

PROJECT SUMMARY

Our objective is to develop the first 3D numerical simulator of *thin-film* photovoltaics (PV) ranging from microscopic, through 1 cm cells and 1 m modules, to 1 km arrays. We propose fundamental theoretical research on two fronts: (1) the physics of charge and heat transport in noncrystalline PV; and (2) solving related partial differential equations with numerical techniques, including finite element and Monte Carlo. The simulator will allow for the creation of cells by specifying material properties and the interconnection of several of them into modules and arrays with all of their inherent nonuniformities.

Intellectual Merit: The disordered nature of noncrystalline semiconductors leads to unique features evident in thin-film PV where common observations are, e. g. performance differences between nominally identical devices, accelerated degradation, and large deviations from ideal diode behavior. Yet, efforts to describe the underlying mechanisms have been largely based on the ‘crystalline’ physics because of simpler descriptions and advanced software products developed to simulate device behavior.

The research of noncrystalline systems advancing since the 1960s recently has been reinvigorated due to applications in PV, as well as the computer memory and communications; the PI for this proposal has been at the forefront of it for three decades; he also led the study of nonuniformity at First Solar LLC, the University of Toledo and national research teams. This project will help to bring the noncrystalline physics into the mainstream by compiling the acquired knowledge in a PV simulation software to serve as a useful tool for advancing the understanding of researchers, educators, and students.

A fundamental problem addressed in this project is the physics of coupled electronic and heat transport in laterally non-uniform non-crystalline (amorphous and/or polycrystalline) thin film structures with electrodes of finite resistivity.

The innovativeness of our proposal is that it is aimed to create the first modeling tool for fundamentally non-uniform structures at all the space scales, and that it introduces the original algorithm of stochastic modeling with parameters chosen in the form of statistical distributions (spatially correlated through the appropriate Monte Carlo routine).

Broader Impacts: The primary utilization of this funding will be to support a postdoctoral researcher to develop the simulator and disseminate the results to the broader community. In accordance with our mentoring plan, the postdoc will participate in multi-disciplinary conferences, publish in peer-reviewed journals, work with PV industry colleagues, and mentor students. We plan to assign one grad student supported by the University funds (beyond this proposal) to collaborate with the postdoc and PI.

The Department of Physics and Astronomy at the University of Toledo has a strong research experience for undergraduates (REU) program and summer camp program for high school students. We will actively participate in these programs by providing research opportunities and conducting presentations. Toledo is an ethnically diverse area and the REU and summer camp programs will allow us to connect with and seek the active participation of underrepresented groups.

The simulator will serve as the core of an interactive pedagogical approach because students will be able to create and observe the effects of variations in operating parameters, as well as the effects of nonuniformities and connecting cells or modules in a circuit. Noncrystalline physics will be more accessible to students and researchers.

One non-traditional broader impact is the use of our future simulator to describe the physics of biological membranes whose ion channels typically have the IV characteristics typical of diodes, and chemical pumps generating charge carriers play the role similar to that of light in PV. We plan to collaborate with biophysicists in order to explore possible applications to biological membranes.

In terms of broader societal impacts, the simulator will play a key role in achieving the goal of bringing the cost of solar electricity on par with fossil fuels and achieving power supply levels on a multi-terawatt scale. It will do so by allowing researchers and students to visualize experiments in-silico and allow for a degree of creativity and risk taking that is not feasible in real experiments.

PROJECT DESCRIPTION

1.0 Objectives, Scope, and Significance

Our objective is to develop the first three-dimensional numerical simulator of thin-film *noncrystalline* photovoltaic (PV) systems of any size scale; from microscopic samples to large arrays. We propose to conduct fundamental theoretical research on two fronts: (1) the physics of charge transport in noncrystalline PV materials; and (2) solving partial differential equations related to charge transport in disordered systems using numerical techniques, including finite element and Monte Carlo methods. The simulator will allow for the creation of compound single-cell devices by specifying individual material properties and the interconnection of several of those single-cell devices into large area PV modules (of ~ 1 m linear size) and arrays of many such modules with all of their inherent nonuniformities.

The research program will explore charge transport in disordered systems relevant to gaining a deeper understanding of the dominant transport mechanisms in modern and future PV technologies. However, the fundamental understanding will go beyond solar energy and will be applicable to any thin-film material with noncrystalline (aperiodic) structure. At a basic level, this research intertwines the fields of electrodynamics, quantum mechanics, statistical physics and numerical methods with the goal of developing algorithms that solve the problem of electronic transport through noncrystalline p-n junctions and metal/semiconductors junctions. Since our aim is to simulate real-world operation of noncrystalline PV devices through a broad range of size scales, we will employ the Finite Element Method (FEM) as our primary numerical analysis tool. Along with the FEM structure will be Monte Carlo type analyses that will allow for random distributions of nonuniform material properties and extensions of single-cell device simulations to large scale PV systems.

Since the inception of the first working silicon solar cell, a great deal of progress has been made in understanding the inner workings of crystalline PV materials. In parallel was progress in the area of noncrystalline semiconductor physics,[1] albeit at a much slower pace. The two fields overlapped upon the creation of 2nd generation PV technology which consisted of thin amorphous or polycrystalline films, such as, amorphous silicon (a-Si), cadmium telluride (CdTe) and copper indium gallium (di)selenide (CIGS). The experimental but promising 3rd generation PV technologies are also typically noncrystalline in nature. These state-of-the-art and future technologies have been explored mostly from the perspective of the well-established theories and concepts of crystalline semiconductor physics, and with great success. Yet, some important issues remain that significantly impede device efficiency and performance, such as the difficulty in scaling up from the lab cell to commercial size, increased degradation rates, anomalous current-voltage characteristics, and statistical variations between identical devices, to name a few. All of those effects are due to the disordered nature of the material.

The natural disorder in noncrystalline systems makes analytical models quite challenging. Over a span of three decades, the PI has made significant strides in understanding the physics of noncrystalline semiconductors through analytical methods. At this point numerical techniques are required to deepen this understanding and convey it to the PV community in an clear and useful format.

Given the disordered nature of thin-film PV, there exists a significant need for advanced PV device simulation. The prevalent thin-film PV device modeling software (called AMPS) is a one-dimensional finite difference package that does an excellent job at simulating device operation under various conditions.[2] However, a 1D model cannot predict the important effects associated with the lateral nonuniformities that are inherent in present and future PV technologies. Also available but not accepted in thin-film PV, are high-end, expensive finite element modeling packages (called DESSIS, or Sentaurus Device) that were developed for the crystalline semiconductor industry.[3]

Although ab-initio based models provide great detail of the dynamics occurring at the atomic scale with minimal tunable parameters, scaling those models up to mesoscopic systems that do not have periodicity is extremely difficult. Since our model is based on the finite element approach it allows for the simulation of nonuniform devices from nano to macroscopic scales, but at the cost of additional parameters. Fortunately, the range of parameter values can be narrowed experimentally which will make

our model practically useful to the PV community. Furthermore, wide dissemination of our results will be made possible by the fact the PV specialists will not require training in density functional theory or Monte Carlo analysis to run the simulator on their own. Our intention is that the numerical schemes we develop be in such a form that they can be utilized through a convenient graphical user interface.

A fundamental issue addressed in this project will be the physics of electronic transport coupled with heat transport in laterally non-uniform non-crystalline (amorphous and/or polycrystalline) thin film structures with electrodes of finite resistivity.

The innovative approach in our proposal is that it is aimed to be the first tool kit modeling fundamentally non-uniform structures at all the space scales ranging from microns (linear scale of nonuniformities in thin film structures) through centimeters (individual cells) and meters (modules) to kilometers (linear scale of modern PV arrays). At the level of implementation, this innovativeness will be implemented through the original algorithm of statistical modeling where some parameters are chosen in the form of statistical distributions spatially correlated through the appropriate Monte Carlo routine.

None of the available simulation packages include the electronic transport mechanisms that are unique to noncrystalline materials, particularly hopping and percolation through a strong potential relief, as discussed in greater detail below. The PI is at the forefront of understanding the physics underlying such mechanisms and it is our aim is to build from that knowledge to fill a significant gap in the PV research and development community. Specifically, PV specialists and educators will have the ability to create virtual 3D noncrystalline solar cells and simulate device performance under various voltage bias, illumination, and temperature conditions. The simulator will elucidate the effects of lateral nonuniformities, such as hot spots due to high current density, large deviations from ideal diode behavior, and significant performance differences between nominally identical devices. Another important consequence that will be observable is the performance dependence on device area, which often leads to drastic efficiency reductions as devices are scaled up from small cells to modules.

Besides simulating device performance for various sizes, compositions and operating conditions, our model will allow for the testing of various techniques for mitigating the detrimental nonuniformity effects by tweaking the interfacial properties. Hence, the simulation capability enabled by our numerical scheme could lead to the invention of greatly improved or new devices.

Finally, the simulator will serve as an effective educational tool because it will provide detailed graphical representations of operating devices and calculation of PV device performance measures.

2.0 Motivation and Background

The main drivers behind our proposed research plan are: (1) the knowledge gap related to the unique charge transport mechanisms in noncrystalline semiconductors; (2) the ever-present but poorly understood effects of nonuniformities in noncrystalline PV devices; and (3) the lack of sufficient computational tools to assist in understanding the previous two points.

2.1 Charge Transport in Noncrystalline Junctions

Charge transport through semiconductor p/n junction or metal/semiconductor junctions often governs the overall performance of PV devices. The current state of understanding is that transport in noncrystalline junctions is similar to the classical band transport of crystalline junctions, with recombination processes limited to band to band[4] or single defect level mechanisms, such as Shockley, Read, Hall (SRH)[5] or Sah, Noyce, Shockely.[6] Our group's recent work[7] presented a theory of electronic transport in noncrystalline junctions which challenged the standard viewpoint and explained many of the typical yet puzzling observations; such as ideality factors much greater than two, differences in identical devices, and rollover recovery in current/voltage (IV) curves under forward bias.

One unique feature of non-crystalline materials is the high density of localized states in the mobility gap. Such states are present in many materials that form junctions of practical significance, such as a-Si:H based structures,[8] polycrystalline CdTe,[9] and CIGS [10] (all used in thin-film

photovoltaics). A high density of localized states [$g_0(E_F)$] at the Fermi level (E_F) in non-crystalline semiconductors is known to give rise to hopping transport which dominates at low temperatures (T). However, at room or higher T of practical interest, the primary transport mechanism in *bulk* materials is typically band conduction. On the other hand, hopping transport can dominate in sufficiently *thin* noncrystalline materials at room temperature or higher, as described below. It is our stance that junctions in noncrystalline PV devices can form such thin structures and the related physics can dictate device operation and explain the observed phenomena.

Transverse hopping through non-crystalline thin films, with thicknesses in the micron or sub-micron range, is known to be qualitatively different and relatively much more efficient than in bulk materials. The concept of gigantic transverse hopping conduction through thin films was introduced by Pollak and Hauser [11] and later developed in a number of works summarized in the review by Raikh and Ruzin.[12] When the film (or junction) thickness L_0 falls below a certain critical value $L_c \sim 1 \mu\text{m}$, the transverse conductivity shows exponential thickness dependence described by[12]

$$\sigma = \sigma_0 \exp\left(-2\sqrt{\frac{2L_0\lambda}{a}}\right) \quad (1)$$

with $\lambda \approx \ln \lambda - \ln(g_0 k T a L_0^2)$, where k is the Boltzmann constant and a is the electron localization radius. The conductivity is governed by ‘untypical’ hopping chains of spatially close localized states, as illustrated in Fig. 1(a). Although comprised of exponentially rare configurations of localized states, these chains are exponentially more conductive than the average hopping pathways of percolation clusters due to the reduced tunneling distance between states. Therefore, these chains are referred to as optimum chains.

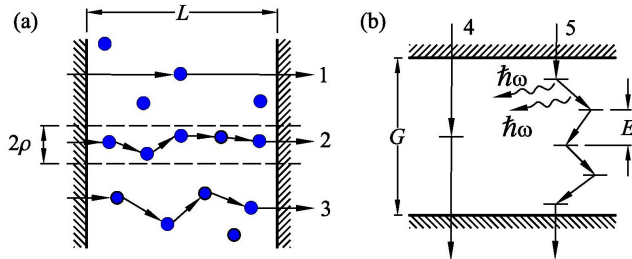


Fig. 1. Charge transport via optimal chains in (a) real space and (b) energy space. (a) three different channels corresponding to: (1) lower than average localized state concentration with a 2-step (one defect) chain; (2) optimum chain having a number of defects greater than the average; and (3) average chain, most likely yet the transmission rate is exponentially low. (b) two different ladders corresponding to recombination through the gap G via: (4) one state located near mid-gap; and (5) optimum ladder with N steps and multiple phonons emitted per step.

Along with the above described hopping in real space, there is a similar hopping process through the energy space of the mobility gap[13] which provides an effective mechanism for nonradiative recombination in noncrystalline semiconductors. As shown in Fig. 1(b), clusters of localized states facilitate recombination by forming ladders in energy space. Recombination via ladders can be orders of magnitude greater than through a single defect.

In our work, we consider optimal chain hopping transport simultaneously in real space (through the junction) and energy space (through the mobility gap) forming ‘hopping channels’, as illustrated in Fig. 2(b). The unlikely yet exponentially efficient *optimum channels* dominate junction transport. Classical recombination mechanisms are illustrated in Fig. 2(a) for comparison purposes.

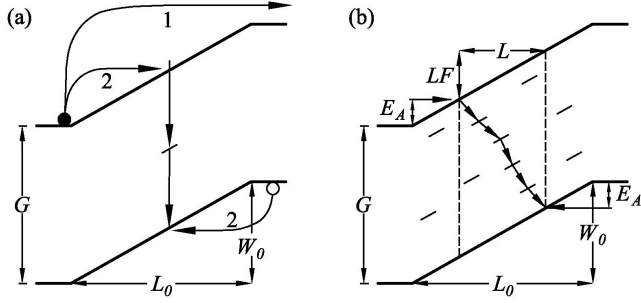


Fig. 2. (a) Arrow 1 represents the classical model of forward current due to thermal activation over the junction barrier W_0 , upon which the electrons and holes recombine; arrows 2 represent the mechanism of forward current due to recombination via a single energy level. (b) Our theory of multi-step recombination channels for a simplified p-n junction of length L_0 , barrier W_0 , and linear built-in field F . G is the mobility gap. An electron is thermally activated to energy E_A and tunnels via N steps through a channel of length L and total energy $G-LF$.

One of the most important results of our theory thus far is an analytical expression for the diode ideality factor A in terms of material properties and operating conditions. We recall the standard photodiode equation relating the current density J to the applied voltage V ,

$$J = J_0 \left[\exp\left(\frac{qV}{AkT}\right) - 1 \right] - J_L \quad (2)$$

where q is the elementary charge, J_0 is the saturation current and J_L is the photocurrent. Our analysis has shown that the ideality factor is given by,

$$A = 1 + \frac{qV - W_0}{kT} \sqrt{\frac{a}{2L_0\lambda}} \quad \text{and} \quad A = 1 + \frac{2a}{L_0\lambda} \left\{ \left[\frac{qV - W_0}{kT} + \ln\left(\frac{v_0}{n\sigma v}\right) \right]^2 - \frac{G\lambda}{\varepsilon} \right\} \quad (3)$$

at low ($T < 100\text{K}$) and high temperatures ($T \sim 1000\text{K}$), respectively. Physically, the two temperature regimes of A are due to a combination of tunneling and activation transport, which we predict are both at work in noncrystalline junctions at standard operating temperatures. Also, Eqs. (3) and (4) predict that the ideality factor increases under illumination (because the depletion width L_0 decreases), which is verified by the data shown in Fig. 3.

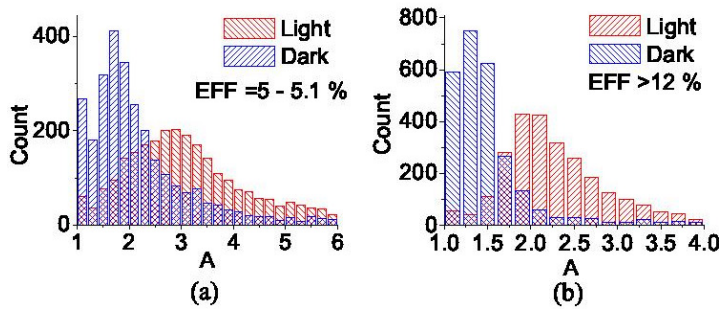


Fig. 3. Ideality factor under ‘dark’ and ‘light’ (1 sun) conditions for two databases (of about 2500 samples each) representing CdTe/CdS solar cells with efficiencies (a) in the interval 5-5.1%, and (b) greater than 12% [7].

Other consequences of our theory are that the saturation current J_0 depends exponentially on A and that there is a negative correlation between V_{oc} and A according to,

$$J_0 = J_{00} \exp\left(-\frac{W_0}{AkT}\right) \text{ and } V_{oc} = \frac{W_0}{q} - \frac{AkT}{q} \ln\left(\frac{J_{00}}{J_L}\right) \quad (4)$$

The latter predictions are verified by the data in Fig. 4.

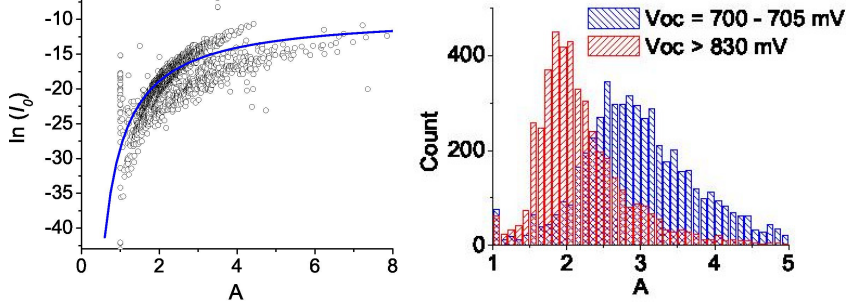


Fig. 4. Right: Correlation between the ideality factor A and saturation current J_0 extracted from a database of approximately 2500 CdTe based PV cells with efficiency greater than 12%. Cells of different recipes used in our experiments exhibit themselves in the form of somewhat different groups of points. Here we show the general trend fit using the first of Eqs. (4), although a more detailed analysis indicates that some rare cells can have J_0 independent of A , corresponding to classical junction transport rather than hopping transport. Left: Statistical distributions of ideality factors for two databases (of about 5000 samples each) representing CdTe/CdS solar cells with $V_{oc} > 830$ mV and in the interval of 700-705 mV. There is a negative correlation between V_{oc} and A as predicted by the second of Eqs. (4). (data and comparison from Ref. [7]).

In summary, our theory leads to the following predictions.

- 1) Depending on material parameters, such as the density of localized states and depletion width, the ideality factor A can be in the range from almost unity to much greater than two at typical operating temperatures. In addition, A has two distinct temperature regimes.
- 2) A generally depends on both T and applied bias V .
- 3) A depends on illumination intensity and increases under light.
- 4) There is a negative correlation between A and V_{oc} .
- 5) At low temperatures, A is inversely proportional to temperature, which results in temperature independent V_{oc} .
- 6) The saturation current J_0 increases exponentially with A .
- 7) Optimum channel transport can dominate the operation of not only photovoltaic junctions, but also back and front barriers, the effects of which appear in the IV curve rollovers at large forward bias. Our consideration predicts that the rollover can either saturate or recover.

We note that based on just fitting the observed IV curves in the operationally important fourth quadrant, it may seem that our approach does not provide much advantage over the classical models. Indeed, the existing “crystalline” modeling software has enough adjustable parameters to fit various observed curves. However, of greater practical importance is a better understanding of the underlying mechanism, which can lead to improvements in device efficiency and stability. In particular, our approach suggests that PV performance can be improved by blocking the entrances to optimal channels, possibly using surface treatments, while “crystalline” models may purport controlling defect chemistry. We know from various sources that all the successful thin film PV manufacturing companies have their proprietary surface treatments, without which their product would not be possible.

Thus far, our analytical approach has been limited to the assumptions of a uniform density of states, a uniform built-in junction field, and uncorrelated localized states. An even more important limitation (to be relaxed in the proposed work) is the lack of heat transfer modeling that may be especially

significant in laterally non-uniform structures. Indeed as the transport is dominated by the rare optimum channels, the corresponding heat generation becomes non-uniform as well increasing those channel temperature and further enhancing their transport abilities. Similarly, the optimum channels in the band transport governed by a strong potential relief in a non-crystalline structure (due to grain boundaries or non-uniform impurity distributions) will be modeled along the lines described in the above for the hopping mechanism.

2.2 The Nonuniformity Problem

The second generation of PV taking over the renewable energy market has always been praised as inexpensive technology. This advantage is based on the use of thin-film structures deposited at high rates. Starting more than 20 years ago at a lab scale of small ($\sim 1 \text{ cm}^2$ or less) dot cells, this technology has now achieved the degree of maturity including large area ($\sim 1 \text{ m}^2$) monolithic PV modules and field installations of thousands of such modules.

One disappointing feature that gradually emerged in the course of development, however, was the omnipresent nonuniformity of thin-film PV revealing itself in differences between nominally identical devices, which had rather detrimental effect on performance and stability. It is in order to mention that the phenomenon of nonuniformity appears generally unavoidable in thin-film PV, exhibiting a hidden price of the otherwise inexpensive, high throughput technology. Indeed, fluctuations in rapidly deposited noncrystalline thin film parameters including thickness, structure, chemical composition, and shunting turn out to be not negligibly small and not self-averaging on that thickness scale. In other words, the amorphous or polycrystalline structure of the film in combination with high-rate deposition leads to profound lateral fluctuations in device parameters.

A systematic study of nonuniformity effects as such was started by this proposal's PI at First Solar LLC and then at the University of Toledo; that activity later expanded over the National CdTe team (managed by the National Renewable Energy Lab (NREL) in the framework of the Thin-Film PV Partnership Program (TFPPP)) where for a number of years the current PI co-chaired the 'Nonuniformity sub-team' and the 'Device Physics' sub-team.

A straightforward observation typical of practically all thin-film PV is the differences between nominally identical ('sister') cells made on the same substrate during the same sequence of technology steps. As illustrated in Figure 5 for the case of thin-film CdTe devices, the nonuniformity shows up in both the initial cell efficiencies and after time evolution under light soak (resulting in either degradation or improvement).

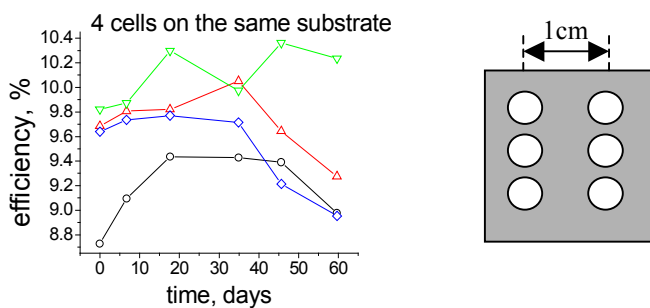


Fig. 5. Typical temporal evolution of CdTe based thin-film 'sister' solar cells [14].

Figure 6 [15] illustrates the electric potential and short-circuit current density (J_{sc}) fluctuations between different but nominally identical pieces on the same substrate and how these fluctuations are not small. The right figure suggests a phenomenological interpretation of many microscopic solar cells connected in parallel, where the fluctuations are less dispersed when the number of such parts is greater, (i.e. for large cells).

Evidence of nonuniformity in CIGS, a-Si:H, and dye-sensitized PV are described in Refs. [16-18]. These and many other examples show that local parameters in thin-film PV fluctuate over different scales ranging from microns (local structure fluctuations) to meters (deposition and other manufacturing

related nonuniformities superimposed on integral effects of local fluctuations) [14], which cause significant concerns in the PV industry.[19]

Local fluctuations in PV parameters can accumulate and result in significant dispersion of PV parameters between integrated modules, as illustrated in Figures 7 and 8, for the cases of CIGS and a-Si:H technology. One detrimental result of such variations is that combining non-identical modules in field installations (or other application) leads to significant mismatch losses.

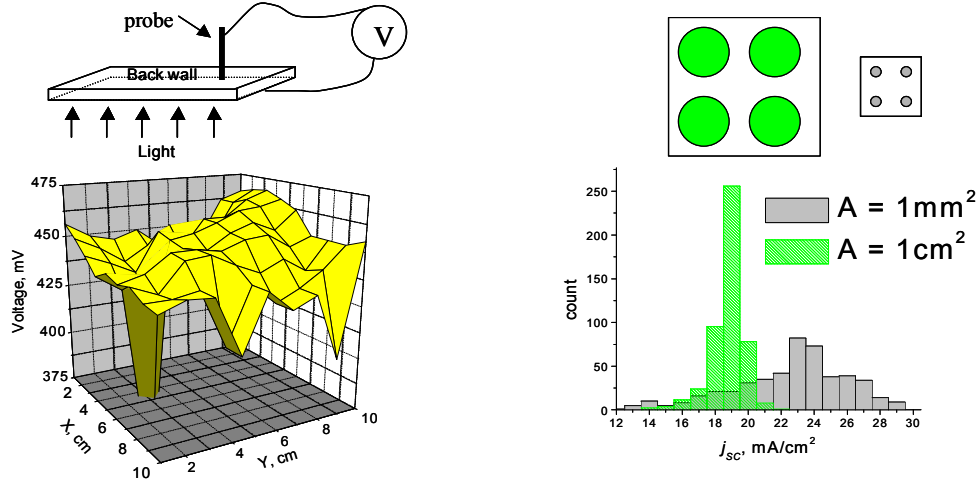


Fig. 6. Left: Nonuniformity evidenced by low light (~ 0.01 sun) voltage mapping of a CdTe PV structure continuously metallized with intentionally high-resistive electrode.[15] Right: Statistical distribution of short-circuit currents in small and large area CdTe cells made on the same substrate.[14]

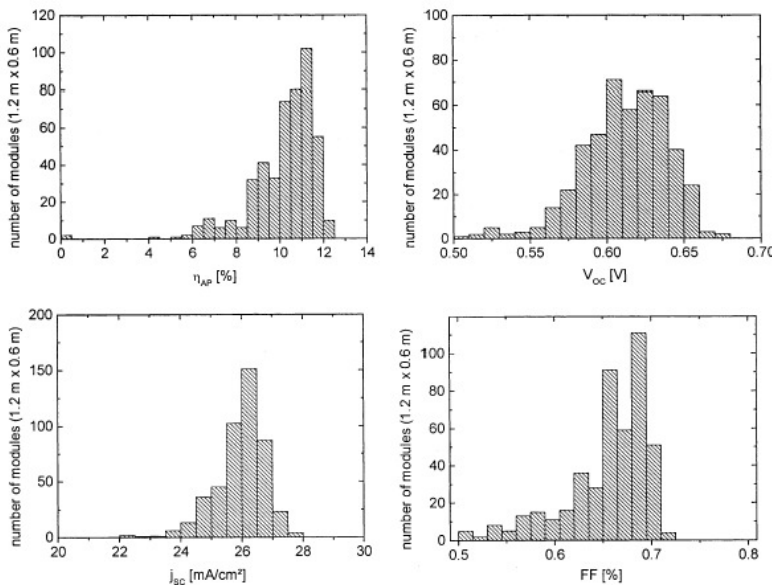
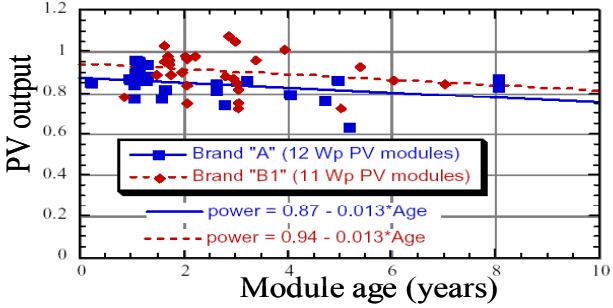


Fig. 7. Distribution of module performance (aperture-area efficiency, open-circuit voltage, short-circuit current density, and fill factor for 1.2 x 0.6 meter CIGS modules).[20]

The mismatch losses are generally due to the fact that electrically connected modules interact and cause each other to operate far from the optimum power conditions, which are different for each module.



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a-Si:H module efficiencies and degradations for a field installation.



Such mismatch loss has long been known for first generation PV [21] and was more recently addressed for the case of thin-film PV by our group, as briefly described below.

Fig. 8. Distribution of

2.3 Random Diode Arrays

The following underlying theoretical concepts are based mostly on our group achievements.[14, 15, 22] We recall a simplified picture of the photovoltaic effect leading to the well-known concept of a photo-diode illustrated in Figure 9.

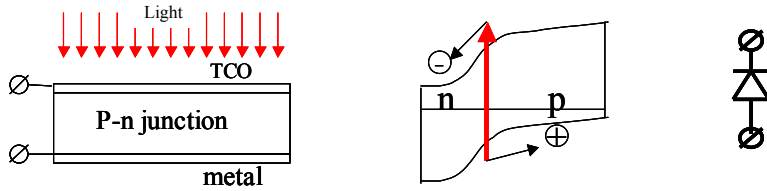


Fig. 9. Sketch of laterally uniform solar cell, its band diagram, and representative circuitry element, which is a photo-diode; TCO stands for transparent conductive oxide electrode whose sheet resistance is much greater than that of the metal electrode.

Different neighboring parts of a polycrystalline cell can be represented by non-identical (random) micro-diodes connected in parallel through a resistive TCO electrode, as illustrated in Figure 10. The random micro-diode circuitry is cumulatively represented again as one effective diode. The parameters of the effective diode are then random, as dictated by the randomness of the underlying micro-diodes.

Weak (low open-circuit voltage V_{oc}) diodes play the most significant role in random diode arrays (RDA). Figure 10 shows how a weak diode can be under forward bias generated by its more robust neighbors. Such biasing results in the weak diode stealing current from a significant area in the neighborhood. It was shown [14, 15] that the area affected by a weak diode has a linear dimension $L = \sqrt{\delta V / J_{sc} \rho} \approx 3 - 10$ mm for the typical PV parameters, J_{sc} (short-circuit current) and ρ (sheet resistance), where δV is the weak diode deficit of open circuit voltage illustrated in Figure 10(b), for $\delta V > kT/q \sim 0.026$ eV. In other words, a microscopically small region of around 10 μm in diameter can rob current from a macroscopically large area of radius $L \sim 3 - 10$ mm.

It was shown that weak diode shunting could be blocked by adding a high enough series resistance,[23, 24] such as that of the back contact. However, a very strong back barrier again leads to local regions that behave as weak diodes (we skip the discussion referring to our work [24]).

Non-identical micro-diodes connected in parallel through a resistive electrode represent the simplest RDA. Such RDAs possess many nontrivial properties [14, 15, 23] including singular electric potential distributions and phase transitions. The latter can switch the system behavior from almost

laterally uniform to strongly nonuniform in response to a relatively small change in parameters, such as the diode statistical distribution or sheet resistance. This behavior can explain the seemingly unprovoked, (without intentional parameter changes) dramatic changes in PV quality occasionally observed in production.

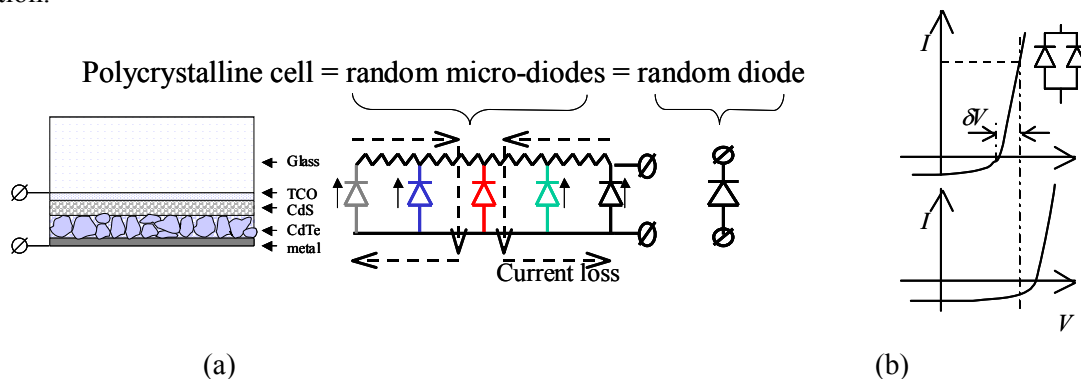


Fig. 10. (a) Sketch of a laterally nonuniform CdTe based solar cell, its corresponding circuitry of random micro-diodes in parallel, and the effective random photo-diode representing the entire cell. Shown in red is a weak micro-diode. Dashed arrows stand for shunting currents as opposed to the ‘useful’ photogenerated currents shown in solid arrows. (b) A weak diode (upper IV curve) in parallel with more robust diodes (lower IV curve).[25]

Note that the standard ohmic shunts can be treated as the limiting case of weak diodes with $V_{oc} = 0$. In what follows we will not specifically separate ohmic shunts from the more general concept of weak diodes, although from the material science perspective, some kinds of shunts, e.g. caused by metal protrusions [26-28], may require separate treatment techniques as described below.

In the present context, it is important consider yet more complex RDAs that appear within integrated modules of many connected cells, as illustrated in Figure 11. At the level of modules each device can again be represented as an effective random diode, whose randomness is an accumulated effect of the variations between its constituting cells. These integral device parameters will vary between nominally identical modules (i.e. ‘sister’ modules created from the same batch in the course of the same technological cycle) leading to variations of the kind shown in Figure 7. At still larger space scales, many modules form field installations spanning mega-areas of square kilometers. From the electric circuitry point of view, these installations are also RDAs composed of strings of individual random diode modules in parallel connected in series.

Summarizing, there is an hierarchy of RDA scales through which the microscopic nonuniformities propagate up to kilometer large installations. Our estimates [27-29] show that the power loss due to RDA nonuniformity including weak diodes, shunting, and mismatch effects can be as large as $\sim 30\%$. Minimization of nonuniformity loss through optimized material choices and circuitry connections is then necessary to maximize power output.

2.4 Existing Computational Tools

AMPS-1D is the current industry standard software package for simulating PV device operation. [2] AMPS employs the finite difference method to solve a system of coupled, nonlinear differential equations which govern charge transport under conditions of external voltage bias and illumination. As with any first-principles approach to this problem, the software numerically solves the Poisson equation coupled with the continuity equations for both electrons and holes. The software is quite general as it allows for degenerate electron systems and both direct band to band recombination and defect level mediated (indirect, SRH) recombination mechanisms. It also allows for a wide variety of defect and dopant states enabling the simulation of a broad range of materials. Being able to handle a high degree of

1D spatial variation in material properties (up to thirty material layers), it can provide some insight on the effects of nonuniformities and the behavior of disordered materials, so long as those variations occur only along one dimension.

AMPS is freely available, it is not demanding computationally, and it has an intuitive, user-friendly interface. It also automatically calculates most of the important PV performance measures and provides simple graphical output of the results. However, it does have several limitations as listed below.

1. Recombination mechanisms only include charge transfer from band to band or between a single defect level and the bands (SRH). We have shown that transitions between multiple defect states via optimum channel hopping can be the dominant recombination mechanism in thin noncrystalline materials. [7, 13]
2. Tunneling of charge carriers is not accounted for. We have shown that this is a significant charge transport mechanism at p-n junctions and interfaces between metals and noncrystalline semiconductors, even at typical operating temperatures. [7]
3. The lateral nonuniformities are absolutely fundamental to understanding the device physics of noncrystalline materials. They allow for the manifestation of optimum hopping channels and many of the related unexplained observations that were discussed in Sections 2.1 to 2.3. The natural disorder results in a statistical pattern of observations which should emerge from a fully 3D simulator that is founded on a deeper understanding of the underlying physics.
4. Even along its 1D domain AMPS does not allow for continuous variations of material parameters. It requires the user to create a new material layer every time a variation in properties is needed.
5. Once a single device is simulated in 1D using AMPS it is not possible to then connect several of those devices in a circuit to observe their integral behavior.

SCAPS-1D is a software package with much similarity to AMPS that was designed primarily for simulation of CdTe and CIGS type PV devices.[30] Although its numerical convergence is not as reliable as AMPS and it only allows for seven material layers, it is slightly more user friendly and allows for the simulation of capacitance-voltage (CV) and capacitance-frequency (CF) measurements. As with AMPS, recombination is limited to SRH type processes.

A well-known software package in the (poly)crystalline Si PV industry is PC-1D.[31] Based on a finite element approach, it can model up to five layers of material and it is limited to one deep defect level per layer. Since it is not possible to define a general density of states in the band gap, it is not suitable for modeling noncrystalline devices.

A more sophisticated software package called DESSIS (recently merged with a newer version called Sentaurus Device) is widely used in the broader, crystalline semiconductor industry.[3] It is a multidimensional, technology computer-aided design (TCAD) package that simulates the operation of silicon-based and compound crystalline semiconductor devices, as well as mixed device connections in a circuit. It employs the finite element method to solve the same basic equations that AMPS does for charge transport in PV devices

Sentaurus has extensive functionality with the ability to conduct steady state, transient, AC signal, and noise analysis with visualization tools that set the industry benchmark. It also employs a comprehensive set of transport models including drift-diffusion, tunneling, hydrodynamic and self-heating, as well as high electric field effects (Poole-Frenkel). Yet, Sentaurus suffers from the same limitations as AMPS with regards to how it handles nonuniformities, with the additional shortcoming that it is extremely expensive and unattainable for most research and education purposes.

In addition to the above software packages that can simulate the operation of a single small device or cell, we must also consider algorithms for connecting many such devices in a circuit to form module and arrays. In the course of our preceding work, we developed several techniques to quantitatively model nonuniformity loss in various RDA, including analytical modeling, PSPICE modeling, and home-developed software (eventually shared with the National CdTe team).

In our PSPICE modeling, we divided the module into a set of individual parts of linear dimension less than 1 cm each, which is less than the above-mentioned nonuniformity length L and justifies the assumption of lateral uniformity within each cell. On the other hand, each uniform part was assigned its

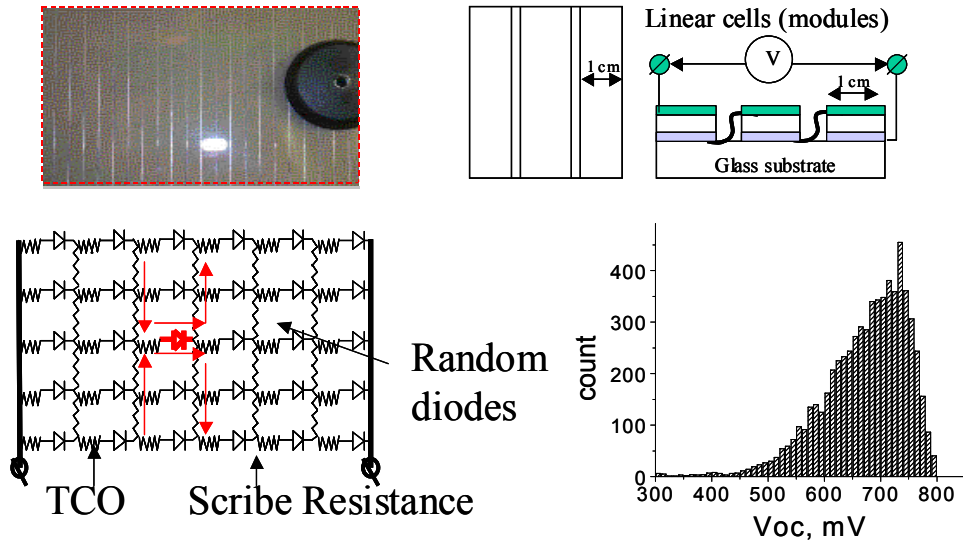


Fig. 11. Top: picture of scribe-integrated CdTe based PV module followed by top and side view sketches of the connection structure where linear cells approximately 1 cm wide are connected in series (top stripes represent metal, bottom stripes are TCO). Bottom: equivalent electric circuit of RDA and realistic statistical distribution of individual diode V_{oc} . Shown in red is a weak diode and its corresponding shunt current.

individual PV parameters, as shown in Figure 12. The list of individual parameters was created to reflect the desired realistic statistical distributions. In this proposed project the PV parameters will be derived from the single-cell device simulator. Some of our previous results are illustrated in Figure 13 for two types of statistical distributions of open circuit voltages.

Several conclusions of practical importance have been derived, such as: 1) details of the geometrical distribution of nonuniformities across the module play only a minor role; 2) mismatch loss is close to a certain fraction of module power and independent of module size; 3) series and scribe resistances interfere with nonuniformity effects and offer a possibility to optimize losses (increase in resistances mitigates nonuniformity loss at the expense of ohmic loss); and 4) rare yet strong local failures, such as weak diodes in combination with low series resistances are responsible for module-to-module variations of the type illustrated in Figure 7.

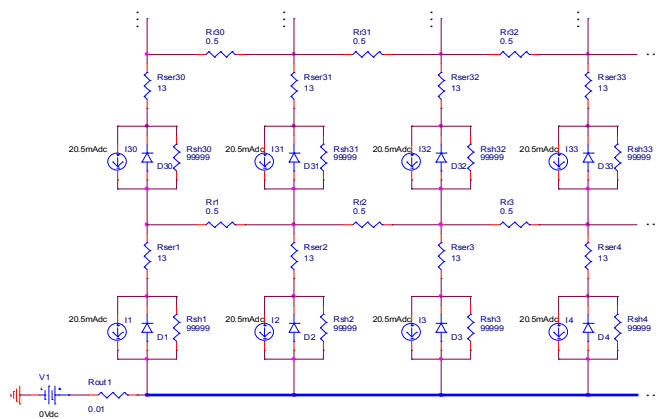


Fig. 12. A fragment of PSPICE circuitry modeling of an integrated PV module based on the circuit of Figure 11. The module is broken into a set of parts, each characterized by its individual diode parameters, shunt and series resistances, and photogenerated current (current generators are shown as circled arrows). Horizontal resistors model scribe resistance.

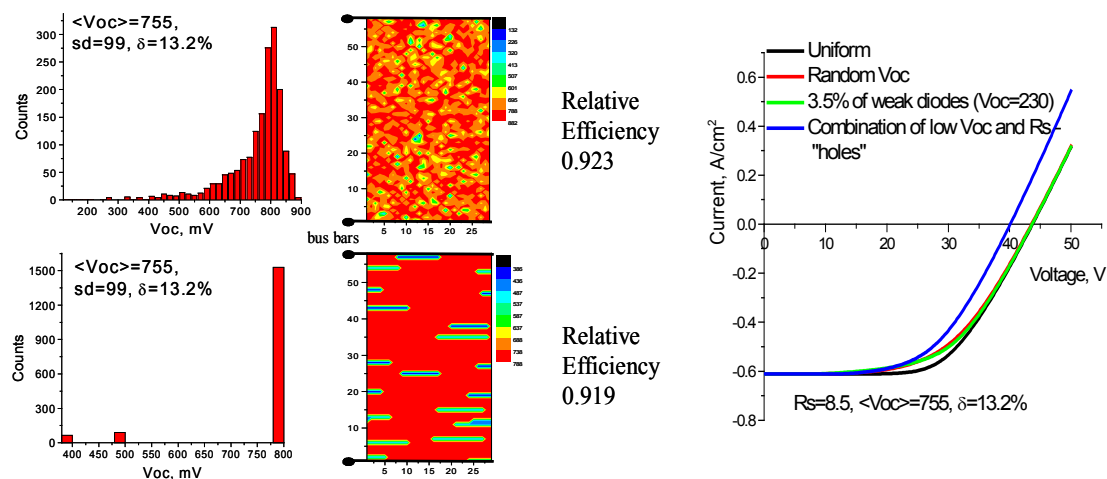


Fig. 13. Examples of two qualitatively different distributions of V_{oc} having the same statistical moments and leading to almost the same integral module efficiency.

Overall, the PSPICE modeling has proven quite reliable, yet has two shortcomings: 1) the circuitry design, parameter definitions, and software tuning would have to be done anew for each particular system; and 2) it does not solve the problem of optimizing the system, in particular, calculating the optimum part parameters and connections.

Along with the above, we have developed our own software for RDA modeling limited to a particular type of RDA, namely that of random diodes connected in parallel through a resistive electrode (illustrated in Figure 10). It has a simple user interface and consists of two functional blocks, one of which generates the desired distributions of individual diode parameters (V_{oc} , J_{sc} , etc.) and then supplies those to the second block which calculates all the currents and voltages in the system. Figure 14 presents an example of the program outputs. Our software allowed for up to 3000 random diodes forming either 1D or 2D arrays. Its main shortcomings were: 1) limitation to a particular type of RDA; and 2) lack of optimization capabilities. Nevertheless it was successfully used to predict RDA properties [26] and to model the results of thermography diagnostic techniques [32]. The software was distributed to the members of the national CdTe team at NREL.

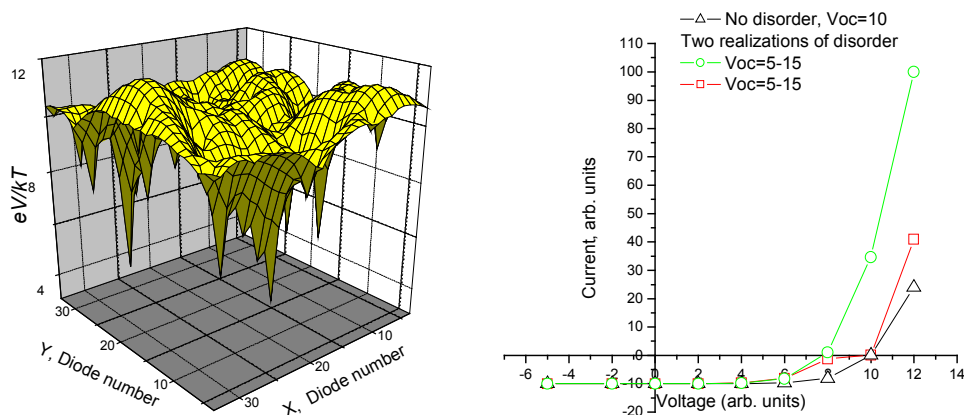


Fig. 11. Left: electric potential distribution in a 2D array of random diodes simulated by our software. Right: Current-voltage characteristics of MDA vs. a uniform system simulated by the same software.

As discussed in the following section, our intention is to incorporate the primary benefits of the software packages mentioned above in our simulator, while compensating for the limitations. One of the most important limitations of all the existing software packages is that they do not include the optimum channel recombination mechanism which is a natural consequence of the disordered nature of thin-film PV.

3.0 Plan of Work

Our plan of work entails the following three major tasks: (1) continued fundamental research and analytical theory development of charge transport in noncrystalline semiconductors; (2) systematic development of the numerical simulation package; and (3) liaison with out industry partners, dissemination of results and outreach for education purposes.

Two problems of fundamental nature will be addressed with the goal of implementing the results into the proposed simulator: (1) band transport through strong potential relief of non-crystalline films; our approach will combine the classical concept of percolation theory with the ideas of optimum channels dominating transversal conductivity in thin structures. (2) Non-uniform heat transport coupled with the non-uniform electronic transport through thin films; such a coupling has a positive feedback on the degree of non-uniformity and will be addressed both analytically and numerically.

The development of the simulation package will start by simply reproducing the capabilities of the existing software packages with the extension to three dimensions. That work is currently underway and some preliminary results are shown in Figure 15. Once that has been successfully completed, we will incorporate our advanced understanding of the physics of charge transport in noncrystalline semiconductors to develop the 3D simulation tool for noncrystalline PV cells. At that point we will have an effective single-cell device simulator.

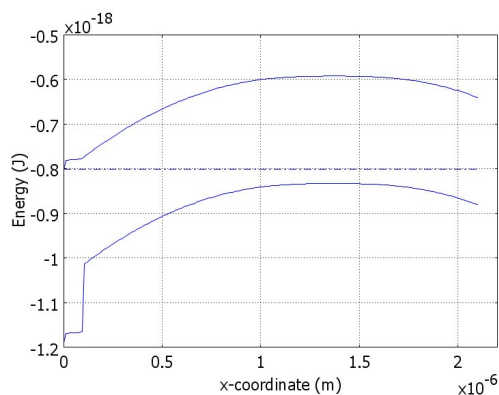


Fig. 15. Preliminary results of our simulation effort showing a simplified band diagram of a CdS/CdTe solar cell with metal contacts. The upper and lower lines are the conduction and valence edges, respectively, and the dash-dot line is the equilibrium Fermi level.

The 3D device simulator will be based on the finite element method and allow the user to input the standard material parameters with the additional features that the material properties can depend on temperature and position in various ways. Inputs will include material types, dimensions, and details on the density of states. The spatial dependencies will be specified as analytical functions, interpolated functions from data tables, or random distributions. Templates will be available for common device types with the ability to adjust the parameters according to user preference. The user will also specify details on voltage biasing and illumination. The simulator output will include all the standard PV measures and IV, CV, Cf, and spectral response data, as well as the ability to visualize the charge, current, and other distributions in the 3D.

The single-cell device simulator will be extended by using Monte Carlo techniques to interconnect several random but statistically correlated single devices into a complete module, followed by the connection of modules into a solar array. That approach is based on the random diode array concept discussed in Section 2.3. Finally, the simulation algorithms will be compiled into a complete package with a graphical user interface.

Ongoing verification of model reliability will be conducted by comparing the simulation results with our readily available experimental data that include the unique features of noncrystalline systems. The software development will be coupled with ongoing discussions and interaction with our existing network of PV specialists.

There are several key challenges that will arise during this research project. First, converting our analytical theory of charge transport into a computational algorithm that can be integrated into an efficient software package will not be trivial, but similar algorithms have been created and we plan to follow their examples. Second, the challenge of accounting for material nonuniformity will be overcome by coupling the meshing engine to the material property distributions so that the final finite element mesh is refined in regions of greater disorder. Finally, dealing with the drift-diffusion equation in situations where the drift velocity (due to the electric field) is much greater than the diffusion velocity leads to poor numerical convergence and inaccurate results. This issue can be mitigated by employing well known numerical corrections (often called artificial diffusion) and smart meshing algorithms that optimize the mesh size in regions of large drift.

The resources required for this project are minimal. The primary resource that is required is a qualified postdoctoral researcher (one is available that has been working with the PI for three years). Also required is medium level computer hardware (double quad-core CPUs), as well as finite element and mathematical software, all of which are already available.

Our results will be disseminated at multi-disciplinary venues, such as the PV Specialists Conference and the Materials Research Symposium, as well as peer-reviewed journals. Outreach to undergraduate and high school students will be conducted as discussed in the broader impacts section below.

4.0 Intellectual Merit Summary

The disordered nature of noncrystalline semiconductors leads to unique features that are not observed in their crystalline counterparts. That fact is evident in state-of-the-art and future PV technologies where common yet puzzling observations, such as performance differences between nominally identical devices, difficulties with technology scale-up, accelerated degradation rates, large deviations from ideal diode behavior, and the performance benefits of thin window layers (e.g. CdS on CdTe). Yet, the efforts to understand the underlying transport mechanisms have been based on the physics of crystalline materials because the theories lend themselves to simpler analytical descriptions and advanced software products have been developed to simulate device behavior. In addition, the knowledge of crystalline semiconductors developed rapidly due to lucrative applications in non-PV industries.

The understanding of noncrystalline semiconductor physics has been advancing independently of its crystalline sibling and a great deal of progress has been made since the 1960s. But only recently has research interest in these ‘dirty’ materials been reinvigorated due to applications in PV technology, as well as the computer memory and communications industries. The PI for this proposed research project has been at the forefront of noncrystalline semiconductor physics research for three decades. Our intent is that this proposed project will help to bring noncrystalline physics into the mainstream by compiling this knowledge in a simulation software package that will serve as a useful tool for advancing the understanding of researchers, educators, and students.

Thus far, our analytical treatment of the recombination mechanism that is at the heart of the charge transport problem in noncrystalline semiconductors has been limited to the assumptions of a uniform density of states in the mobility gap, a uniform built-in junction field, and uncorrelated localized

states. A numerical simulator that embodies the underlying physics of transport in noncrystalline systems is required to advance our understanding and serve as the next-generation PV model.

The PI for this proposal has over 100 peer-reviewed publications related to noncrystalline materials physics. The study of nonuniformity effects was started by the PI at First Solar LLC and then at the University of Toledo; that activity later expanded over the National CdTe team (managed by the National Renewable Energy Lab (NREL) in the framework of the Thin-Film PV Partnership Program (TFPPP)) where for a number of years the PI co-chaired the ‘Nonuniformity’ sub-team and the ‘Device Physics’ sub-team. Those experiences have resulted in an extensive network of PV specialists, many of whom have identified this proposed work as a significant knowledge gap in the industry. In addition, the PI receives research funding from Intel Corporation for the study of noncrystalline semiconductor memory devices.

5.0 Broader Impacts Summary

The primary utilization of this funding will be to support a postdoctoral researcher to develop the model and disseminate the results to the broader research and education community. The postdoc will be encouraged to participate in multi-disciplinary conferences, publish in peer-reviewed journals, work with PV industry colleagues, and mentor students. The postdoc will be mentored by the PI according to the Mentoring Plan submitted as a supplementary document to this proposal. We plan to assign one grad student supported by the University funds (beyond this proposal) to collaborate with the postdoc and PI.

The Department of Physics and Astronomy at the University of Toledo has a strong research experience for undergraduates (REU) program and summer camp program for high school students. We will actively participate in these programs by providing research opportunities and conducting presentations to convey to students that high-level science plays an important role in the energy challenge. Toledo is an ethnically diverse area and the REU and summer camp programs will allow us to connect with and seek the active participation of underrepresented groups.

Our intent is to make the simulator as user-friendly as possible so that it can be used throughout the PV community by researchers and educators at all levels. The simulator will serve as the core of an interactive pedagogical approach because students will be able to create and observe the effects of real-time variations in operating parameters, such as temperature, surface reflectivity, and carrier lifetimes, as well as the effects of nonuniformities and connecting cells or modules in a circuit. The enhanced post-processing capabilities and 3D graphics should improve the student learning experience.

The PI has an extensive network of colleagues throughout the PV community, in industry, national labs, and academia; many of which have expressed the need for the type of simulator proposed here. Through collaboration with these groups, we hope to enhance the infrastructure for research and education by developing and disseminating the next-generation PV simulation tool.

In terms of broader societal impacts, the simulator will play help in achieving the goal of bringing the cost of solar electricity on par with fossil fuels and achieving power supply levels on a multi-terawatt scale.[33] It will do so by allowing researchers to visualize experiments in-silico and allow for a degree of creativity and risk taking that is not feasible in real experiments and the existing computational tools.

Finally, one non-traditional broader impact anticipated for this proposal is the use of its results in the physics of biological membranes where ion channels have the IV characteristics typical of diodes and are randomly distributed along the membranes. This makes such systems similar to the random diode arrays described in connection with PV problematic above as we have mentioned earlier [34]. We plan to collaborate with biophysicists in order to explore possible applications of our tools for modeling of the biological membranes.

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