML) to the lower. Oscillation of the wave occurs along the *y*-axis.

Unlike ray tracing (RT) modelling methods, EMWO requires a very dense mesh as defined by the Nyquist criterion. A minimum of two elements per complete wavelength, 600 nm in this case, must be created within the geometry's mesh for adequate simulation accuracy. An adaptive meshing strategy was employed, whereby the mesh was automatically adapted to yield enough accuracy for the study.

RESULTS: In order to quantify light propagation direction, we first applied a streamline graph indicative of the average power direction from the incident wave.

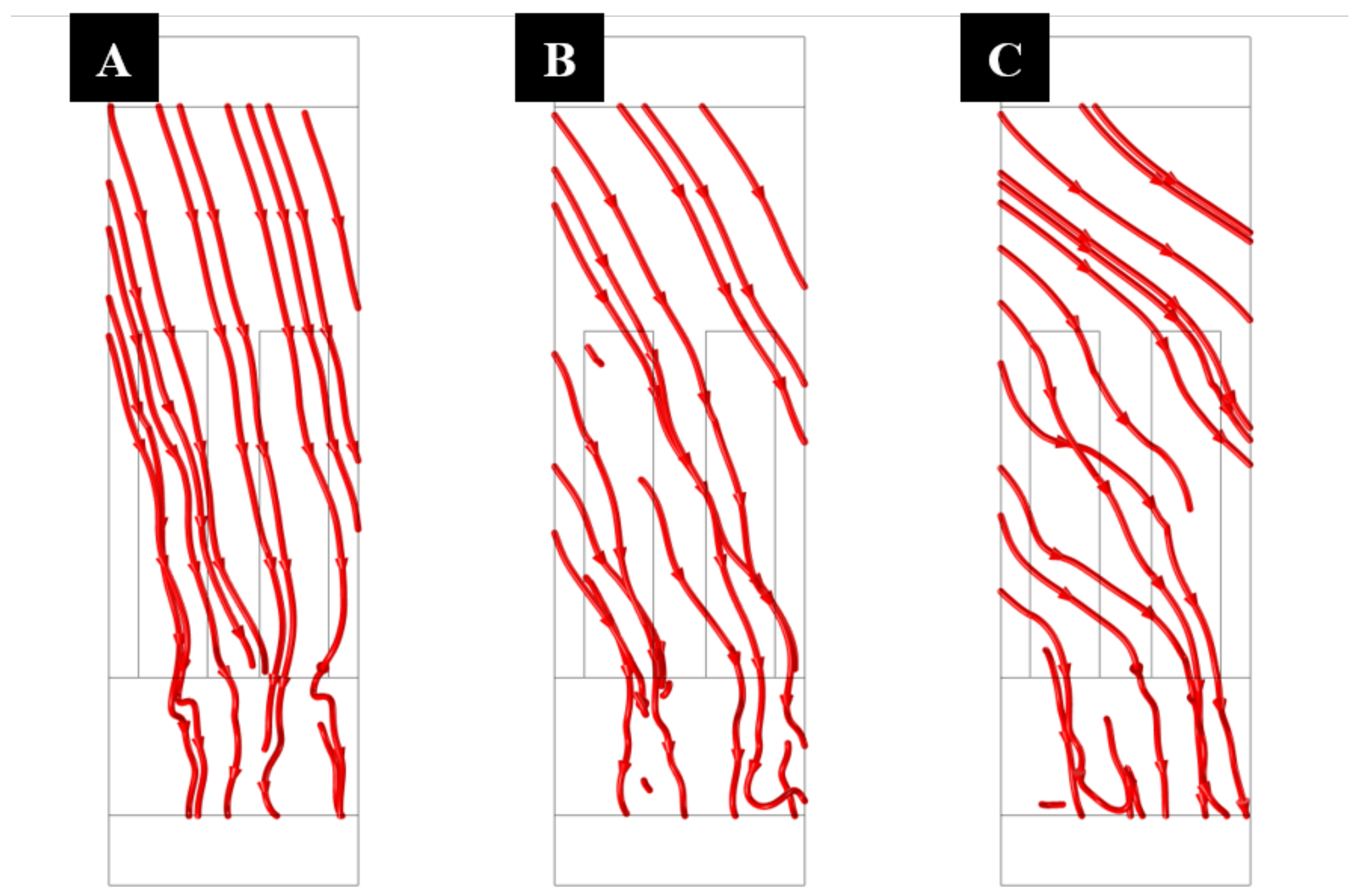

Figure 2. Demonstrating how SiNWs distort the power delivery direction for 15 (a), 30 (b), and 45 (c) degree angles of incidence.

It can be seen how, particularly for high angles of incidence as in figures 2a and b, incident power is directed downward toward the normal of the substrate surface. This forms a brief demonstration of the affect, and subsequent benefit, of nanoscale texturing for photovoltaic applications, for example.

CONCLUSIONS: Current software limitations prevent us from releasing rays, using the ray tracing module, at various angles indicative of the wave scattering demonstrated using the data shown in figures 1 and 2. Currently, COMSOL only permits rays to be release from an electric field interface at the normal to said interface - negating the ability to model scattering.

Given the active interest in this field of study, and the initial computation functioning as expected, we are actively working with COMSOL to model this angular scattering in the form of rays instead of solely relying on waves.

REFERENCES:

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