Process Control Advancements for Flexible CIGS PV Module Manufacturing

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ABSTRACT

ITN Energy Systems, Inc., and Global Solar Energy, Inc., with the assistance of NREL's PVMaT program have continued the advancement of CIGS production technology through the development of trajectory oriented predictive/control models, fault tolerance control, in-situ sensors, and process improvements. Modeling activities to date include the development of physics-based models for CIGS and Mo deposition processing; implementation of model-based control for CIGS processing, and application of predictive models to the construction of new evaporation sources. Reliability improvement activities include implementation of preventive maintenance schedules; detection and reconfiguration of evaporation source thermocouples and other sensor failures; and systematic development of fault prevention and reconfiguration strategies for the full range of CIGS PV production deposition processes. In-situ sensor development activities have resulted in improved control and indicated the potential for enhanced process status monitoring and control of all deposition processes. In spite of the short time since the program was initiated, substantial process improvements have been made, including significant improvement in CIGS uniformity, thickness control (e.g., 71% reduction in Cu variability), yield, and throughput.

INTRODUCTION/BACKGROUND

Interest in thin film photovoltaics (PV) has expanded dramatically, but wide-scale commercial use remains limited by performance and cost. These factors are often interrelated and negatively impacted by the lack of reliable and accurate process control. ITN Energy Systems, Inc. (ITN) and Global Solar Energy, Inc. (GSE) are using a comprehensive and systematic program to integrate intelligent process control into the manufacture of flexible, lightweight copper indium gallium diselenide (CIGS) based PV modules. Process control has been a priority since the outset of this endeavor, enabling the development of a fully integrated CIGS module manufacturing facility in only four years. The PVMaT program aims to enable GSE/ITN to complete a fully integrated process control development program with models and diagnostic tools (sensors) for intelligent processing of PV modules, with the ultimate goal of improving CIGS module performance, process throughput, and yield.

To capitalize on the potential cost reductions that thin film processing methods can provide for polycrystalline PV modules, every manufacturing step must be controlled at a level where quality and yield are maximized. Depending on the complexity and extent of fundamental scientific understanding of each process, the transition to large-scale manufacturing can be more difficult and costly than anticipated. A critical requirement is the development of diagnostic tools and associated predictive models that can quantitatively assess the relationship of processing conditions to product properties.

In general, diagnostic capabilities for manufacturing thin films are rudimentary, and manufacturers can only assess their product after module completion. Inadequate diagnostics and predictive models result in sub-optimal control and correspondingly lower quality and yield. For system failures, the most common strategy consists of sophisticated interlocking and alarm mechanisms to stop the process when a fault is detected. Process models/simulators are required for unanticipated process upsets, reactor variability/drift, and operation in unstable processing regimes where repeatability can be achieved only through dynamic feedback/feed-forward control. Similarly, in-situ, real-time process diagnostics development, in the form of sensors, is also required since their use has been proven to improve process yield/quality and reduce module costs.

The essence of our PVMaT effort is to develop trajectory oriented and fault tolerance based intelligent process control using predictive physics-based process models and strategic process/film property sensors to significantly improve yield, throughput, and performance of flexible CIGS PV modules. Trajectory oriented modeling activities include development of mathematical relationships between control variables one can activate and final product properties (system identification), reduction of these relationships into more computationally efficient forms, and establishment of optimum trajectories for film properties during deposition. Fault tolerance activities include detection, location, and isolation of faults, and implementation of appropriate corrective actions that prevent faults from becoming critical failures. Diagnostic tool activities involve integration of existing and alternative sensors to increase reliability and/or provide process information. All effective model/sensor features will be incorporated into a robust control platform that will enable autonomous and continuous manufacturing, with automatic data storage and presentation for operator monitoring.

OVERVIEW OF CIGS MANUFACTURING

GSE's production facility is fully equipped for manufacturing flexible, lightweight CIGS PV products. Key equipment includes: molybdenum back contact, large-area CIGS absorber layer, cadmium sulfide, and transparent conductive oxide deposition systems; fully automated laser

scribing; module lamination, and PV product finishing equipment. Each production deposition system is capable of processing 12-in. wide 1000-ft. long polymer or stainless steel in a low cost, automated fashion. GSE's present annual manufacturing capacity is 5 MW, with 2003 production anticipated to reach 2 MW.

CIGS based PV is being sold to commercial and military customers who require flexible, lightweight, and high performance products. GSE's Portable Power Packs (P3s) are examples of true foldable and rugged, portable, lightweight self-sustaining power sources (Figure 1). Standard P3s are available in a number of configurations for 12 and 24 V loads up to 56W at exceptional power/weight ratios of up to 12.1 W/lb. In addition, GSE's intelligent product concept allows products to be made to customer specifications, as well.

Figure 1. Example of flexible CIGS PV product being manufactured at GSE: 12V, 30W P3-60 at 9.7 Watts per pound

Of the thin film PV materials, CIGS has demonstrated the greatest potential for achieving high performance at a low cost. To ensure the cost-reduction goals necessary for profitable manufacturing at Global Solar are achieved, the activities performed under the PVMaT program must be successfully completed.

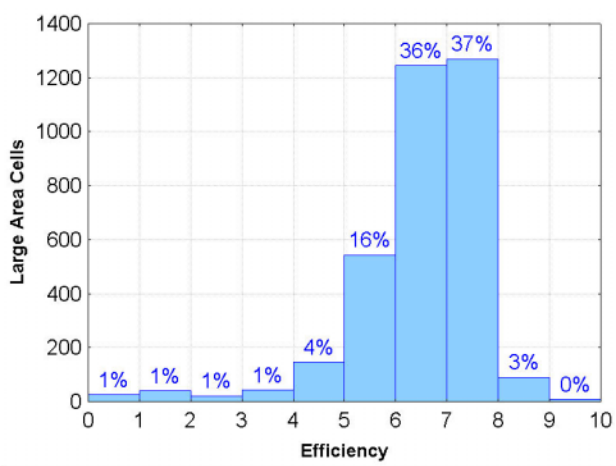

Figure 2. Device efficiency distribution over a production web for cells of 68.8 cm^2

Since the start of the PVMaT program, GSE has steadily improved processing and increased the yield of large area cells with efficiencies between 6 and 10% (Figure 2). Initial efforts to improve process control and fault tolerance along with preventive maintenance schedules have already lowered fault events (Figure 3) and provided well controlled deposition of individual CIGS elements (Figure 4).

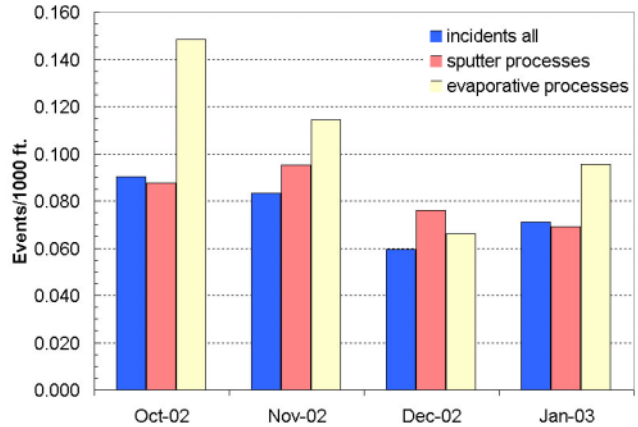

Figure 3. Frequency of anomalies or unplanned deviations (incidents) per 1000 ft. for different deposition processes

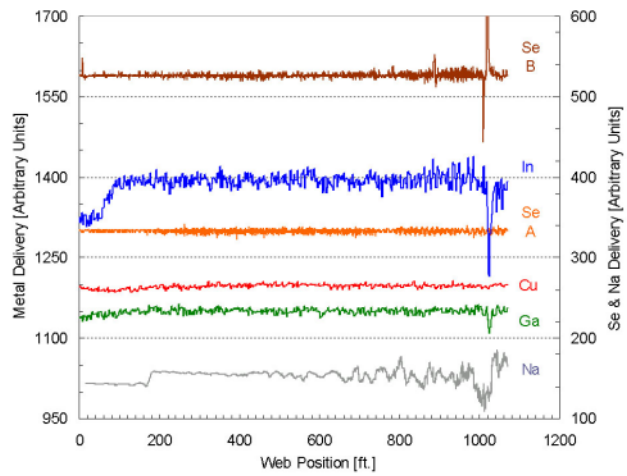

Figure 4. Real-time composition and flux signals monitored by in-situ sensors during a 1000 ft. CIGS deposition on stainless steel with active process control

DISCUSSION AND RESULTS

Physics-Based Model Development

Process control is based, to the greatest extent possible, on physically derived models of the reactor system and its environment. This requires significant *a-priori* information to determine internal system behavior. The models give insight into important physical processes such as droplet nucleation and plume uniformity that can be used for re-designs or adjustments. Furthermore, the models allow determination of the fast transient dynamics and interaction terms that are necessary for feedback control design. Finally, the models determine if longer-term dynamic effects will require the set-points of the feedback control system to be non-constant trajectories.

The process models are modular, with a decomposition that is relevant for many different deposition processes. In particular, the model components are mass source (or mass generation), mass transfer and deposition. Generally, the modules are feed-forward, so that outputs from one model become boundary conditions for the next (Figure 5). The physics-based models are validated using production data;

however these models are generally too complex to be used directly for process control. Therefore, a model reduction step is performed to obtain low order dynamic or static models. For the CIGS production systems, several modules were developed and integrated.

Finite Element (FE) Thermal – A physics-based finite element thermal model of the effusion cells, with 2606 nodes, was developed in ABAQUS.

Melt Convection – A reservoir flow model is used with the heat transfer model to determine the vapor flow in the source above the melt and to determine the conditions at the source outlets. From this vapor flow model, the conditions at specific points within the source are determined (pressure, velocity, and mass flow rates).

Boundary-layer Flow – The vapor flow model results are then put into a source outlet boundary-layer flow model, based on one of the codes in the CHEMKIN suite.[1] This model is used to determine the nucleation behavior of droplets forming in the source outlet.

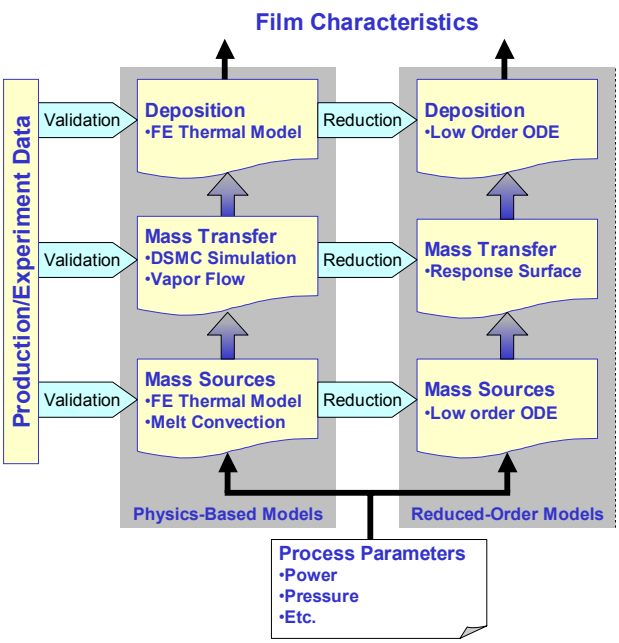

Figure 5. Outline of the individual modules combined to provide an overall model of CIGS processing

Plume Interaction – The vapor flow results are also used as inputs to a Direct Simulation Monte Carlo (DSMC)[2] module of the effusion source plumes. This enables investigation of plume interaction effects (including back-pressure at the source), and provides predictive plume shape capabilities to improve thin film thickness uniformity across the substrate.

Deposition – Initial modeling efforts of the heat transfer to the web include effusion source surroundings, reactor geometries, and web/heater assembly configurations. This model was created and analyzed using ABAQUS; results from the effusion source models were simplified and applied as boundary conditions. Model results will provide insight to web heating changes with source outlet geometry changes, as well as an effective heater model to predict thermal gradients throughout the web.

Model Validation/Reduction – Even for physics-based models, a number of parameters must be determined to best match the physical process. These parameters are tuned to a particular reactor by perturbing process inputs and recording the response with available process sensors. A related process occurs for model reduction, where the reduced model structure is a generic low order differential equation or response surface, rather than specific physical laws. Representative data comparing the reduced and physics-based models are shown in Figure 6 and indicate that the reduced models needed for real-time process control accurately emulate the higher order models and therefore the system dynamics from input (power) to output (effusion rate). Note that the control system is model-based in two ways: the models are used to determine input trajectories and to determine internal states given sensor measurements.

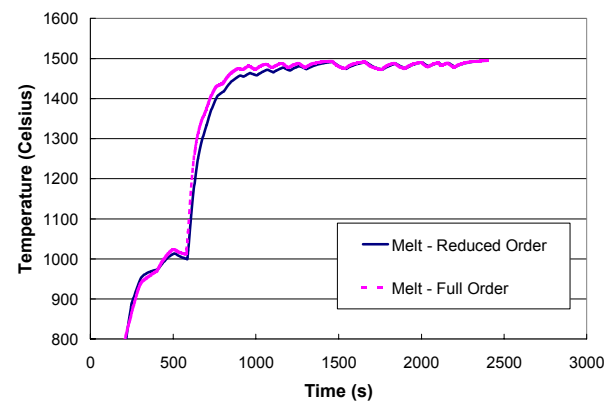

Figure 6. Comparison of full and reduced models indicates good agreement

Sputtering – In addition to the CIGS process, the Mo sputtering process was modeled using PVD Pro software (a commercially available sputter deposition modeling package based on Monte Carlo simulations), produced by Reaction Designs. This sputtering chamber software has been modified for CIGS PV production systems and continuous deposition processes.

Source Design – To validate the ABAQUS effusion source models, temperature measurements were systematically obtained from strategic positions inside and outside an operating source. Experimental data was compared with corresponding source model predictions to validate the model inputs and assumptions. Once validated, the source models provided temperature relationships between the melt and source outlet, predicted outlet dynamics including condensation, and predicted system time constants for transient input conditions. Therefore, these source models were used to predict quantifiable differences in source design changes to identify/validate improvements. Initial source design improvements resulted in significantly enhanced side-to-side uniformity and considerable reduction in the potential for recondensation in the effusion source outlet. Source redesign efforts have eliminated several undesirable operating characteristics and have substantially improved stability of the flux delivery, thus minimizing thickness variation, as shown in Figure 7.

Model-Based Process Control – In addition to providing predictive information about each component in the process, models were utilized to provide improved control of individual element deposition from each CIGS source. Model-based control has been implemented for all the deposition sources (NaF, In, Ga, Cu, and Se) based on sensor input and non-linear dynamic models. Compared to simple PID control, model-based control is advantageous for decreased thickness variation of individual constituents, as shown in Figure 7, corresponding to better control of film properties including Cu/(In+Ga) and Ga/(In+Ga) ratios. Process modifications resulting from model-based control combined with improved source design have begun to show improvements in overall yield. Additional gains in average efficiency and yield are expected with parameter optimization and further refinements in process control.

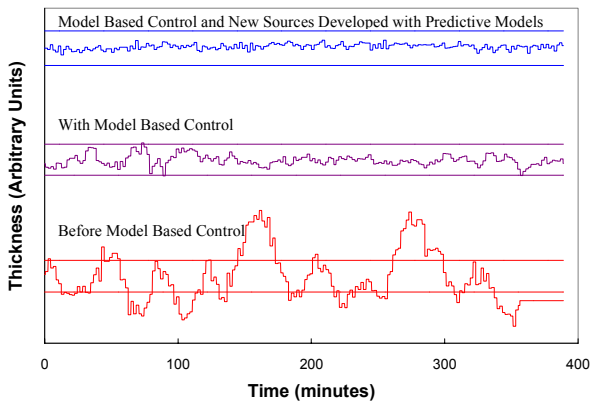

Figure 7. Comparison of thickness variability improvements with improved model developments; the solid lines indicate +/- 5% from the average

Reliability: Fault Prevention and Fault Tolerance

A CIGS deposition system is typically operated continuously for long periods of time, and system components are exposed to harsh environments, thus, decreasing reliability. System reliability can be improved by fault prevention and fault tolerance. For example, operator-induced faults can be prevented through sophisticated interlocking mechanisms. However, to increase reliability further, the system must be designed to provide service in the presence of faults. Fault tolerance enhances system reliability by continuing to perform specified tasks correctly in the presence of failures and errors. A typical fault tolerance technique consists of four basic steps: fault detection, fault location, reconfiguration, and recovery.

Initial diagnostic evaluations of reconfiguration strategies for all levels of the CIGS PV production deposition systems were performed In addition, specific subsystems were identified where implementation of fault tolerance methodologies could be beneficial. These fault tolerance issues include:

- Source thermocouple accuracy and failures
- Sodium fluoride sensor reliability
- Substrate heater failures
- Line voltage regulation
- Source power and current, and
- Sputtering source arc detection.

To enhance system reliability, a systematic evaluation of equipment failures was performed and a preventive maintenance schedule developed. In addition, redundant operator input was implemented to decrease the relatively high incidence of system faults induced by input error. The main reconfiguration strategies incorporated to date include redundant components and alternative sensor control. Several examples of fault tolerance/reconfiguration strategies are provided below to illustrate the complexity and unique approaches needed to provide robust operation. However, even the limited implementation of some of these reliability strategies has already resulted in improved operation (Figure 3).

Mo Arcing – The molybdenum deposition system tended to be shut down when an arc was detected. Hence, detection algorithms were developed and implemented to track arcing events and to provide information used to identify arcing types and eliminate some of the causes. In addition, a target fault identification strategy was designed to take corrective action. Further recovery methodologies are under investigation.

Thermocouples – Since thermocouples in the effusion sources, especially for copper, are prone to failures (low mean time between failures), the design and implementation of fault-tolerant controllers will enhance the reliability of this critical sensor, increasing throughput and yield. A fault detection algorithm has been successfully developed to identify abnormal changes in temperature measurements. Once an abnormal change is detected, a consistency check is performed and, if confirmed, a redundant thermocouple is used to perform the temperature measurements. Figure 8 shows data that shows the signature of a faulty thermocouple that can be used for fault detection.

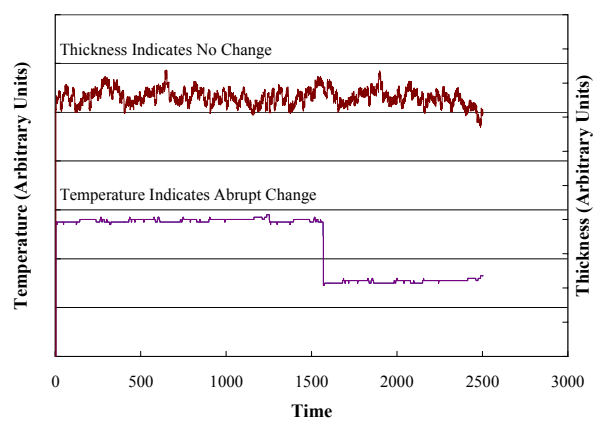

Figure 8. Representative thermocouple data where the corresponding algorithm would indicate a faulty thermocouple

Quartz Crystal Monitor (QCM) – A sensor for controlled sodium fluoride delivery provides primary set-point control. However, due to harsh processing environments, these sensors have demonstrated susceptibility to frequent failures. Model-based algorithms were designed and simulated to predict NaF flux and to

detect faulty sensors. The model and control methodology are combined with both a primary sensor that measures NaF flux and a thermocouple that measures source temperature. The flux measurement provides a more accurate correlation to film thickness. However, the temperature measurement and model are used to provide real-time primary sensor error monitoring and, when necessary, thermocouple-based control.

Sensors

To achieve the next level of cost reductions and increase product quality, yield and performance, intelligent outer loop control, based on in-situ film property diagnostics, will need to be implemented for the Mo, CIGS, CdS and ITO deposition processes. Furthermore, since GSE processes require hours of continuous operation, sensor robustness and fault detection/tolerant control are mandatory. As part of the initial PVMaT effort, several specific control parameters of all the PV production deposition systems were identified where benefits could be realized with in-situ diagnostics. Once specific concepts were identified, importance and feasibility criteria were applied to narrow the scope of effort to provide maximum results with the given resources. In the CIGS deposition systems, for example, thermocouples provide information about source temperatures and physics-based models provide guidance about expected effusion flux and anticipated film properties. In general, effusion source temperature and flux measurements enable more direct and simple process control but are less closely tied to desired film properties, whereas in-situ measurements of film properties provide information directly but require more sophisticated process control. After considering all of the different factors, several sensor development activities were initiated for Phase I, including:

- Investigation of RGA, OES, and QCMs to provide flux and chamber health monitoring for the Mo and ITO sputtering systems
- Development of pyrometry to improve source and substrate temperature monitoring
- Investigation of emissometry to measure film temperature, roughness, and emissivity
- Development of Se flux monitoring
- Development of alternative input current/voltage measurement methodologies to monitor system health and provide process control
- Investigation of reflectometry to provide characteristics of the various coatings, and
- The use of visible imaging for CdS film thickness.

Voltage/Current Monitoring – As in the semiconductor industry, input power quality was determined to be critical for both the deposition sources and sensors. Besides monitoring input power, additional sensors were integrated within the evaporation and sputter deposition systems to provide system monitoring and control information. Monitoring electrical contributions to the sources also provides equivalent control capabilities to thermocouple-based control. This strategy enables accurate and robust control of the effusion flux without the need for expensive in-situ sensors that can fail due to a myriad of physically induced mechanisms.

Sputter System Flux Monitoring – An initial set of tests was performed to provide side-by-side comparison of RGA, OES, and QCM sensors for Mo system health and/or flux rate monitoring. Previously, OES and QCM measured flux rates have provided only marginal film thickness control, especially as the sputtering target reaches the end of its usable life. While film thickness correlations may require substantial effort, the conclusion from this initial evaluation is that OES should be further investigated to better assess system performance. This will be especially important for ITO deposition, but could provide useful control for Mo deposition, as well.

Pyrometry – A commercially available pyrometer and a custom IR thermometer were evaluated as in-situ temperature monitors for CIGS processing. In addition to calibration issues, the commercial instrument also required the input of emissivity values for accurate temperature measurement. The lack of accurate emissivity data for the materials of interest limited the value of data from this instrument. To remove the emissivity and calibration issues, an IR spectrometer was used to provide a spectral measurement of the IR light emitted from heated surfaces. By fitting the obtained spectrum, an accurate emissivity independent temperature measurement of the source, pool, and substrate was obtained. The results from the initial experiments indicated that pyrometry can be used to accurately provide temperature measurements of the effusion sources/pools/substrate and may be more sensitive to dynamic changes than thermocouples.

Emissometry – Presently, no film property monitors are used close to or during deposition. The main issues include high temperatures, coating of optical surfaces, and corrosion of materials due to the Se environment. A commercially available emissometer was evaluated as an in-situ sensor in the CIGS process to provide surface temperature, roughness, and emissivity information for process control. Initial tests indicated that the CIGS films exhibit only minor emissivity changes with temperature. The tests also demonstrated that the emissometer is capable of providing reproducible results and precise discrimination in emissivity, roughness and film temperature. A decrease in emissivity with increase in Cu/(In+Ga) ratio was observed, as well. While these initial results are encouraging, additional experiments must be performed to determine if the emissometer can provide useful process control information for continuously moving CIGS thin film production inside a Se containing vacuum deposition system.

Se Flux Measurements – A proprietary method for monitoring Se in the CIGS deposition process has been developed at GSE, and has been successfully implemented for real-time feedback process control. Further development in the Se source-sensor combination is expected to enhance reliability and control for extended runs.

Visible Imaging – CdS thickness-to-color correlation is being investigated as an indirect in-situ product performance feedback. Figure 9 depicts this correlation for five clearly distinguishable CdS coating colors on production material. In conjunction with digital image analysis algorithms, 100% of the CdS coated CIGS can be analyzed to determine if CdS coating thickness is within the lower and upper specification limits. These limits have been determined via statistical design of experiment studies. The value of incorporating this technique into a feedback control system is under investigation.

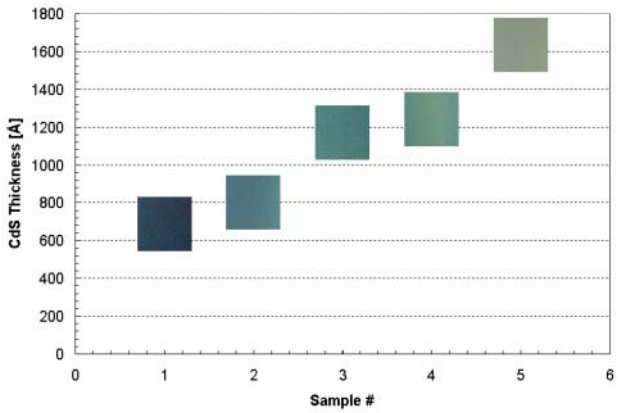

Figure 9. CdS film thickness as determined by cross-section FE-SEM at 60,000 magnification as a function of CdS color on CIGS

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[2] DS2V software by G.A. Bird (G.A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows,* (Clarendon, Oxford, 1994)

SUMMARY/CONCLUSION

To date, models have been used to provide both revolutionary new evaporation source and substantial process control improvements. In addition, initial fault prevention and tolerance activities have increased reliability (Figure 3) and identified several areas where reconfiguration/recovery methodologies can be applied. Finally, initial development activities have identified several sensors that could or have improved process control. Even in the short time period since this PVMaT program started, substantial yield, efficiency, throughput, and reliability improvements have been obtained for CIGS PV manufacturing as a direct result of program activities. ITN/GSE will continue process control and reliability development efforts to increase performance and decrease costs to produce cost competitive PV products for commercial and military applications.

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