BAPVC Annual Project Report

Project Title: Exploratory Photovoltaic Modeling and Simulation: An End-to-End, Technology-Agnostic Approach
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Summary:

In 2013, Purdue's team pursued simulations of contactless in-line characterization techniques and light-trapping in solar cells. For the first project, they created a detailed opto-electronic multiphysics simulation tool suitable for directly simulating two photoluminescence (PL)-based characterization methods: time-resolved PL (TRPL) and PL steady-state excitation (PLE). In the second project, they created an online capability of simulating light trapping through two distinct freely-accessible tools on nanoHUB/PVhub: S4 and MEEPPV, and optimized designs for c-Si thin films.

Key Accomplishments:

For the first project, Purdue created a detailed opto-electronic multiphysics simulation tool suitable for directly simulating two photoluminescence (PL) characterization methods: time-resolved PL (TRPL) and PL steady-state excitation (PLE). Purdue's simulation approach links optical and electronic transport mechanisms together in an integrated framework. This strategy is particularly important for high-performance materials, in which photon recycling can play a significant role. Applying this simulation approach to TRPL on a VLS-grown Indium Phosphide thin-film sample grown by Ali Javey's group at Berkeley was shown in Fig. 1(a) to match well with measurements. Furthermore, the simulation of PLE using the same tool also achieved a strong match to experiment, as shown in Fig. 1(b). More generally, it was shown that TRPL and PLE provide complementary information on the surface recombination velocity and Shockley-Read-Hall (SRH) lifetimes in thin-film samples. For example, in Fig. 2(a), the TRPL simulation provides best fits localized to a restricted range of SRH lifetimes, while Fig. 2(b) shows that the PLE simulation provides the best fits within a narrow range of surface recombination velocities.

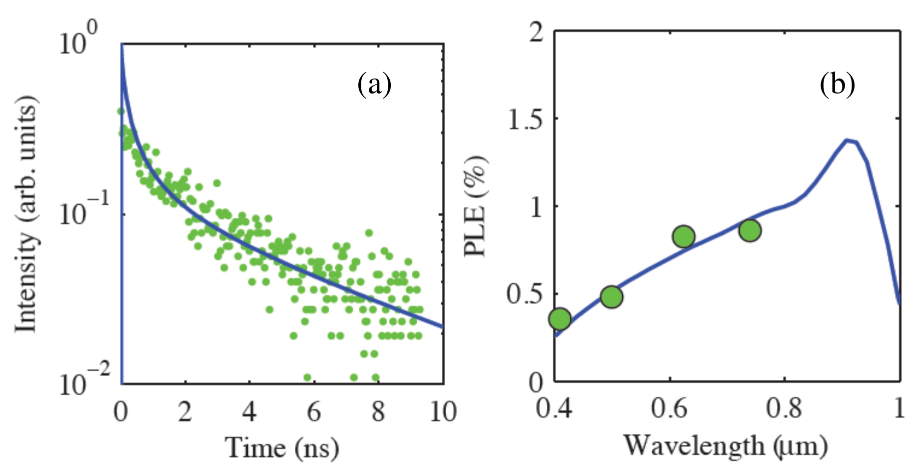

Fig. 1. (a) Best overall fit between experimental measurements (green dots) and simulations (solid blue curves) for time-resolved PL; (b) Best overall fit between theory and experiment for PL excitation.

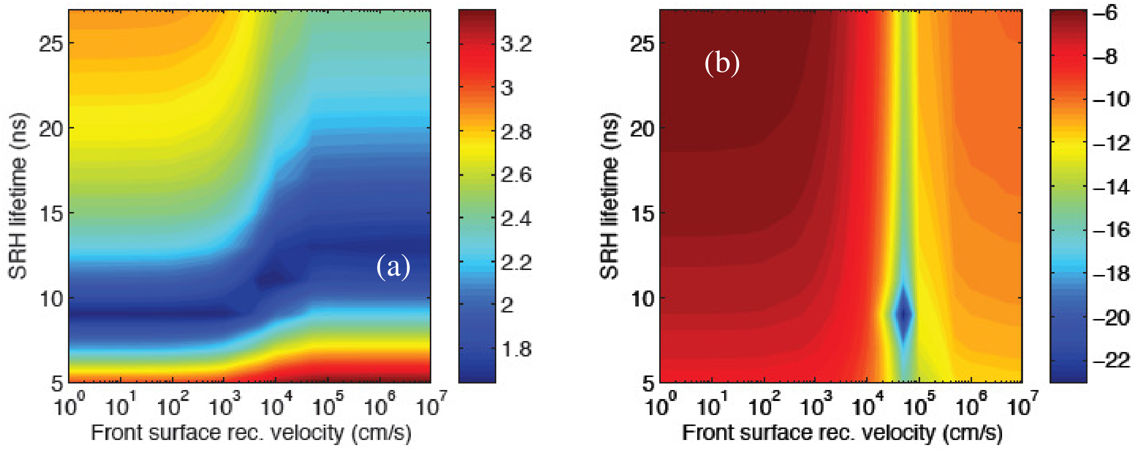

Fig. 2: (a) Least-square error as a function of SRH lifetime and front surface recombination velocity when fitting to data from TRPL; (b) Least-square error with respect to the same variables for PLE. The most likely values of each variable (corresponding to the lowest error) are depicted in blue.

In the second project, Purdue created an online capability of simulating light trapping through two distinct freely-accessible tools on nanoHUB/PVhub: S4 (from Stanford) and MEEPPV (from MIT). This was used to create a detailed simulation of correlated random texturing, found in a variety of thin-films grown in commercial applications. These tools were used to find an optimal design for texture-based light-trapping in multijunction crystalline silicon (c-Si)-based thin film solar cells – the result is depicted in Fig. 3(a). The relative enhancement of the normalized light trapping of the c-Si thin-films compared to standard planar or random textures, as shown in Fig. 3(b), illustrates the potential usefulness of this approach.

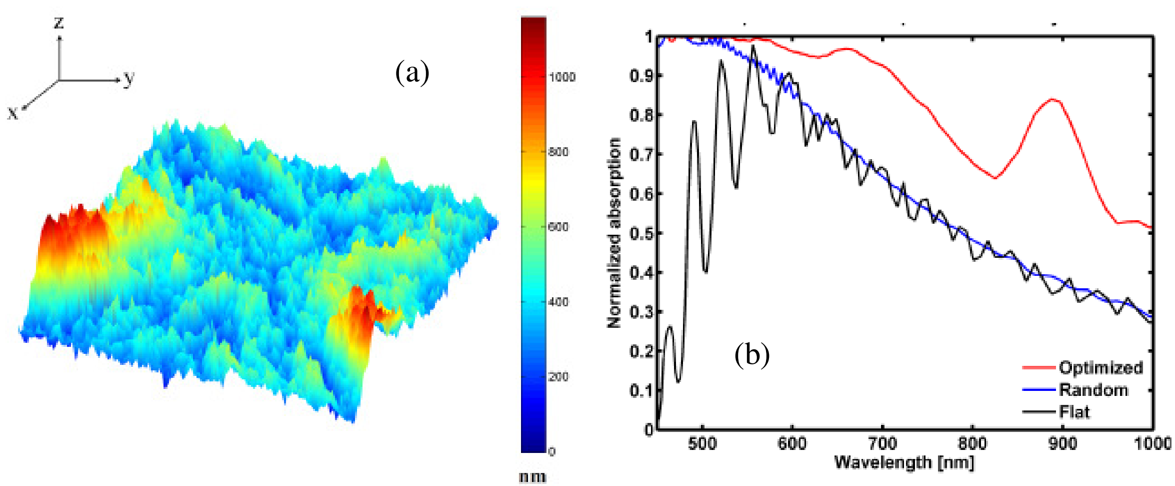

Fig. 3: (a) Portrayal of the optimal correlated random texturing found in Purdue's FDTD simulations; (b) Relative enhancement of normalized absorption for c-Si thin-film –optimized absorption spectrum is in red.

Future Work:

Purdue will extend its recent characterization work to related material systems to assist in rapid prototyping and quality control, and will work closely with experimentalists and industry partners to translate modeling work into useful results, developing additional tools where needed.