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Silicon nanowire

Aim of this numerical experiment was to calculate local absorption in different parts of a silicon nanowire (NW) based solar cell, with possibility of evaluating different geometrical parameters influence on cell performance.

Two different models were constructed as shown on the right image. They always consist of several materials (TCO that was handled as ITO, amorphous silicon, crystalline silicon that was treated as Si 100 and eventually also a Sn nanoparticle on the top of the NW that was treated as perfect electric conductor). In model “A” a periodic array of structured is created using single NW/aSi/ITO column and periodic boundary conditions. This can be used to evaluate effect of column spacing films thicknesses, length or tilt on resulting structure performance. In model “B” 3×3 differently tilted columns are used as basic building block for periodic array construction. This is useful to estimate effects of random column orientation. In principle this could be expanded up to 7×7 array basic building block, however for even larger building blocks the computation would be too long and memory demanding.

All the optical data were taken from SOPRA database. Structure was illuminated from top or from bottom by a linearly polarised plane wave. Glass at the bottom of the structure was treated as infinitely extending. Voxel spacing was 7 nm.

Geometrical parameters of a single column were as follows in first set of simulations (radii of nested cylinders capped by spheres and apparent thickness of the film if seen from side):

material cylinder radius film thickness Si NW 28 nm (i) a:Si-H 161 nm 67 nm (n) a:Si-H 182 nm 11 nm TCO 350 nm 84 nm

Bottom ITO thickness was 630 nm. All these parameters can be changed and were considered only as initial values, a bit smaller than ideal values, to speed up the first test calculations.

Images below show how the models look in parameter files visualiser XSvit that is part of the FDTD package. Left to right: Single column, ideal 3×3 array, randomized 3×3 array.

Numerical results

Here we show resulting time averaged spatial distribution of absorption in single column structure illuminated from top (left) and bottom (right), for 500 nm illumination wavelength. Visualisation was performed using Paraview.

Time averaged spatial distribution of absorption in 3×3 column structure illuminated from bottom, for regular (left) and irregular (right) column geometry for 500 nm illumination wavelength:

Similar calculation can be performed for any wavelength within range of our optical data (and reasonable ratio between wavelength and voxel spacing). Here a set of simulation snapshots for different wavelengths is shown for single column structure illuminated from bottm:

If we run full spectral calculation, we can get also dependences of summed local absorption in different parts of the solar cell, for distinct materials. A preliminary result for bottom illuminated regular structure is shown below (note that number of steps for longer wavelengths was too small for reaching steady state). Spectral calculations using optical database are performed for each wavelength separately, so this type of calculations is already computationally demanding - we had used CMI high performance computing system for these preliminary calculations.

Geometrical model can be made even more complex, e.g. by adding scanning probe microscope tip to the structure. This geometry is similar to what we use in photoconductive AFM measurements. After adding simple tetrahedral tip we get this snapshot and volume absorption (tip only sketched on absorption image).

The same model 3D view including better probe sketch is shown below: (left) geometry, (center) 400 nm illumination, (right) 600 nm illumination,