DuraMat Capability 3:
High-Throughput Materials Discovery and Forensics

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)
20	DuraMat Capability 3: High-throughput materials discovery and forensics	This capability will develop new functional materials for PV modules and establish methods for forensic materials characterization to provide empirical information for module failures and degradation mechanisms. This capability will use Materials Genome Initiative (MGI)-based tools including: high throughput computational materials design, combinatorial synthesis and fabrication, high-throughput materials characterization and forensics, advanced manufacturing for rapid prototyping of materials and new processes, and new operando tools for forensics during accelerated environmental stress tests. To guide and inform module materials design and discovery, these capabilities will interface with Data Analytics and Predictive Simulation. In addition, module prototyping and Field Deployment will help guide and interact through the accelerated stress testing development and their application to existing and developed materials. For advanced manufacturing, the capability will be informed by Predictive Simulation, to guide the process development, and will interface with Data Analytics for management of large data sets. Additionally, the capability will provide empirical tests of the Predictive Simulation capability materials and processes predictions through characterization and screening of materials using the capabilities' forensics tools and the operando accelerated testing facilities. This will be used in a feedback loop to improve the accuracy of the Predictive Simulation capability tools. In terms of high throughput materials design and discovery, we will work to define design rules for new functional module materials and develop in-situ and inline characterization tools for rapid validation, testing and prototyping. For characterization of materials properties against design, the capabilities will provide an understanding of the physics and chemistry of failure, and validate failure and performance analysis in MGI based materials design. A new forensic testing system - operando characterization for accelerated materials validation - will be designed allowing for environmental control (including atmosphere, humidity, temperature, light, electric field bias, mechanical loads) during module characterization.	Mike Toney, mftoney@slac.stanford.edu	NL- SLAC National Accelerator Laboratory	3. High-throughput Materials Discovery and Forensics	(1 year) Create and develop the MGI feedback loop between synthesis, characterization, modeling, prototyping, and deployment for PV module materials. This capability will be the first demonstration of the MGI methodology in applied PV module research. (5 year) Enable fundamental understanding of the physics and chemistry of materials degradation across mechanical, chemical and other stressors simultaneously. This will create the ability to rapidly screen of new materials and processes for quick assessment of new technologies in collaboration with industry, extensive data analytics, deployment, and technology to market efforts.	http://www-ssrl.slac.stanford.edu/toneygroup/duramat
21	High-Throughput Experimental (HTE) combinatorial capabilities to development of inorganic materials for durable modules	The High-Throughput Experimental (HTE) Capabilities be suitable for development of new inorganic materials that would increase durability of photovoltaic modules (Capability 5). In general the HTE combinatorial capabilities consist of combinatorial synthesis, spatially-resolved characterization, and semi-automated data analysis. The current combinatorial synthesis capabilities feature multi-element thin film deposition chambers with intentional and well-controlled composition-, and temperature gradients using sputtering. The existing spatially-resolved characterization techniques include chemical composition (XRF), crystallographic structure (XRD), microstructure (AFM), surface properties (PES, KP), electrical transport (4-point probe), optical properties (transmittance/reflectance), all as a function of position on the thin film, and hence as a function of the graded composition or temperature. The data analysis tools include custom-written processing and visualization routines for user-assisted data analysis, and data warehouse connections and project-specific databases The HTE combinatorial capabilities established at NREL for semiconductors, are proposed here to be extended to handle metals (e.g. electrical connections such as solder bonds) and insulators (e.g. multifunctional coatings for anti-soiling, antireflection etc).	Andriy Zakutayev	NL- NREL	3. High-throughput Materials Discovery and Forensics	In 1 year, demonstrate that the HTE combinatorial capabilities established for semiconductors can be extended to handle metals (e.g. electrical connections such as solder bonds) and insulators (e.g. multifunctional coatings for anti-soiling, antireflection etc). In 5 years, discover new durable module materials using HTE combinatorial approach, and scale up the discovery to large coating area or bulk metallic material	http://www.nrel.gov/materials-science/materials-discovery.html
22	Multi-scale investigations of solder bond failures	According to the module field failure literature, interconnects failures are the third most common module failure mechanism after discoloration and back sheet/EVA delamination. Solder bonds can fail due to stresses induced by thermal cycling or vibration during the long life cycle of modules. Early modules typically only had 1 solder bond per interconnect per cell. Hence, failure of this solder bond resulted in an open circuit failure of the whole module. Even today, non-cell solder bonds often have little or no redundancy so failure of one of these bonds can lead to drop out of a cell string, a whole module or even a whole string of modules. Further, the transition from lead-containing to lead-free solder and electrically conductive adhesives in modules could exacerbate the problem, as the adhesion characteristics of these new materials are less well understood. Thermomechanical fatigue in ideal cases may be modeled, however, grain coarsening associated with aging, the formation of intermetallics, corrosion, delamination, and the stress states particular to all aspects of the PV module including the bus interconnects and junction box must be considered as well to ensure durability. We propose to investigate the metallurgical, chemical, adhesive and electrical properties of solder bonds using a multi-scale approach that spans the length scale from millimeters to sub-nanometer. This approach will be based on an NREL-developed suite of AFM-, SEM- and TEM-based techniques that have been successfully applied to Si and thin film modules. This multi-scale approach is being further refined in a currently funded reliability project entitled "From Modules to Atoms: Increasing Reliability/Stability of Commercially Relevant PV", where the focus is module power loss mechansism such as potential-induced degradation.	Mowafak Al-Jassim	NL- NREL	3. High-throughput Materials Discovery and Forensics	In year one, we will demonstrated the materials and failure analysis techniques that show the nature of metallurgical, chemical, and adhesive properties of the solder bond as it degrades in accelerated stress testing and in the field. In year five, best practices for materials selection and formation of electrical interconnects with solder and electrically conductive adhesive bonds for PV modules based on the understanding of the observed degradation mechanisms and material interactions will be shown such that the confidence in the performance and reliability of PV systems will be greater.	http://www.nrel.gov/pv/measurements/about_mc.html
23	Materials Characterization at Sandia	The Materials Center at Sandia National Laboratories draws from extensive experience in assessing aging and reliability relevant to the nuclear weapons stockpile. This core capability spans expertise in accelerated aging and testing to manufacturing troubleshooting to root-cause failure analysis. In DuraMat, fundamental analysis with advanced characterization tools will be critical for developing new materials and for forensic investigations of degraded modules. At hand are comprehensive surface science facilities including photoemission spectroscopy, Auger, AFM, profilometry, and SIMS. Surface analysis allows for characterization of the entire periodic table at nanometer scale depth resolution. Several aging-specific capabilities have been developed that are directly applicable to the DuraMat mission and MGI development, including in situ thermal treatments and depositions. Depth profiling can be performed to evaluate buried layers and interfaces revealing information on diffusion, corrosion, or potential-induced degradation. A newly installed XPS is uniquely equipped with a gas cluster ion source for depth profiling organic materials, potentially relevant to understanding delamination or polymer degradation. The instrument also has IPES and UPS for examining electronic state information, as well as several X-ray sources for interrogating different depths in the near surface. Ambient pressure XRF for examining large area modules, interconnects, and solder has also recently been installed. Electron microscopy capabilities include several SEMs, FIB-SEMs, and WDS microprobe. SNL has state-of-the-art AC-STEM (with 0.8 Å resolution) and multi-STEM (for large area (~cm) imaging at nanoscale resolution). Electron microscopy can be used to assess structural changes in module materials, at interfaces, and at grain boundaries. Extensive X-ray diffraction, Raman, IR, ICP, and other capabilities add to the comprehensive capabilities in the Materials program. A unique core competency at SNL is the co-location of numerous advanced instruments coupled with a breadth of materials characterization experience and a culture of awareness for aging-related reliability.	Michael Brumbach	NL- Sandia National Laboratories	3. High-throughput Materials Discovery and Forensics	Near term: • Analysis of interfacial dynamics of new materials and how they age in relevant environments • In situ thermal treatments while imaging to determine effect on new module materials from coatings to interconnects • Depth profiling to evaluate buried layers and interfaces revealing information on diffusion, corrosion, or potential-induced degradation. • Large area multi STEM and critical high resolution SC-STEM could be used to assess structural changes in materials, at interfaces, and at grain boundaries. Long term: • Combine relevant advanced analytical techniques with module prototyping to validate new module materials. • Use analytical forensics and predictive simulation to influence new module materials.	
24	Bottom Up Synthesis of Energy Materials for Digital Direct Write and Roll to Roll Printing at the Advanced Materials Laboratory	TTo overcome thermal and electrical materials issues that affect PV reliability requires an integrated understanding of component fabrication, from materials development to printing/processing using relevant manufacturing modalities. The Advanced Materials Laboratory (AML) provides expertise in synthesis of nano-colloids and printing inks to develop interfacial coatings and bulk materials with tailored properties (thermal, electrical, and optical). We are an integrated laboratory comprising synthetic chemistry (molecular precursors, nanomaterials, etc.), colloidal-dispersion/ink development and materials coating and printing. Our digital printing capability consists of a suite of direct write and coating deposition platforms including an ultra-high resolution 3D laser printer (Nanoscribe), a multi-layer registration gravure/flexo printer (GT+W), roll-to-roll based test machines (RK meter bar, gravure systems) and a model-based discovery and design capability. Importantly, our R2R-scalable micro-gravure printing and coating capabilities moves from an R&D scale to small lot production while maintaining fine feature control. Robotic controlled dip-coating facilities (SNL), expertise in Layer-by-Layer and solution deposition (spray, casting, or related) rounds out our abilities to specifically address needs in the arena of printed module materials including electrical contacts, encapsulants, sealants, backsheets, optical materials and scratch-resistant surfaces. Coupons of these printed components and tailor made polymer composites can be evaluated at Sandia's Photovotaics System Evaluation Laboratory.	Bernadette A. Hernandez-Sanchez	NL- Sandia National Laboratories	3. High-throughput Materials Discovery and Forensics	Near term: • Formulation of new printing inks with tailored thermal and electrical properties; and optimization using combinatorial techniques • With materials predictive simulation at SNL, target new colloids and dispersion chemistries • With SNL's extensive Materials Characterization Capability, optimize ink-interface interactions at relevant conditions Long term: • Mature developed inks from R&D scale to lot production and ensure compatibility with relevant industrial printing and coating capabilities • With module prototyping capabilities at SNL, test material coupons in accelerated and actual conditions	

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25	Advanced Manufacturing and Prototyping for understanding of the processing-structure-property relationship	Properties of module packaging components, such as backsheets, encapsulants, and sealants, are critical in preventing module failure caused by delamination, degradation of absorbers and discoloring of light path materials. In the efforts of reducing module manufacturing cost while trying to improve module lifetime, property control under high-throughput processing will be key challenge. This is true in order to expand the lifetime of the c-Si solar cells to beyond 30 years; it is even unambiguous for thin film based modules that can be roll to roll processed for greatly reduced cost. Being able to understand the processing-structure-property relationship for these materials is fundamental in order to achieve the property that outperforms the state-of-the-art. In this work, we will combine efforts in printing from SLAC, Sandia, and NREL to develop a greater understanding of the processing-structure-property relationship in both existing module materials as well as new materials. SLAC has previously demonstrated in-situ x-ray scattering capability combined with roll-to-roll solution printing processing for thin film materials. For DuraMat this platform will be expanded to module packaging components, such as, but not limited to, backsheets, encapsulants, and sealants. The material’s structural evolution during film formation and solution drying can be monitored in real time. This versatile platform at SLAC could incorporate either flexible (plastic or glass substrate) or rigid flat substrates (for enhanced signal-noise ratio). Sandia and NREL have also both been leaders in developing coating and printing processes for PV development and will partner in this effort. Work at Sandia’s AML laboratory also focuses on developing new materials for printing and coating processes, and accelerates process development with high-fidelity process simulations. Additionally, NREL has excelled in developing in-line metrology for greater understanding of printing processes. Together this team will provide DuraMat and the PV industry with a platform for rapidly prototyping new processing methods as well as rapid validation of new printable materials.	Hongping Yan, Hyan@slac.stanford.edu, Laura Schelhas Schelhas@slac.stanford.edu, Bryan Kaehr bjkaehr@sandia.gov, Maikel van Hest Maikel.van.Hest@nrel.gov	NL- SLAC National Accelerator Laboratory Sandia National Laboratory - NL, National Renewable Energy Laboratory - NL	3. High-throughput Materials Discovery and Forensics	(1 year) Within the first year the team will work together to define a process challenge with the guidance of industry. The team with modify and update any current capabilities to meet these challenges. (5 year) This capability team will provide rapid validation, testing, and prototyping of new processing protocols and new functional materials. (5 year) More widespread adoption of RTP in module manufacturing to drive down cost.	http://www-ssrl.slac.stanford.edu/toneygroup/duramat
26	In situ rapid thermal processing / X-ray diffraction for materials forensics	Rapid thermal processing (RTP) is widely used for processing a variety of materials, including photovoltaics and electronics. Optimization of RTP is often done based on ex-situ studies. As a consequence, the precise reaction pathways and phase progression during the RTP remain unclear. More awareness of the reaction pathways would better enable process optimization and foster increased adoption of RTP, which offers numerous advantages for materials production. To achieve this, we have designed and developed an RTP instrument that enables real-time collection of X-ray diffraction data with intervals as short as 100 ms, and while heating at ramp rates as high 100 ºC/s up to 1200 ºC. The system is portable and can be installed on a synchrotron beamline for X-ray diffraction. The unique capabilities of this instrument are demonstrated with in-situ characterization of the Ag-Si contact formation process during firing or heating with ramp rates 5^0Cs-1 and 100^0Cs-1, revealing numerous phase changes. Direct observation of etching by lead- and silver-oxide during firing using in-situ XRD reveals the contacting sequence. A series of studies have been done on a silver, frit, silicon, and silicon-nitride model systems resulting in the clear elucidation of the reaction pathways that enable screen-printed contact formation. Silver dissolution into the glass frit – a key for obtaining low contact resistance – shows strong oxygen-dependence. Ultimately, understanding the temperature thresholds for each of these competing mechanisms accurately clarifies the nature of screen-printed, fast-fired contacts.	Mike Toney, mftoney@slac.stanford.edu	NL- SLAC National Accelerator Laboratory	3. High-throughput Materials Discovery and Forensics	(1 year) Ability to rapidly test and screen new materials for front and back contacts in Si cells. (5 year) More widespread adoption of RTP in module manufacturing to drive down cost.	http://www-ssrl.slac.stanford.edu/toneygroup/duramat
27	Operando characterization for accelerated materials validation	for DuraMat. Here we will develop collaboration between NREL’s reliability and systems engineering group and SLAC to develop a greater understanding of the degradation mechanisms in module materials that can lead to loss in efficiency and module failure. These teams, with input from industry, will work together to identify, design, and ultimately down select the relevant experimental parameters to investigate. This collaboration will closely link NREL’s experience and guidance with accelerated testing with SLAC’s beamline capability development. SLAC will develop in-situ and operand,o forensic capabilities to study the structural and microstructural (3-dimensional) changes for both long and short term effects. A new forensic testing system will be designed allowing for environmental control (including atmosphere, humidity, temperature, light, electric field bias, mechanical loads) during module characterization. For example, such as the change that occurs with repeated thermal cycling through the glass-transition of encapsulant materials and the evolution of materials during a life time of aging. To demonstrate this capability EVA will be used. To achieve this, an initial survey of EVA samples that are currently available at NREL will be characterized by SLAC. There already exists a breadth of knowledge about EVA; therefore, starting with a known system will help refine our approach that can then be applied to newer materials. This capability will allow for correlation to be made between module degradation and structural changes to encapsulant materials, providing a route to lower degradation rates and higher end-of-life efficiency. Once developed, this capability will be quickly available to encapsulant materials suppliers (such as DuPont, 3M) for rapid assessment of new materials degradation. Finally, the in-situ and operando forensics system that we build will serve as a model for similar capabilities for a host of other module components. This capability will also be used for validation of models developed in the predictive simulation capability group.	Laura Schelhas, schelhas@slac.stanford.edu, Mike Toney, mftoney@slac.stanford.edu	NL- SLAC National Accelerator Laboratory	3. High-throughput Materials Discovery and Forensics	(1 year) Complete design and build of the operando capability and demonstrate operando characterization of one new and one established PV material under at least two stresses. (5 year) The long term value of the operando capability will provide validation of failure mechanisms modelled within DuraMat. Additionally, this capability will generate structural forensic characterization to develop design rules for new materials discovery.	http://www-ssrl.slac.stanford.edu/toneygroup/duramat
28	Multiscale Characterization of Advanced Metallization for Microcrack Reduction	During the process of laminating a module, high enough temperature is applied to melt and cure the encapsulant– cross-link in the case of EVA, in conjunction with high pressure to remove trapped air bubbles. The encapsulant’s solidification usually comes with a degree of shrinkage, which directly translates on stress on the solar cells. This effect combined with the soldering of bus bars, which have thicknesses of a few hundred micrometers could cause serious local deflection. The concentration of stress is known to promote the formation of microcracks and this in combination with real operating conditions inevitably leads to crack propagation. Smart wire technology has been proposed to reduce this type of failure and the recent development at ASU of a metallization technology with a low profile and compatible with solderless contacts can pave the way to significant reductions in crack formation. We propose here a multi characterization approach to evaluate the effect that different encapsulants and module aging have on contact resistance and crack formation for two types of metallization processes (1) Standard screen printed metallization with soldered tabs and (2) 3D Printed Metallization with solderless tabs. The novel approach relies on correlating the stress that the cells see under encapsulation and its evolution with the microstructural changes of the metallization. This will be achieved using stress field measurement methods available at ASU and operando and in-situ structural measurements at SLAC. Aging profiles will be applied as a variety of stressors including thermal, mechanical, and atmospheric (humidity, gas, etc.) loads. This methodology will create a comprehensive library correlating Materials (Encapsulates, metallization) – Properties (stress, microstructure, microdefects) – Performance (module output) that will help optimize the module stack with the ultimate goal of minimizing microcracks and mechanical stress. This framework and results will be readily available to industry to evaluate new materials and processes for use with solderless flexible contacts.	Mariana Bertoni Mariana.bertoni@asu.edu and Laura Schelhas schelhas@slac.stanford.edu	AI- Arizona State University NL- SLAC National Accelerator Laboratory	3. High-throughput Materials Discovery and Forensics	(1 year) Optimization of encapsulation processes using ASU metallization methods to minimize stress in the module. Use of this methodology will ultimately minimize microcracks and lower stress within modules. (5 year) Long term this work will provide a route for industry to vet new encapsulation methods and materials with solderless contacts. The flexible of these contacts could also lead to development of more flexible modules.	https://defectlab.engineering.asu.edu/ , http://www-ssrl.slac.stanford.edu/toneygroup/duramat
29	X-ray Diffraction Imaging for Crystalline PV Modules	X-ray diffraction imaging or topography, an over 50 year old technique, provides a fast non destructive method not only to detect a crack of a PV cell within the module package but also to visualize details of the crack environment including material defects such as grain boundaries, contacts, Ag fingers, and other cell features, the crack structure with its relaxed surfaces and its origin, and most importantly the distortion of the cell yielding to the strain and stress. This distortion is the cause that drives many degradation processes. A specific example is the characterization of the mechanical properties of the glass-EVA-cell compound using in-situ bending tests combined with Finite Element Analysis (FEA). Synchrotron facilities provide a unique resource of instrumentation and X-ray experts to the research community. Our collaboration, combining about 10 experts in the field of PV characterization, X-ray topography, instrumentation and data analysis development, will provide easy access not only to the tool but also to the analyzed data for the members of the DuraMAT consortium and their partners. The experiments will be performed at the ISS beamline at NSLS-II, a high flux, wide energy beamline, which is optimized for fast energy scans over a wide energy range. Using a unique low divergence large beam mode we will be able to provide about 3000 wafer measurements with a resolution of 5-10 □ This estimation assumes that a dedicated setup will be build allowing the characterization of full PV-panels. The currently existing system can only handle single cell test modules. The existing access modes allow long term projects with multiple visits per year as well as a rapid access mode providing a fast response to urgent research needs and industrial partners. Our tool will help to rationally optimize processing parameters by displaying the mechanical properties of the compound and the cell while using new materials and new processing methods. It will also display the degradation effects of the compound by building on the non-destructive nature of the probe allowing repeated measurements on the same sample during the aging process.	Alessandra Colli	NL- Brookhaven National Laboratory	3. High-throughput Materials Discovery and Forensics	Near term use (1 year): Capability to scan a full commercial module at the ISS beamline at BNL-NSLS II, with high throughput data analysis capabilities. Long term use (5 years): Providing high throughput services for research and industrial partners and developing FEA models for specific compund (module structures). Development of in-line tools in collaboration with industry to support a better module quality at manufacturing level and improved reliability in time.	Reference paper: http://ieeexplore.ieee.org/document/7513426/
30	Bi-functional anti-reflective and anti-soiling coating	To address the DuraMat’s mission of accelerating the development and deployment of new, high performance materials for photovoltaic modules to lower the cost of electricity generated while increasing field lifetime, there is an increasing need in developing bi-functional inorganic anti-reflective and anti-soiling coating that can lower the cost of electricity generation through the improvement in energy conversion efficiency and the reduction of maintenance costs. While the current state-of-the-art coatings are largely based on organic molecules and the lifetime of these coatings is strictly limited due mainly to the UV radiation, inorganic coatings offer both lifetime and simplicity advantages. However, there are key challenges in engineering these inorganic nanoparticles, particularly in controlling nanoparticle size and distribution, as well as the composition uniformity. Idaho National Laboratory (INL) has expertise and capability in nanomaterial engineering and coating through the strategic hiring of industrial experts and the Laboratory Directed Research and Development (LDRD) investment. INL capability experts also have experience and knowledge in manufacturing nanoparticles at industrial scale. We will apply combinatorial high-throughput methodology in the development of the bi-functional inorganic costings. Our combinatorial high-throughput capability has been demonstrated by the discovery of oxygen reduction catalysts for fuel cells, hydro-carbon reforming catalysts for hydrogen production, and conjugated co-polymers for organic photovoltaics.	Ting He ting.he@inl.gov 208-526-1165	NL- Idaho National Laboratory	3. High-throughput Materials Discovery and Forensics	The near term goal is to demonstrate that bi-functional anti-reflective and anti-soiling coatings can be developed and applied for solar modules to improve the conversion efficiency and reduce the maintenance effort. The long term goal is to economically manufacture and coat the coatings in a roll-to-roll process.	https://bios.inl.gov/Lists/Researcher/DisplayOverrideForm.aspx?ID=255&ContentTypeId=0x0100DB1D67D981610A45BA27930D30FED203

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31	Design and development of enhanced light capture in solar modules	Our key expertise is the design and development of solar architectures for enhanced light collection and light-trapping. This is an area we have extensively demonstrated for thin film solar cells, and can be fruitfully utilized for enhancing PV modules. Design simulations utilize our rigorous scattering matrix method. We have the capability to design/fabricate advanced multilayered optical coatings for anti-reflection and infrared rejection, that can cool modules and improve reliability. We can measure infrared rejection with local FTIR spectrometers. We aim to design and develop shaped interconnect lines and metal vias on the module that collect light through oblique reflectance and reduce shadowing, increasing module performance. We can design and fabricate diffracting solar architectures that trap near-IR photons in solar modules. The frame of solar modules in an inactive area, and we have the capability to design/develop novel architectures that increase peripheral light capture, and increase efficiency. Our preliminary measurements found a substantial photo-current gain (>20%) for peripheral light capture. We can design modules to generate enhanced infrared emission, cooling the module and improving reliability. A large portion of the solar spectrum (beyond 1100 nm) is not collected in Si-modules. An attractive scheme to harnessing the IR portion is to utilize up-conversion nanoparticles. We have the capability to design and fabricate structures that can focus light within the module, on nanoparticles that can up-convert infrared to visible light. Our local collaborator (A. Mudring) has capability for fabrication of rare-earth nanocrystals, that can be incorporated into modules. Module improvements can be best combined with industrial partners and measurements at NREL's outdoor test facility. We have capability to measure accelerated light soaking effects. Our capabilities build on our DOE-supported Photonics research that has designed, developed and synthesized unique photonic structures for energy conversion.	Rana Biswas (biswasr@iastate.edu; biswasr@ameslab.gov)	NL- Ames Laboratory	3. High-throughput Materials Discovery and Forensics	Near Term: Demonstration of module designs that enhance light capture. Long term: Development and fabrication of commercial solar modules with increased performance from enhanced light collection. Development of modules that can operate cooler –increasing reliability.	https://www.ameslab.gov/users/biswasr ; https://www.ameslab.gov/dmse/fwp/photonic-systems http://www.mrc.iastate.edu/NewStaff/RanaBiswas.htm
32	Defect Laboratory	Characterization and modeling capabilities to evaluate the 2D stress distribution and levels seen by the solar cells after encapsulation. The lab has the capabilities and expertise to evaluate and produce unusual encapsulations, e.g. curved surfaces, multiple layers of encapsulants, filters and substrates. We can perform unconventional mechanical testing as a function of ilumination and electric fields.	Mariana Bertoni	AI- Arizona State University	3. High-throughput Materials Discovery and Forensics	We can evaluate the impact that metallization, soldering, glass, encapsulants and backsheet material have on the stress distribution across the solar cells and link them to performance.	http://defectlab.engineering.asu.edu/
33	Module-level Power electronics durability and lifetime testing	MLPE, such as microinverters (MI), DC power optimizers (DCO) and newly emerging module-embedded electronics , are power electronic devices integrated or attached with the module so that there is one power-conditioning unit per module. This sort of power handling topology offers numerous advantages on the system level such as reduced power handling of components, partial shading gains, and piecemeal failure of the array via distributed architectures. Similarly to PV modules, MLPE will be exposed to operation in a variety of environmental conditions, as well as exposed to wide diurnal temperature variations. Offering a 25-year warranty for a power-handling device in a cost-competitive environment is challenging. Consequently, durability and lifetime of MLPE components is of significant importance to the overall durability and lifetime of PV modules. This work will concentrate on materials-based analysis of understanding specific failure mechanisms which are already present in MLPE devices, and how those failure mechanisms do (or do not) propagate and exhibit in fielded units under real operating conditions. Furthermore, we will work with our consortia and industry partners to analyze, predict and offer solutions to future module-embedded electronics durability. As emerging solutions develop, we anticipate that more and more of electronic functions will be merging into PV module, therefore this aspect of durability will start playing more and more important part of the PV module durability and lifetime projections. This capability focuses on (1) reliability/durability of module-level power electronics, and (2) reliability/durability of connectors, solder and other electrical bonds.	Lavrova, Olga <olavrov@sandia.gov>	NL- Sandia National Laboratories	3. High-throughput Materials Discovery and Forensics	First year work will zoom in onto specific material-related failure modes of the construction stack of the PV module electronics. This analysis will identify parts most susceptible to the thermal cycling stresses present in field-usage environments. The at-risk parts and their subsequent materials stack will be used to develop a predictive simulation of the solder joints in the MLPE via the Sandia-developed solder joint simulation tool, TurboSip v2.0. This modelling tool utilizes constitutive relationships of the specific materials stack present to accurately determine stress conditions and predict failure much more accurately than a generic cumulative damage model, such as Coffin-Manson. Later work (five year), as emerging solutions develop, will focus on electronic functions merging into PV module, which will start playing more and more important part of the PV module durability and lifetime projections.	
34	New magnetic and dielectric materials for compact and reliable micro-inverters	Power density and reliability of photovoltaic (PV) micro-inverters will be significantly increased through the use of newly developed magnetic and dielectric materials in passive components (capacitors, inductors, and transformers). Iron nitride, specifically □’- Sandia Labs for the first time ever, has a saturation polarization (Js) almost 4 times greater than soft magnetic ferrites. This translates to a power density 16X greater than ferrites in transformer and inductors. Additionally, the enhanced Js of current spikes and high ripple current. Inductor fabrication using spark plasma sintering (SPS) has already demonstrated the net-shaping of devices, converting raw powders into fully dense parts in only three minutes. This will ensure that component prices are kept low. Complementary developments in high reliability and high temperature compositions of ceramic dielectrics will enable affordable high energy density multilayer ceramic capacitors (MLCCs). Ceramic capacitors will eliminate the slow switching speeds and questionable reliability associated with electrolytic capacitors while achieving higher power densities. Sandia's expertise in power electronics, packaging, and wide bandgap (WBG) semiconductors will be leveraged in implementing these enhanced passive components in compact topologies capable of operating for lifetimes of 50+ years. Sandia National Laboratories is a multi-mission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.	Todd C. Monson, Harlan Brown-Shaklee, Jack Flicker, Olga Lavrova	NL- Sandia National Laboratories	3. High-throughput Materials Discovery and Forensics	1 year: Improved micro-inverter design and components 5 year: Micro-inverters the size of a quarter constructed with revolutionary components	
35	Multi-beam SEM for High Throughput Imaging of Materials	Multi-SEM (mSEM) represents a new imaging paradigm. No longer will we have to search for the significant features or ideal areas. High-throughput imaging will allow the true statistics of the sample to be determined over large areas while maintaining excellent resolution. With this instrument, 61 focused electron beams are focused on a surface at a resolution of 4 nm and images are collected in parallel (1.22 GPixels/s). This instrument has been used to image relatively large surface areas, and search for needle-in-a-haystack irregularities or specific areas of interest. In addition, now statistics for each sample can be reliably calculated. This technique could be ideal for investigating structural surface changes of coatings on panels or on interconnects over time using comparative techniques. The mSEM instrument at SNL represents a unique imaging capability, one of only 3 in the world.	Joe Michael	NL- Sandia National Laboratories	3. High-throughput Materials Discovery and Forensics	Imaging of a mini module surface looking specifically for irregularities in the interconnects, for instance, and then subjecting the module to accelerated testing and again imaging the surface to detect changes could be an interesting near-term use.	
36	Polymer-Clay Nanocomposite Materials as Encapsulants and for Arc Fault Mitigation.	Application of polymer clay nanocomposite barrier coatings as photovoltaic encapsulants represents a unique extension of known polymer clay nanocomposites such as the transparent montmorillonite composites developed by Professor Grunlan (Texas A&M) as effective fire retardants and packaging for foods and electronics. We have expanded this inexpensive materials system to create transparent environmentally stable gas vapor barriers desirable for photovoltaic encapsulants. Leveraging expertise from Professor Grunlan we used Layer-by-Layer growth to sequentially deposit alternating layers of charged polymers or copolymers (e.g. tailored polyacrylic acid, polyethyleneimine) and oriented oppositely charged exfoliated clay platelets creating impermeable "brick and mortar" assemblies of clay platelets in a tailored polymer matrix. This project has investigated: 1) Tailoring clay particle chemistry to optimize platelet geometry (size range of 1 nm x50nm to 1 nm x 2 μm), dispersion, dopant metals in the clay layer such as Fe, Ni, V for contaminant affinity, and optical transparency; 2) Design and integration of the polyelectrolyte matrix to control film adhesion, composite integrity, and gas permeation; 3) Scalable LbL deposition on module sized surfaces, and 4) Arc Fault passivation on energized circuits.	Margaret Gordon (Erik Spoerke, PI)	NL- Sandia National Laboratories	3. High-throughput Materials Discovery and Forensics	Near term, the coating would need to undergo accelerated testing and further barrier proerty testing on the functionalized and doped coatings. Long term success would devise a commercially viable application of the coating technology, as an encapsulant enhancement, relpacement, or as a strategy to prevent arc-faults elsewhere.	

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37	Probing changes in the optical properties and chemical composition of soft materials and metal films	We will present three case studies conducted at NREL to demonstrate the applicability of spectroscopic techniques to probe chemical transformations and modifications of the optical properties in soft, polymeric systems and thin metal films of relevance to solar photoconversion technologies. The first case study explores the impact of the diiodooctane (DIO) processing additive on the photostability of a polymer-based light-harvesting material. Fourier-transform infrared (FTIR) spectroscopic measurements, coupled with elemental analysis by X-ray fluorescence, suggest that illumination of materials containing DIO can result in the generation of highly reactive free radicals that can rapidly attack the polymer, resulting in severe degradation of the optical properties. Radical-initiated reactions on the polymer side-chains lead to oxidation products such as esters and carboxylic acids and eventually to ring opening on the polymer backbone. This study suggests that the chemical nature of processing additives should be considered for polymer-based materials that will be exposed to solar radiation. The second case study employs FTIR and UV/Vis/NIR spectroscopies to probe the exposure of poly(ethylene terephthalate) (PET) foils to a simulated solar irradiance spectrum. This study suggests that the severe discoloration (yellowing) of the PET foil is due to chemical modifications associated primarily with the aromatic ester moiety (carboxylic ester bound to an aromatic ring). An increase in the spectral linewidths suggests that the aging process results in the formation of more heterogeneous chemical environments. Analysis of the carbonyl (C=O) and C–H/O–H stretching regions provide clear evidence for the formation of carboxylic acid groups associated with the aromatic ester moiety. Finally, we probe the effect of exposing bare silver films to a simulated solar irradiance spectrum under ambient conditions. Variable angle spectroscopic ellipsometry (VASE) measurements suggest that exposure results in the formation of an overlayer with optical properties similar, but not identical, to silver oxide (AgOx), which increases in thickness with prolonged aging. Deposition of an ~250 nm thick aluminum oxide (Al2O3) layer onto the silver surface completely inhibits the photoactivated degradation of the optical properties of the silver film.	Andrew J. Ferguson, Bertrand J. Tremolet de Villiers, Robert Tirawat, Ross E. Larsen	NL- NREL	3. High-throughput Materials Discovery and Forensics	The near term (1 year) goal for these capabilities is to further demonstrate that the spectroscopic tools are capable of probing and identifying the degradation mechanism(s) of existing PV module materials. The long term (5 year) goal is to develop high-throughput variants of these spectroscopic tools to allow industrial partners to deploy them for rapid material screening and real-time production line testing of PV components and modules.	
38	LLNL Capabilities in Materials Modeling, Characterization, and Synthesis for Module Reliability Improvement and Cost Reduction	LLNL maintains leading capabilities in materials modeling that span and couple the atomic-scale, mesoscale, and macroscale. Those modeling capabilities leverage world-class high-performance computing resources available both internally and to collaborators through the Multiprogrammatic & Institutional Computing Program (M&IC), the High-Performance Computing Innovation Center (HPCIC), and the High Performance Computing for Manufacturing Program (HPC4Mfg). Expertise in applying atomistic and mesoscale modeling techniques has recently been exercised in several relevant areas, including polymer encapsulant degradation, transparent contact degradation, and structural material design. General capabilities are maintained in kinetics of phase transformations; modeling of interfaces and materials defects; modeling of alloy properties; and coupling of atomistic-scale models to macroscopic device response models. These computational capabilities would be leveraged to help find and design improved materials for module components to enable longer lifetimes, higher reliability, and/or reduced cost. Several novel experimental capabilities also are available. A capability in infrared spectroscopy of water ingress into polymer encapsulants has been developed, which further leverages predictive simulations for calibration. This capability would be used by module manufacturers to study and qualify long-term reliability, primarily of flexible modules, related to water ingress. The dynamic transmission electron microscope (DTEM) is a unique instrument invented at LLNL for direct imaging of materials transformations at the sub-nanosecond and sub-nanometer scales. This capability enables the study of reactivity, stability, and strength of materials, especially across interfaces. A major capability in additive manufacturing of hierarchical materials leverages computational design of structures as well as unique integrated validation of manufactured parts. Engineering (meta)materials with properties surpassing those possible with simple bulk materials can be fabricated reliably; recent demonstrations have included ultra-wide-angle and broadband anti-reflective coatings, highly absorptive materials, negative and zero thermal expansion materials, and high-stiffness/high-strength ultra-lightweight materials, bypassing many property tradeoffs encountered with traditional bulk materials.	Vincenzo Lordi, lordi2@llnl.gov, 925-423-2755	NL- Lawrence Livermore National Laboratory	3. High-throughput Materials Discovery and Forensics	On a 1 year timescale, these capabilities can help identify failure mechanisms and characteristics of material aging leading to reliability problems. Also, prototype metamaterials can be designed and fabricated for testing as suitable replacement materials for targeted module components. On a 5 year timescale, success would include the development and potential integration at lab-scale of a new material with properties that improve reliability and/or lower cost. The highest probability of success would result from synergistic leveraging of both computational and experimental capabilities.	
39	Surface science methods and their application to the study of PV module soiling	Module soiling has recently gained prominence as a major consideration in the large scale deployment of photovoltaic power systems. This is true not only because the semiconductor engines of modules have generally neared their theoretical limits, but also because soiling itself is a complicated, difficult to solve issue. Soiling and the related phenomenon of cementation involve a large number of physical and chemical processes that occur over wide range of spatial and temporal scales. The complexity of soiling is exacerbated by the fact that it is dependent on climate and location. Despite this complexity, an NREL team funded by SuNLaMP has made significant progress understanding some of the mechanisms that govern the soiling of glass surfaces typical of PV modules. One key part of this work has been viewing aspects of the problem from the standpoint of surface science. In this contribution, we present recent results showing how surface analysis methods can be used to probe chemical aspects of module soiling. X-ray photoelectron spectroscopy results show that surfaces of module glass aged in the field for ~15 years are depleted in alkali and alkaline earth metals, and in some cases are enriched in iron. A method to accelerate aging and intentionally deplete surfaces of these ions was used to test the hypothesis that surface-segregated sodium contributes to adhesion of particles. Adhesion testing involved using the tips of an atomic force microscope as a proxy for dust particles. These nano/micro-scale measurements are connected to larger scale adhesion tests involving real dust particles and particle counting experiments based on white light optical profilometry. More recently we have developed an objective criterion for the widely used but poorly defined term "cementation". We believe that cementation in particular presents a massive opportunity to research at the nexus of applied surface science and module soiling.	Craig L. Perkins	NL- NREL	3. High-throughput Materials Discovery and Forensics	Our efforts have the end goal of reduced LCOE. This will be accomplished by gaining a fundamental understanding of soiling of PV modules, which in turn will lead to cost-effective soiling mitigation strategies.	
40	Roll-to-roll printing and coating	Eastman Kodak has deep technical expertise in the science of materials, imaging, and deposition. A broad patent portfolio and a history of ground breaking inventions, including OLED and organic photoconductors, makes Kodak an ideal partner in the solar energy industry. With over 100 years' experience formulating and manufacturing coated films, Kodak offers prototype, pilot, and full scale manufacturing. Aqueous and solvent based solutions are roll-to-roll (R2R) coated and printed onto paper, plastic, glass, and metal webs. Examples include, a R2R manufacturing line developed to print eight solvent-based layers as thin as 0.1 microns onto substrates down to 4.5 microns at speeds up to 330 m/min. For printed electronic applications, e.g. touch screens and touchless solar cleaners, R2R printing, plating and coating line were developed to manufacture passivated copper electrodes <5 micron in width. Optical grade film manufacturing features three in-line coatings per side with dimensional stability of 0.2%. Functionalized topcoats (e.g. sol-gel and aluminum oxide) have also been commercialized. Ongoing research and development efforts include metal and polymeric based conductive inks, functional polymeric powders, antimicrobial materials, and spatial atomic layer deposition. Kodak also excels in developing and manufacturing complex equipment as demonstrated by our commercial printing products: Prosper 6000 inkjet press (world's fastest) and NexPress SX toner press (best-in-class image quality and substrate capability). Both have leading image-to-image and image-to-sheet registration. A wide variety of ink jet inks, offset and flexographic plates, and toners are developed and manufactured at our U.S. facilities which include a 1200-acre industrial park with >16 million square feet of manufacturing, lab, and office space. With custom chemical manufacturing services, more than 500 distinct molecules are made annually with a library of over 1500 manufacturing processes, an archive of >30,000 procedures, and reactor systems from 22 to 3780 liters for pilot batches to multi-ton commercial quantities.	Thomas N Tombs, Ph.D. Program Director Eastman Kodak Company 1999 Lake Avenue, Rochester, NY 14650 thomas.tombs@kodak.com, Office: 585-726-3419, Mobile: 585-764-1100	C- Eastman Kodak Company	3. High-throughput Materials Discovery and Forensics	Near term, Kodak expects to increase the external use of its formulating, coating and printing services and to form partnerships with material developers with the intent of developing roll-to-roll (R2R) solar energy products. Long term Kodak plans to manufacture solar energy products. One potential product is a touchless electronic solar cleaner made by R2R printing electrodes on flexible film and/or glass. A second potential product is a low cost, PV module R2R printed on flexible film and/or glass.	www.kodak.com

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41	NREL Surface Analysis Cluster Tool, Time of Flight Secondary Ion Mass Spectrometry (TOF-SIMS)	The NREL surface analysis cluster tool integrates deposition, processing and characterization capabilities with an ultrahigh vacuum sample transfer system, as illustrated in Fig. 1. A dedicated glovebox facilitates air-free sample transfer into and out of the system. Key analytical capabilities include: • X-ray and ultraviolet photoelectron spectroscopies (XPS/UPS): XPS/UPS quantifies near-surface compositions (~1 atomic % composition & above) and chemical states, and correlates these with surface valence-electronic structure and interfacial band alignments. • Auger electron spectroscopy (AES); scanning Auger microscopy (SAM); scanning electron microscopy (SEM): Auger electron spectroscopy (AES) provides surface-sensitive compositional measurements and depth profiling of matrix elements (~1 atomic % composition & above). Scanning Auger microscopy (SAM) measurements permit compositional imaging with spatial resolution of ~ 50 nm, as well as correlations between composition maps and SEM images of sample morphology, as illustrated in Fig. 2. • Omicron surface-science platform: This instrument is geared toward fundamental studies of materials using techniques including XPS/UPS, low-energy electron diffraction (LEED), scanning-tunneling and atomic-force microscopies (STM/AFM), and ion-scattering spectroscopy (ISS). Time-of-flight secondary ion mass spectrometry (TOF-SIMS) is a versatile UHV surface analysis technique which provides surface spectrometry of both inorganic and organic materials with detection limits in the sub-ppm range. TOF-SIMS combines excellent chemical imaging capabilities (> 80nm lateral resolution) with high mass resolution spectroscopy ($m/\Delta m > 9000$). Combining high-resolution imaging with depth profiling (3-D tomography) allows for 3-D imaging of elements. This can allow for quantitative 3-D representation of modules or materials degradation, as illustrated for potential induced degradation in poly-silicon modules in Fig 3. TOF SIMS is an ideal tool to investigate material degradation and failure mechanisms at the micro to nano-scale.	Glenn Teeter, glenn.teeter@nrel.gov, Steve Harvey, Steve.harvey@nrel.gov	NL- NREL	3. High-throughput Materials Discovery and Forensics	Successful use of the NREL Surface analysis capabilities in the near term (1 year) would be to establish partnerships with at least one industry partner to help them investigate either diffusion of problematic species for module failure or degrading of module components. A 5 year successful use would be to form a collaborative R&D effort with an industrial partner which leads to a more stable module component.	