

DuraMat Capability 2: Predictive Simulation

Poster Number	Capability Name	Short Paragraph Description of Capability (300 words same as the abstract. Summarize what it does and value to DuraMat and Module Materials)	Capability Expert (principal contact)	Organization Name and Type - (National Laboratory - NL, Academic Institution - AI, Company- C)	Which Capability Area Best Fits This Work (Select One)	Define from an industry perspective what near term 1 year and long term 5 year successful use of the capability would be. (100 words)	Link to Your Website (if available)
7	DuraMat Capability 2: Predictive Simulation	This capability will be a suite of modeling and simulation tools, model workflows, and a community of experts who work in concert with experiments and data analytics across length and time scales. The capability will be organized through four key work areas: 1) PV systems/stressors, 2) manufacturing stressors/excursions, 3) PV packaging materials, and 4) material defects. Module and material failure mechanisms have origins that span multiple length scales. Similarly, failures induced by external stressors must be understood based on accurate descriptions of environmental or process conditions. Computational materials tools for atomistic and mesoscale modeling will establish thermophysical properties and dynamical processes at the nanoscale, thus providing fundamental, molecular-scale limits on materials performance and enabling high-impact materials design. This capability leverages in-house developed production software, commercial tools, and physics-based and performance models being developed under DOE's SuNLAMP and PREDICTS programs. All tools are readily available to industrial and academic partners through open source or commercial licenses, and model workflows will be developed to help transfer the modeling/simulation capabilities to the consortium partners. PV module-level thermal-electrical-mechanical (T-E-M) and manufacturing process simulators will provide a unique connection to other consortium capabilities. PV T-E-M simulators will enrich PV damage databases and expose the origins and magnitudes of thermal and structural stressors on modules, materials, and materials interfaces. The manufacturing-process simulators will connect manufacturing modes/parameters to materials and interface residual stresses and composition, which, in turn, can lead to latent defect and performance degradation. This capability suite is foundational to the materials-by-design framework and will link to experimental data for validation and uncertainty quantification by the DuraMat data hub. Tools, components and SMEs from Sandia, NREL, SLAC, and LBNL underpin this capability. Possible additional resources from academia and industry will be brought in as needed.	P. Randall Schunk, Sandia National Laboratories	NL- Sandia National Laboratories	2. Predictive Simulation	In the short term, industry will benefit by working with tool SMEs with an improved understanding of the molecular origins of common degradation mechanisms, including the effects of micro- to macro-transport of oxidative, hydrolytic, and electrochemical by-products. Early capability components will also enable the prediction of thermal-mechanical stressors on material(s) in a PV module, thereby allowing better understanding of material requirements. Within five years, industry will benefit from tools and workflows that allow for multiple degradation/damage mechanisms to be analyzed simultaneously and tools for designing new materials and processes that might mitigate these stressors.	
8	Mesoscale modeling of multi-phase/multi-component materials	The theme of this thrust can be stated as "Durability, microstructural stability, and performance of PV components". The fundamental question we will address is: can we predict how PV microstructures evolve under given operating conditions over extended time scales? Under operation, microstructures and local compositions of multi-phase/multi-component materials systems evolve over time in response to a multitude of physical, chemical, and/or mechanical cues. In order to understand and quantitatively predict the stability and durability of morphologies, a mesoscale approach is required, which accurately incorporates both atomic scale information and evolving microstructures. The mesoscale method we will employ here falls under the rubric of diffuse-interface approaches. The fundamental idea is to introduce a set of order parameters (OP), defined everywhere in space, which describes the local state of the system. The dynamics are driven by the minimization of a free energy functional written in terms of the OPs, and no explicit tracking of the interfaces is required as they are implicitly coded into the evolution of the OP fields. This set of OPs are then augmented by additional variables such as temperature, local composition fields for multi-component systems, elastic deformations etc., and simulation of the coupled governing equations provides the means to investigate the spatio-temporal evolution of such systems. As inputs, these frameworks require (a) the relative free energies of bulk phases, (b) interfacial free energies, and (c) kinetic coefficients, all of which can be obtained from atomistic calculations and/or experiments.	Fadi Abdeljawad	NL- Sandia National Laboratories	2. Predictive Simulation	In the short term, the modeling capability will benefit industry by providing an improved understanding of the relevant factors affecting the phase stability of polymer blends. More specifically, the framework is capable of exploring the phase space of parameters, such as compositions and temperature level and cycles, that lead to instability and phase separation processes. The resulting morphologies greatly influence a wide range of properties and the proposed modeling capability provides a tool to explore which are the optimal ones. Within five years, the developed capability can be coupled to other relevant processes/mechanisms, which allows for the direct analysis of the role of microstructure on performance.	
9	Evolving Morphologies in Polymer Blends	The theme of this thrust can be succinctly described as: "Can we predict evolving morphologies in polymer blends under various external physical stimuli." Polymer blends can be unstable to perturbations, such as thermal, mechanical, or compositional, which lead to complex pattern formation dynamics. Of particular interest are phase separation and crystallization processes, which involve a strong coupling between mass transfer, flow and evolving morphologies, and greatly influence the properties and performance of such systems. Here, we propose to develop a mesoscale theoretical and computational framework for phase separation dynamics in pseudo-binary blends. The framework is based on time-dependent-Ginzburg-Landau (TDGL) formalism and is capable of incorporating the free energies through a Flory-Huggins-like description, and accounting for the kinetics of such processes. Within this proposed framework, various effects and stimuli can be probed, such as chemically reactive additives, thermal cycles and temperature levels. As inputs, the framework leverages atomistic studies for the kinetic and/or thermodynamic parameters of the model. For example, atomistic studies can be used to investigate the composition, temperature and phase dependence of the TDGL kinetic parameters. In addition, appropriate statistical sampling methods allow us to separately estimate enthalpic and entropic contributions to the relevant parameters, allowing temperature variations to be included without requiring full atomistic simulations for all state points.	Fadi Abdeljawad, Ross Larsen and Lauren Abbott	NL- Sandia National Laboratories NL- NREL	2. Predictive Simulation	In the short term, the modeling capability will benefit industry by providing an improved understanding of the relevant factors affecting the phase stability of polymer blends. More specifically, the framework is capable of exploring the phase space of parameters, such as compositions and temperature level and cycles, that lead to instability and phase separation processes. The resulting morphologies greatly influence a wide range of properties and the proposed modeling capability provides a tool to explore which are the optimal ones. Within five years, the developed capability can be coupled to other relevant processes/mechanisms, which allows for the direct analysis of the role of microstructure on performance.	
10	Multiscale molecular simulations of PV encapsulants	Molecular simulations can provide important information about nanoscale structure and phenomena in PV encapsulant materials, such as local packing and interactions and dynamics of additives and contaminants within the encapsulant. With a multiscale approach, quantum mechanical (QM) calculations and atomistic and coarse-grained molecular dynamics (MD) simulations can be performed to capture a broad range of length and time scales. For example, MD simulations could yield insight into where UV absorbers and stabilizers accumulate in polymer encapsulants and how the nanoscale structure is affected. Subsequent QM calculations on representative structures from the MD simulations may shed light on how incorporation of additives into an encapsulant matrix alters material properties and stability. In addition, MD simulations can capture the dynamics of O ₂ and H ₂ O in encapsulant materials, which can negatively impact the performance of PV modules. For instance, simulations may identify internal binding motifs for H ₂ O that would require dual sorption rather than purely Fickian models for water transport and sorption. In particular, this capability will leverage Sandia's LAMMPS MD package and NREL's STREAMM toolkit to setup, run, and analyze molecular simulations of PV encapsulant materials. When necessary, chemically specific coarse-grained models will be developed from atomistic models via methods like iterative Boltzmann inversion or force matching to access longer length and time scales. A reverse "fine-graining" may also be used to restore atomistic resolution for subsequent QM or MD simulations of small regions of interest, such as at interfaces.	Lauren Abbott (SNL), Ross Larsen (NREL), and Stan Moore (SNL)	NL- Sandia National Laboratories NL- NREL	2. Predictive Simulation	In the short term, this capability will develop computational models incorporating molecular-level detail of PV encapsulant materials, including additives and contaminants, for an improved understanding of material structure and properties, which will be demonstrated for exemplar systems. In the long term, this capability will make tools and workflows available to industry and academia to aid in a high throughput approach to screening encapsulant materials, as well as connect models and results to related capabilities that address other length/timescales or components of PV modules.	
11	Thermal-mechanical-electrical model for PV module-level mechanical failure	Thermomechanical stress induced in a PV module is a leading driving force of module failure. These failures include delamination, cell fracture, and solder bond fatigue, among others. Each of these failure modes depend on the specific deployment environment (temperature, humidity, etc) and electrical characteristics (e.g. temperature non-uniformity) of the module. A predictive thermal-mechanical-electrical simulation capability is desired to quantify loads on PV module interfaces and materials as the result of the environment and stressors. The model will be three-dimensional in order to capture details of the module configuration. As a part of the Predictive Simulation Capability, this model framework should integrate predictive simulation with capabilities in materials discovery and module durability testing. Thermal loads (from environmental cycling or from electrically-generated temperature non-uniformities) will drive mechanical deformation, and the mechanical component of the model will predict generated stresses, interface and material failures. A major part of this effort will include the development of appropriate constitutive models for the complex thermo-visco-elastic/plastic behavior of many materials. Model validation is also critical, both at the materials and module scales. This capability will be a computational code (model), documented workflow, and a community of practice for industry and academia to characterize environmental thermomechanical loads on PV modules. This model will enrich PV degradation databases to expose the origins and magnitudes of thermal and structural stressors on modules, materials, and materials interfaces. Successful Capability Use: Near term, this capability will establish a viable computational path for solving this complex thermomechanical module-level problem. Longer term, this capability will make the code, workflow, and community of practice available to industry and academia to help better design PV modules and to assess failures of currently-fielded modules.	Scott A. Roberts (SNL)	NL- Sandia National Laboratories	2. Predictive Simulation	Near term, this capability will establish a viable computational path for solving this complex thermo-mechanical module-level problem. Longer term, this capability will make the code, workflow, and community of practice available to industry and academia to help better design PV modules and to assess failures of currently-fielded modules.	

DuraMat Capability 2: Predictive Simulation

Poster Number	Capability Name	Short Paragraph Description of Capability (300 words same as the abstract. Summarize what it does and value to DuraMat and Module Materials)	Capability Expert (principal contact)	Organization Name and Type - (National Laboratory - NL, Academic Institution - AI, Company- C)	Which Capability Area Best Fits This Work (Select One)	Define from an industry perspective what near term 1 year and long term 5 year successful use of the capability would be. (100 words)	Link to Your Website (if available)
12	Process simulators for manufacturing process design, scale-up, and process/material-property understanding	Material quality of module packaging components, such as backsheets, encapsulants, and sealants, is critical in preventing module failure from delamination, degradation, discoloring and related environmental effects. In the efforts to improve module lifetime while reducing costs, manufacturing process effects on material quality (compositional or microstructural variations or defects) must be understood. Process models developed together with experiments designed to validate those models will be offered as a component of DuraMat's Predictive Simulation capability. Process simulators will be assembled/built for deposition/coating, thermal, lamination, and printing processes that are most prone to mechanisms undermining materials and packaging quality. The validated models in some cases exist but otherwise can be built with SNL's SIERRA codes or commercial software COMSOL, and will be aimed at prediction of materials composition and stress state defects. Sandia has a long history of developing and applying manufacturing process models for component encapsulation, welding/printing, coatings, polymer processing, and more. One key benefit that these simulators will provide to all research thrusts is the ability to assess "designs" for manufacturability, and how manufacturing quality can lead to module failure (e.g. stresses on interfaces from manufacturing, compositional heterogeneities from coating defects, etc.) Predictive models require rigorous validation with actual on-line or at-line process metrology that measure resultant material microstructure uniformity, residual stress, and other product quality attributes. NREL and SLAC have unique facilities to gather this data in for precision film coating processes, as does Sandia for printing processes. The capability includes a close integration with these experimental operations.	Randy Schunk (SNL)	NL- Sandia National Laboratories	2. Predictive Simulation	Within the first year, existing process models will be developed or advanced depending on their current maturity and relevance to assist DuraMat industry-led projects with manufacturing emphasis. In the long term, this capability will consist of models and workflows and easy user-interfaces for industry/academic DuraMat partners to deploy to help with design and scale-up of PV manufacturing processes.	
13	STREAMM: Simulation Toolkit for Renewable Energy and Advanced Materials Modeling	A wide range of current energy and materials modeling applications rely on combining simulation methods that cross multiple length and energy scales. For example, to understand both mechanical and electronic properties of a single polymeric material, a multi-step process often is needed, including: (1) performing a large-scale molecular dynamics simulation of hundreds of oligomers comprising hundreds of thousands of atoms; analyzing the structure and dynamics from this simulation; (2) extracting sub-regions from the simulation and computing quantum mechanical properties in these regions; and (3) putting the sub-regions together in some coarse-grained manner (e.g., with an effective Hamiltonian for charge transport) to predict properties of the entire system. Materials discovery efforts would then require the aforementioned steps to be repeated many times for many different materials, but doing all of these steps typically involves significant hands-on effort that makes performing a high throughput multi-scale modeling effort difficult. To remove the intensive "by hand" aspects of running materials simulations across these scales, we have created a set of scripts and programs called Simulation Toolkit for Renewable Energy and Advanced Materials Modeling (STREAMM) to automate steps (1)-(3) based on scripts that produce input and output files for a variety of classical and quantum mechanical systems (e.g., LAMMPS, Gromacs, Gaussian, and NWChem). STREAMM uses an internal "structure container" object to allow facile inter-conversion between data formats and scripts have been written so that the molecular dynamics/quantum mechanics pieces can be done automatically. STREAMM also contains scripts to auto-generate candidate molecules combinatorially that we have used to produce a large (1,000,000+ structure) set of molecules and compute their electronic structure in vacuum. These auto-generation scripts also could be used as the first step to produce materials for a true high-throughput materials discovery effort based on emergent properties of realistic, bulk systems or thin films, ultimately allowing durability-relevant properties to be understood and predicted in silico.	Ross Larsen, National Renewable Energy Laboratory	NL- NREL	2. Predictive Simulation	In the short term, industry will benefit by being able to rely on extensive in-house expertise and domain knowledge to be able rapidly screen industry-relevant materials for interesting and useful properties. Over the longer term success would result in adding tools and methods to the STREAMM functionality to allow the other predictive simulation tools developed within DuraMat to be driven in an automated way to allow high throughput materials discovery based on stability and durability criteria.	http://streamm.nrel.gov
14	Transformative approach to inverse modeling of photovoltaic module failures in solar fields	Packaging materials are critical to the long-term reliability of photovoltaic modules, since premature failures directly increase LCOE. Unfortunately, it is quite challenging to develop new approaches to packaging. Despite the adoption of qualification tests, ultimate validation against many years of field data is generally required for new module designs. Recent work has even identified failure probabilities at the level of individual materials and interfaces. However, this approach is statistical and empirical in nature, and as a result, cannot directly provide reliable extrapolation to new geographies and longer time periods. To address this gap in the literature, we have developed a physics-based framework for assessing the reliability of novel module designs. It consists of two components: a forward and an inverse model. The forward model can use environmental data and thorough knowledge of the underlying materials to faithfully predict the performance and reliability of solar modules. Using real or synthetic environmental data, the forward model can provide a faithful prediction of the environment-specific performance and reliability for a perfectly understood module. In the presence of uncertainty, however, an inverse modeling approach can provide a much more accurate picture of the key degradation components to analyze time-series field data to extract the dominant degradation components. We have shown that synthetic aging time-series module performance data can be reliably deconvolved into its underlying failure components if these components have a non-negligible impact on the performance during the time of data collection. We are now in the process of applying this approach to real field data collected across the world to demonstrate the relative importance of certain failure modes for given photovoltaic modules in various environments, and to predict the energy yield in future time, validate this result against future data collection, and ultimately use this data to inform future module package design.	Muhammad Ashraf Alam, Jai N. Gupta Professor of Electrical & Computer Engineering, Purdue University Peter Bermeel, Assistant Professor of Electrical & Computer Engineering, Purdue University	AI- Purdue University	2. Predictive Simulation	Within one year, this model will be applied to qualification and field installation data from national laboratories, academia, and industry, particularly for crystalline silicon and CIGS modules, to extract key failure mechanisms and predict future power production. Within five years, this model will be extended to other manufacturable technologies (notably, cadmium telluride, as well as emerging technologies gaining significant traction). The results of these studies will be fed back to industry R&D groups through freely available web-enabled tools on nanoHUB.org to help design new modules with emerging materials, and can also be used to inform PV plant installations.	https://nanohub.org/groups/pvhub
15	Predictive Network Modeling For Design of PV Module Materials with Increased Durability, Performance and Lifetime	The ability to accurately model the lifetime and performance of current installed and next generation PV modules is essential for predicting the leveled cost of energy. Generalized network models provide quantitative predictions while serving as the framework for integration of multiple experiments, data types, and study designs. In this scenario nodes of a network represent process, performance and response variables and the edges represent data-driven submodels, which are guided by domain science. This network model has predictive capability in that the individual sub-models are subject to optimization techniques to quantify the multivariate relationships amongst variables and predict the changes to the entire network and system performance. Backpropagation is utilized to predict process variables to describe how to build the material in a guided manner. Network model development encapsulates a big data analytics approach combining data from PV modules exposed to real-world and accelerated, lab-based weathering of components and materials from a diverse set of studies with differing study designs and data types [French, 2015]. Our recent advances in predictive network modeling [Bruckman, 2013] have demonstrated how to accomplish this integration of data and insights to produce system level predictions. A system of equations is developed from these models encompassing degradation pathways which provide a statistical method for prediction of lifetime and performance and can include the cost of materials and components. We now are incorporating graph-theory informed network modeling for larger complex systems such thousands of PV plants spread across diverse Köppen-Geiger climatic zones, to enable more precise understanding of the stressors PV plants actually spend their lifetime under.	Prof. Laura S. Bruckman	AI- Case Western Reserve University	2. Predictive Simulation	1 Year: Harness the broad experiments and simulations done by PV research community, so the aggregated research, captured in predictive network models, helps guide development of DuraMat materials. 5 years: Broad use data science methods, such as machine learning and predictive network modeling, to aggregate and integrate DuraMat research results into common systems-level models of PV modules exposed to real-world conditions and lab-based accelerated exposures.	http://sdle.case.edu
16	High-fidelity simulations of diffusion induced aging of PV modules	According to the Report IEA-PVPS T13-01:2014, CdTe modules undergo an initial 4-7% degradation over the first 1-3 years and a 0.5-0.7%/year degradation thereafter. While this has been attributed to the grain boundary diffusion of copper from the back contact, progress to reduce this degradation has been slow due to the long cycle of aging experiments. Current accelerated aging tests rely on the use of elevated temperatures and cell bias, which necessarily activate different degradation mechanisms. Sandia's unique capabilities may enable this problem to be solved through advanced computations. First, we have large scale atomistic simulation methods that approach the accuracy of quantum mechanical calculations [PRB, 85, 115206, 2012; PRB, 86, 245203, 2012; J. Phys. Chem. C, J. Mater. Sci., 50, 2859, 2015]. Second, Sandia, our new algorithms have overcome the time scale of atomistic simulations and at the same time accounts for the statistics of atom diffusion on all lattice sites [J. Phys. Chem. C, 120, 7500, 2016]. When leveraged with Sandia's computing power, we can study not only copper diffusion on all possibly encountered grain boundaries, but also grain boundary evolution under the thermal and mechanical cycles. As a result, these computational studies can be used to design new chemistry and to engineer new grain boundaries that minimize diffusion and therefore extend lifetimes. They can also be used to derive relations that connects experimental aging data obtained under accelerated conditions to real conditions, which will impact a variety of current efforts to improve PV modules.	Xiaowang Zhou xzhou@sandia.gov	NL- Sandia National Laboratories	2. Predictive Simulation	In the near term, this project will answer the question as how diffusion impact properties of PV modules as a function of time, how PV properties measured from accelerated aging experiments can be accurately converted to those under the operating conditions, and how materials' chemistry and microstructure can be engineered to improve durability. Between 1 and 5 years, the capability will be made available to improve durability of CdTe PV modules. In five years, this tool will be made available to other PV modules.	

DuraMat Capability 2: Predictive Simulation

Poster Number	Capability Name	Short Paragraph Description of Capability (300 words same as the abstract. Summarize what it does and value to DuraMat and Module Materials)	Capability Expert (principal contact)	Organization Name and Type - (National Laboratory - NL, Academic Institution - AI, Company- C)	Which Capability Area Best Fits This Work (Select One)	Define from an industry perspective what near term 1 year and long term 5 year successful use of the capability would be. (100 words)	Link to Your Website (if available)
17	Predictive modeling and testing of the long-term performance of building integrated photovoltaic (BIPV) systems	<p>The Sustainable Engineering & Materials Laboratory in the Carleton Laboratory of Columbia University has developed research capabilities to characterize, simulate and analyze the long-term performance of solar panels at macro-, micro-, and nano- scales through interdisciplinary research methods covering mechanics, materials, structures, green technologies, and accelerated testing. The following three ongoing research thrusts contribute to our goal for durable BIPV systems:</p> <ol style="list-style-type: none"> 1. Fracture and delamination of solar panels: As a multilayered structure, solar panels are generally made of brittle PV laminated with glass and substrate. We have developed fracture model to study the opening-mode fractures, block cracks, and delamination, which can be caused by the mechanical and environmental loading. The elastic, elastoplastic, and viscoelastic behavior of the silicon materials, encapsulant, and back-sheet can be considered in multiple time scales and loading cycles, respectively. 2. Accelerated testing and modeling for lifetime prediction and extension: To understand the life-cycle performance of a solar panel, reliable accelerated testing methods and models are necessary. We have designed and developed a multifunctional environmental chamber to reproduce various service environments, provide accelerated aging stresses, and measure energy and mass flow in the system. Fundamental research is conducted to discover the similarity of material behavior at different time scales under different loading levels and environments, so that we can predict the long-term behavior by short-term tests. 3. Environmental impacts of solar panels: Thin-film PV cells are commonly made of toxic heavy metal compounds, e.g., cadmium telluride (CdTe) and gallium arsenide (GaAs). Both cadmium and arsenic are well known carcinogens. Solar panels often use ethylene vinyl acetate (EVA) to encapsulate thin film, which is degradable under UV exposure. We can model and measure the metal pollutant levels in leachate with our environmental chamber. In sum, we have developed an effective research approach to characterization and prediction of the long-term performance of BIPV systems. 	Huiming Yin	AI- Columbia University	2. Predictive Simulation	In the near term of 1 year, through collaboration with industry engineers and NREL researchers, we can apply our mechanical models to fracture modeling and prevention in solar panel manufacture and installation and develop standard test methods for quality assurance. In the long term 5 years, we will establish accelerated testing and modeling methods for life-cycle analysis of emerging solar panels and investigate the long-term performance of the 2nd and 3rd generation PV panels, including both the mechanical failure and environmental impacts.	http://www.columbia.edu/cu/civileng/yin/
18	Experiments and Simulations for the Development of Durable Interconnect and Encapsulant Materials for Photovoltaic Systems	<p>Failure mechanisms such as cracking and corrosion in metal solder interconnects and delamination of packaging materials lead to both module degradation and shortened lifetimes of photovoltaic systems. At present, qualification tests by IEC standards involve the use of stress tests such as thermal cycling (TC) and damp heat exposure (DH) which are intended to accelerate and mimic long-term field-use performance. However, such test conditions may not accurately stress modules in the same manner as seen in the field. Thus the current industrial practice of accelerated tests lack physics-based underpinnings to mimic field-use performance and failure modes, and such tests are time-consuming and cost-ineffective.</p> <p>Georgia Institute of Technology has done extensive work in understanding and predicting the cracking failures of metallic interconnects as well as interfacial debonding of polymer materials. Through accelerated stress testing, crack propagation in solder interconnects has been studied and correlated with physics-based simulations. Similarly, the propagation of crack in polymer/metal and polymer/glass has been studied through experiments and simulations. Such experiments and simulations provide design guidelines into how the geometry, material, and process parameters can be modified to enhance the overall system reliability. The work will also provide insight into the correlations between accelerated testing and field performance.</p>	Prof. Suresh Sitaraman, suresh.sitaraman@me.gatech.edu; Dr. Scott Grutzik sjgrutz@sandia.gov	AI - Georgia Institute of Technology NL- Sandia National Laboratories	2. Predictive Simulation 4. Module Prototyping and Accelerated Durability Testing	In the near term, the models will help identify key material, geometry, and process parameters that lead to performance degradation of PV modules. In the long term, the models and experiments will provide guidelines to select material, geometry, and process parameters that will result in PV modules with enhanced reliability and reduced degradation in operational efficiency.	
19	Predictive Brittle and Interfacial Failure in PV Modules	<p>Sandia National Laboratories has a history of success in modeling stress and failure in systems involving brittle materials. A system of particular interest to Sandia involves a metal pin concentric in a metal cylindrical shell with glass filling the space between. Although the geometry is very different, the material response and failure modes seen in this system are directly applicable to a photovoltaic (PV) device (e.g. tempered glass - polymer interface). Sandia's BritMAP program is a collection of current efforts devoted to exactly this set of problems dealing with lifetime prediction and reliability of brittle materials. Because of the brittle glass and silicon materials and many interfaces, a fracture mechanics and interfacial fracture mechanics based lifetime prediction will be needed. Such an analysis would involve prediction of both initiation and growth of cracks and interfacial flaws in a PV cell module. Correctly modeling crack growth is important because even if a crack is present a PV cell may be operational for some time depending on where and how quickly the crack propagates. A PV system with a design lifetime of 30 or more years will experience many cycles of thermomechanical loading and phenomena such as creep, fatigue, and failure at interfaces will play a major role in predicting component failure. Sandia has proven success in viscoelastic modeling of glass and other brittle materials and mode dependent failure at interfaces. By applying this expertise to a model of a representative set of PV modules subject to the heat faults seen in field tests we anticipate success in predicting mechanical failure modes and providing a statistical estimate of operational lifetime.</p>	Scott Grutzik (Sandia)	NL- Sandia National Laboratories	2. Predictive Simulation	The short term (1 year) deliverable of this project would be the ability to determine whether a given mechanical flaw will remain the same or get worse under normal operating conditions. The long term (5 year) deliverable would be the ability to provide a statistical estimate of lifetime given a description of PV module structure and operating conditions.	