Master internship/thesis project - Year 2019-2020

Numerical optimization of ultrathin solar cells

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The ultimate success of photovoltaic (PV) cell technology requires substantial progress in both cost reduction and efficiency improvement. An actively studied approach to simultaneously achieve these two objectives is to leverage *light trapping* schemes. Light trapping allows solar cells to absorb sunlight using an active material layer that is much thinner than the materials intrinsic absorption length. This then reduces the amount of materials used in PV cells, which cuts cell cost in general, and moreover facilitates mass production of PV cells that are based on less abundant materials. In addition, light trapping can improve cell efficiency, since thinner cells provide better collection of photo-generated charge carriers. Enhancing the light absorption in ultrathin film silicon solar cells is thus of paramount importance for improving efficiency and reducing cost.

The theory of light trapping was initially developed for conventional solar cells where the light absorbing film is typically many wavelengths thick. From a ray optics perspective, conventional light trapping exploits the effect of total internal reflection between the semiconductor material (such as silicon) and the surrounding medium (usually assumed to be air). By roughening the semiconductor-air interface, one randomizes the light propagation directions inside the material. The effect of total internal reflection then results in a much longer propagation distance inside the material and hence a substantial absorption enhancement. For such light trapping schemes, the standard theory, first developed by E. Yablonovitch, shows that the absorption enhancement factor has an upper limit of $4n^2/sin^2\theta$, where θ is the angle of the emission cone in the medium surrounding the cell. This limit is referred to as the Yablonovitch limit or the $4n^2$ limit, since one is primarily concerned with structures with $\theta = \pi/2$ which has a near-isotropic emission cone. For nanophotonic films with thicknesses comparable or even smaller than wavelength scale, the ray optics picture and some of the basic assumptions in the conventional theory are no longer applicable. In that case, it can be shown that the absorption enhancement factor can go far beyond the $4n^2$ limit with proper design.

There is significant recent interest in designing ultrathin crystalline silicon solar cells with active layer thickness of a few micrometers. Efficient light absorption in such thin films requires both broadband antireflection coatings and effective light trapping techniques, which often have different design considerations. Recently, researchers from several physics institutes in Europe have jointly proposed a strategy based on multi-resonant absorption in planar active layers, and have reported a 205-nm-thick GaAs solar cell with a certified efficiency of 19.9% [CCD+19]. This solar cell uses a nanostructured silver back mirror fabricated by soft nanoimprint lithography. In such a structure, broadband light trapping is achieved with multiple overlapping resonances induced by the grating and identified as FabryPerot and guided-mode resonances.

The general objective of this internship is to revisit the numerical study realized in [CCD+19] by developing a framework for the *inverse design* of the nanostructuring of the silver back mirror in view of possibly improving the light trapping properties of the solar cell. In order to do so, we will combine the use of a high order DGTD solver [Viq15] from the DIOGENeS software suite[1] for an accurate and efficient optical characterization of the solar cell, with statistical learning-based global optimization strategies [DC12] namely, CMA-ES (Covariance Matrix Adaptation Evolution Strategy) and metamodeling-based EGO (Efficient Global Optimization) methods, which are offered by the DiceOptim libray[2]. The candidate for this position is expected to start a joint Ph.D. project between Inria and C2N, which will constitute a follow-up of the present study. This Ph.D. project will be conducted in close collaboration with Total Gas, Renewables & Power and Total R&D Computational Science and Engineering.

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Monthly gratification: ≈ 600 €

References

[CCD+19] H.-L. Chen, A. Cattoni, R. De Lépinau, A.W. Walker, O. Höhn, D. Lackner, G. Siefer abd M. Faustini, N. Vandamme, J. Goffard, B. Behaghel, C. Dupuis, N. Bardou, F. Dimroth, and S. Collin. A 19.9%-efficient ultrathin solar cell based on a 205-nm-thick GaAs absorber and a silver nanostructured back mirror. *Nat. Energy*, 4:761–767, 2019.

[DC12] R. Duvigneau and P. Chandrashekar. Kriging-based optimization applied to flow control. *Int. J. Num. Fluids*, 69:1701–1714, 2012.

[Viq15] J. Viquerat. *Simulation of electromagnetic waves propagation in nano-optics with a high-order discontinuous Galerkin time-domain method.* PhD thesis, University of Nice-Sophia Antipolis, 2015. https://tel.archives-ouvertes.fr/tel-01272010.

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[1] https://diogenes.inria.fr/

[2] http://dice.emse.fr/