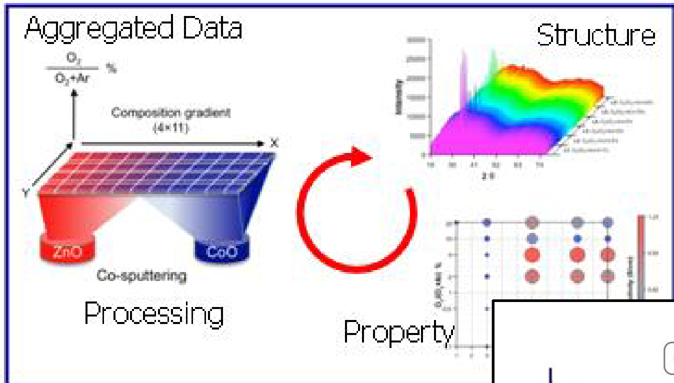
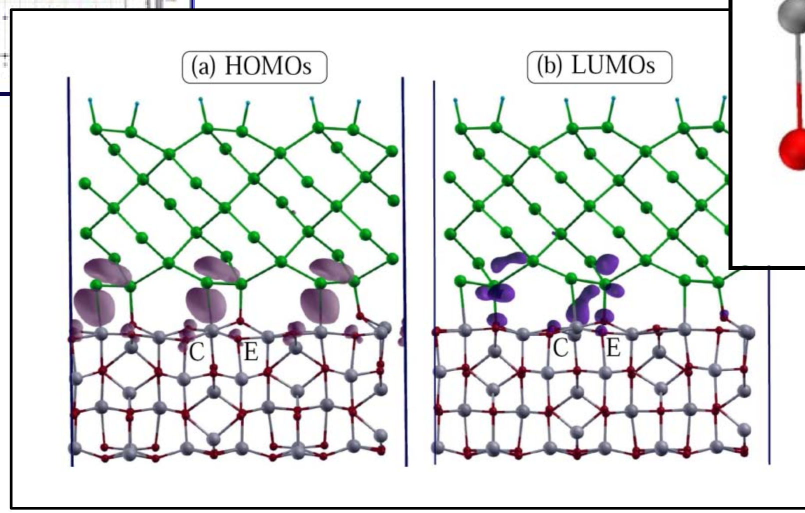
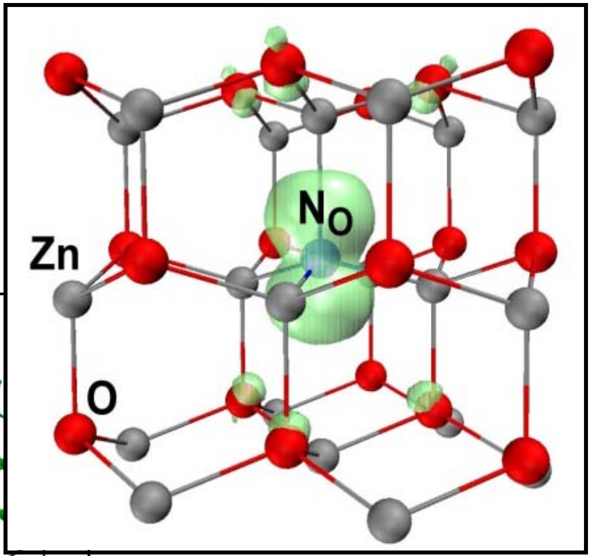






Theory and Computational Science

(Agreement leader: William Tumas)

PV Program

Presenter:
Stephan Lany

National Renewable Energy Laboratory
Stephan.Lany@NREL.gov

May 27, 2010

Challenge

Build a fundamental knowledge base of PV materials for the SETP

Timeline

- Project start date: FY08
- on-going

Budget

- Total project funding
  - DOE share: 100%
  - Contractor share: n/a
- $915k received in FY09
- $970 for FY10

Partners

Chemical and Materials Science Center
Scientific Computing Center
at NREL

- Task 1 ($200k), Lead: Wesley Jones
  Scientific data management and mining
- Task 2 ($250k), Lead: Alex Zunger
  Solid State Theory
- Task 3 ($390k), Lead: Su-Huai Wei
  Theory of PV materials
- Task 4 ($130k), Lead: Angelo Mascarenhas
  Ultrafast imaging of defects

Challenges, Barriers or Problems

This agreement integrates unique cross-cutting NREL capabilities to build an essential ***knowledge base*** for the Solar Energy Technologies Program:

(1) Scientific data management and mining

(2) Solid State Theory

(3) Theory of PV materials

(4) Ultrafast imaging of defects in PV materials

This agreement plays a key role in building a strong link between theory, characterization, and application.

Importance for Solar Program mission

Develop scientific understanding of PV relevant materials properties; Address barriers facing existing PV technologies; Provide theory guidance for promising directions of PV R&D; Accelerate the advances in the long-term goal of employing solar cell technology efficiently and cost-effectively.

Task 1, Scientific data management (Wes Jones)

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

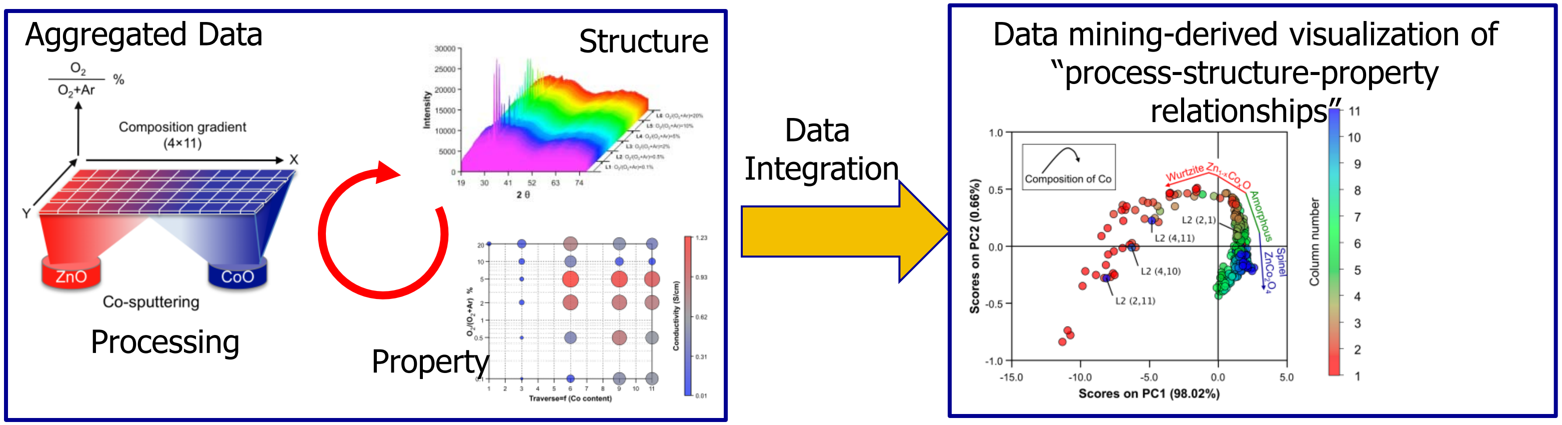
Relevance

<u>Objective and goals:</u> Provide robust scientific findings using advanced data analysis, data mining and optimization approaches.

Integrate and explore complex experimental information, accelerating the design and discovery of new materials, and improvement of process via data management and advanced data analysis methods

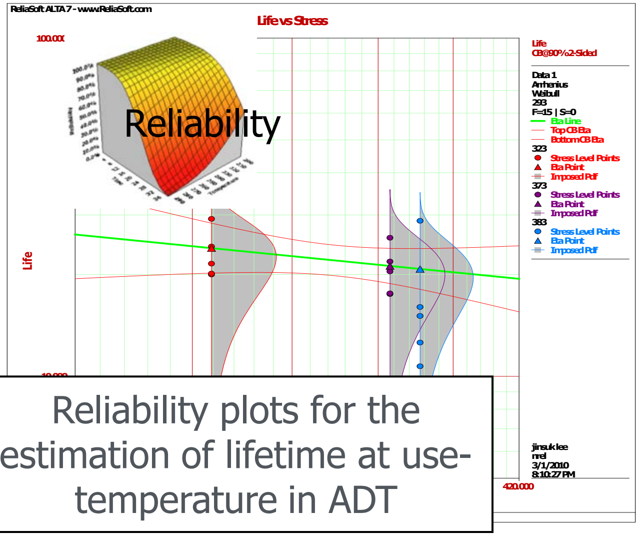
Approach

Construct data aggregation methods enabling the integration of data across different experimental tools. Integrate PV characterization such as XPS with data mining techniques.

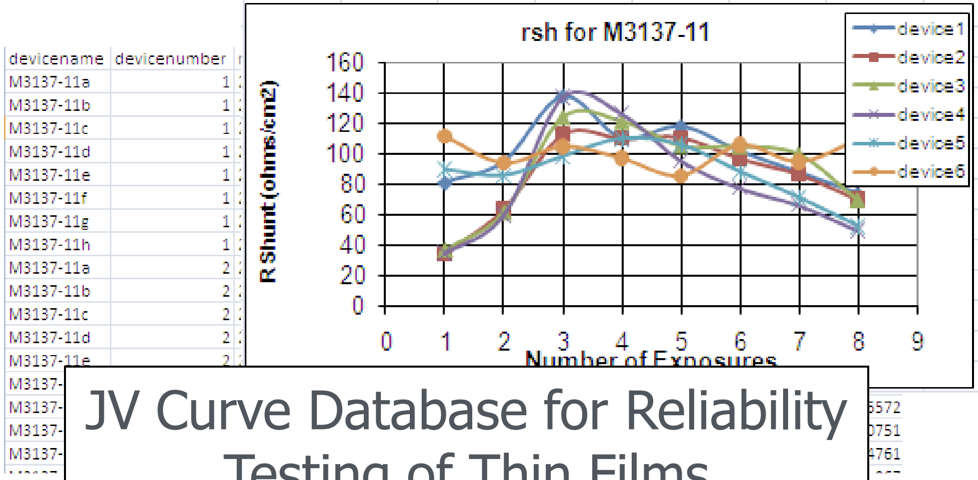


Accomplishments

- **Data management and data aggregation:** 1) For thin film (CIGS), prototyped J-V curve data collection and query 2) Researched improving data aggregation for TCO data sources, 3) Developed workflows for thin film reliability and device testing, 4) Maintained film Silicon and FTIR databases.
- **Enabled AMpulse Collaboration within Film Silicon Database.**
- **Paper Submission to ACTA Materialia: "**Strategy for the maximum extraction of quantitative information generated from combinatorial experimentation of Co-doped ZnO thin films" with John Perkins (TCO).
- **Applied advanced statistics for PV systems:** 1) Investigated the characteristics of the thermal fatigue damage of CPV cells, 2) Preliminary white paper on step-stress accelerated life testing (SSALT) for PV modules, and 3) Introduced strep-stress accelerated degradation testing (SSADT) models to CIGS.



Reliability plots for the estimation of lifetime at use-temperature in ADT



JV Curve Database for Reliability Testing of Thin Films

Task 1, Scientific data management (Wes Jones)

Budget Status and Potential for Expansion

- On budget: Current budget 200k
- Additional funding opportunities: J-V Curve data mining; Reliability testing in multi-failure modes

Collaborations and Technology Transfer

Collaboration with NCPV

Future Plans

- Construct data aggregation methods enabling the integration of data across different experimental tools.
- Investigate data mining techniques using the J-V curve repository to uncover hidden relationships between performance from CIGS reliability testing and processing factors.
- Develop an analytical SSALT model and investigate appropriate experimental designs for reliability testing of PV devices (CIGS and encapsulation).
- Study reliability testing problems due to multi-failure modes, which lead to different characteristics and patterns of failures, by understanding complex reliability system models.

Task 2, Solid State Theory (Alex Zunger)

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

Team (FY10)

Alex Zunger	0.1 FTE (task leader, research fellow)
Stephan Lany	0.5 FTE (senior scientist)
Koushik Biswas	0.5 FTE (post-doc)

Relevance

Objective and goals: Provide scientific underpinning, modeling, and predictions pertaining to PV materials and phenomena. Identify promising directions and guide experimental efforts. Maintain NREL's ~30 yr ***leadership in theory*** for PV absorbers and transparent conductors.

*Distinction from OS-BES funded EFRC "**Center for Inverse Design**":*

- The EFRC addresses the development of ***general*** design capabilities for ***entirely new*** materials with functionalities that include but are not limited to PV Those materials do not necessarily fit into today's PV technologies.

- In contrast, the present SETP effort addresses ***specific*** problems in ***existing*** technologies, e.g., open-circuit voltage limitation in CIGS, replacement of Indium in PV thin-film absorbers, *p*-type doping of ZnO, work-function engineering in TCOs, electron trapping in TiO_2, …

Task 2, Solid State Theory (Alex Zunger)

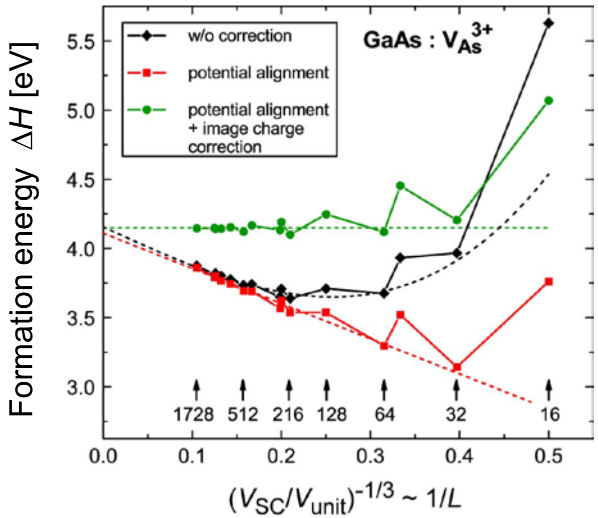
U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

Approach: Apply electronic structure theory to model PV relevant phenomena in solar absorbers and transparent conductors: Band-structure, atomic structure, defects, doping, interfaces, grain boundaries, …

Maintain NREL leadership in theoretical predictions of PV materials properties, advance existing models and theories on an as-needed basis

Example:
Defects cause detrimental recombination centers
$\Rightarrow$ Need accurate defect formation energies ΔH

Assessment of correction methods for the band gap problem and for finite-size effects in supercell defect calculations: Case studies for ZnO and GaAs
S. Lany and A. Zunger, Phys. Rev. B **78**, 235104 (2008).



Impact: Recent SST work that is ***important and relevant*** to PV technologies:

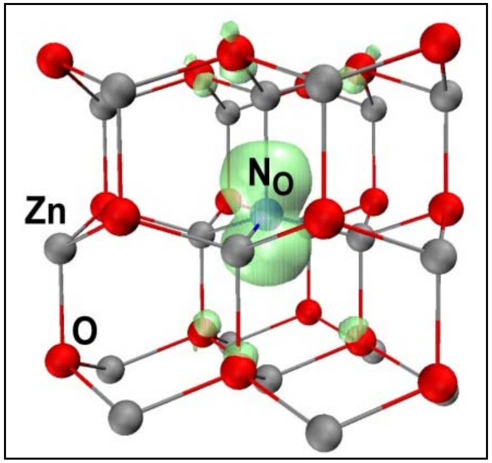
- Limitation of the **open-circuit voltage** due to defects in $Cu(In,Ga)Se_2$ absorbers
- Predictive theory for ***p*-type doping** of transparent conducting oxides
- Electronic consequences of **multivalent elements** in PV materials

Task 2, Solid State Theory (Alex Zunger)

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

Accomplishments

Generalized Koopmans density functional calculations reveal the deep acceptor state of N_O in ZnO



p-type doping in transparent conducting oxides (TCO) is desirable for a range of PV applications, including tandem cells and organic PV. However, shortcomings of standard DFT led to “false positives” in previous predictions of *p*-type doping of TCO. Here we apply a ***corrected theory*** to show that contrary to common perception, nitrogen in ZnO is a deep acceptor that does not release free holes.

Conclusion: Our theory will aid truly predictive calculations of *p*-type TCO in the future.

The electronic consequences of the existence of multivalent elements in inorganic solar absorbers

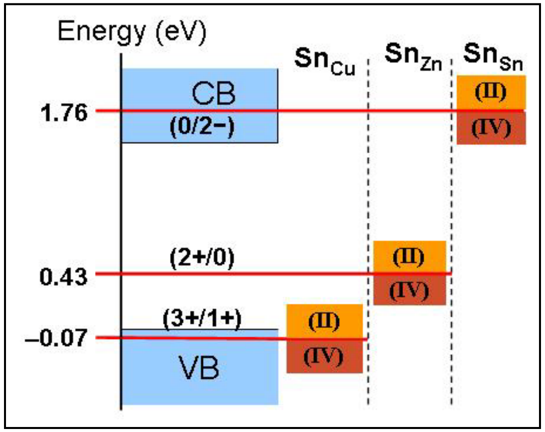
There is a rapidly increasing interest in renewable energy applications employing earth-abundant materials, many of which contain multivalent elements. As we demonstrate for the In-free Cu_2ZnSnS_4 PV absorber, multivalent elements (e.g., like $Sn^{+IV/+II}$ in CZTS) can cause detrimental deep levels that promote electron-hole recombination. The presence of ***multivalent elements*** (e.g., Sn, Fe, Bi, …) in new PV materials deserves particular attention towards the possibility of ***detrimental defect*** states.

Conclusion: Theory can direct efforts to identify showstoppers at early stage or mitigate detrimental defects via doping principles.

possible *e-h* recombination

$Sn^{+IV} + 2e \rightarrow Sn^{+II}$

$Sn^{+II} + 2h \rightarrow Sn^{+IV}$



Task 2, Solid State Theory (Alex Zunger)

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

SST Milestone (FY10 AOP)

Provide theory guidance to overcome bottlenecks in PV materials. Support SETP by state-of-the-art theory for PV materials of current technologies.

Budget Status

Budget ($250k for FY10) is on target

Collaborations and Technology Transfer

Collaboration with experimental groups in the NCPV

Potential for Expansion

- Study the potential of materials for thin-film solar cells made from ***abundant***, ***non-toxic***, and ***inexpensive*** elements
- Model structure and formation energies of electron-producers in ***amorphous*** *n*-type TCO (e.g., Zn-Sn-O)

Future Plans

- Apply unique theory capabilities for prediction of carrier trapping to TiO_2, study issues of electron transport through the TiO_2 layer in Dye Sensitized Solar Cells
- Alloying of Mg to ZnO to better match conduction band offsets (e.g. in OPV). Use theory to overcome the deterioration of Al-doping following Mg addition

Task 3, Theory of PV materials (Su-Huai Wei)

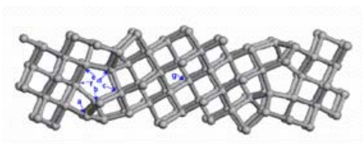
Relevance

<u>Objective and goals:</u> The Theory of PV Materials task provides critical cross-cutting components in a wide range of PV device structures. The objective of the task is to perform fundamental research to establish the theoretical knowledge base of PV materials using the state-of-the-art computational tools. It is aimed at accelerate the advances in the national PV technology and R&D program by improving solar cell efficiency and reducing its cost through understanding and control of PV material properties.

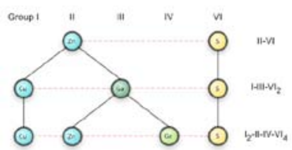
Approach

Use state-of-the-art computational tools to establish the fundamental knowledge infrastructure of PV materials. The study is two-fold: (i) explain experimental results and provide guidance for future experimental investigation, and (ii) propose design principles of PV materials which are potential candidates for future PV applications. Work was done in close collaboration with NCPV experimental groups. Calculated results are shared with them for test and confirmation. Experimental results are in turn used to guide future theoretical research activities.

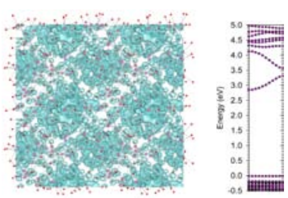
Accomplishments



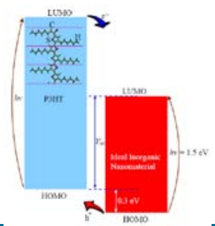
- Effective impurity gettering is important for low-cost c-Si solar cell. Using first-principles method, we have investigated the mechanism of Fe segregation into Si S5 <310> grain boundary. We find that the segregation is site-selective, determined by the strain and crystal field splitting at each site.



- $Cu_2ZnSn(S,Se)_4$ is one of the most promising quaternary absorber materials for low-cost thin-film solar cells. We have studied systematically its defect properties and proposed approaches (e.g., grow samples under Cu-poor and Zn-rich conditions) to optimize its performance.



- Studied crystal structure, electronic structure, and doping properties of oxides for possible transparent conducting oxide applications. Explained why amorphous TCO can be good electronic materials even without passivation.



- Using first-principles method, we have searched semiconducting nanostructures for possible organic-inorganic hybrid solar cell applications. We suggest that chalcopyrite $MgSnSb_2$ quantum wire could be a low-cost material for this application.

Task 3, Theory of PV materials (Su-Huai Wei)

Budget Status and Potential for Expansion

Budget ($390k/year) is on target.

Collaborations and Technology Transfer

Strong collaboration with experimental groups at NCPV.

Future Plans

- Understand the role of Cu and Cl diffusion in CdTe-based solar cell system, calculate the diffusion barriers of Cu and Cl in CdTe, CdS, ZnTe, $CdTeO_3$, CuO.
- Understand microscopic structure and passivation mechanism of the c-Si/a-Si heterojunction interfaces in order to improve the cell efficiency.
- Obtain the electronic and optical properties of the crystalline and amorphous phases of the homologous $InMO_3(ZnO)n$ (M=Al, Ga, In) alloys for possible TCO application.
- Study the electronic and defect properties of quaternary chalcogenide absorbers [$Cu_2ZnGe(S,Se)_4$ and $Cu_2ZnSn(S,Se)_4$]. Identify the best quaternary materials for PV applications.

Task 4, Ultrafast imaging of defects (Angelo Mascarenhas)

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

Team (Project start date Feb. 1, 2010)

Brian Fluegel 0.2 FTE

Angelo Mascarenhas 0.05 FTE

Relevance

Objective and goals: A recently developed new technique enables nearly instantaneous capture of an entire photoluminescence (PL) map, allowing to study polycrystalline or epitaxial PV materials with submicron spatial resolution, selectable spectral resolution, variable sample temperature and tunable excitation sources. The plan is to utilize and perfect this apparatus for the study of defects in CdTe and III-V based solar cell materials.

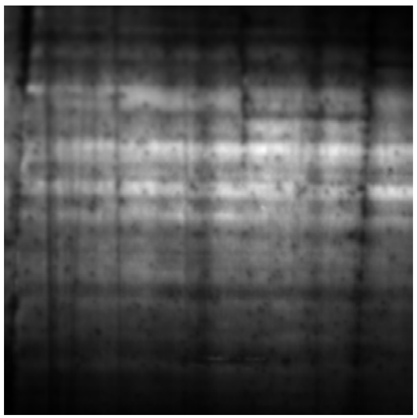
Approach

To meet these goals, two relatively new technologies are drawn upon: (a) instantly tunable LCD bandpass filters that provide high or low spectral resolution of an entire image, and (b) electron-multiplying CCD cameras with high-speed readout that combine high-sensitivity with video-rate output. The system in quite flexible, but typically a sample is cooled to liquid nitrogen temperature and illuminated over 100 microns laterally with a defocussed laser. The resulting wide-field PL is filtered and imaged, providing data as quickly as the operator can move the sample.

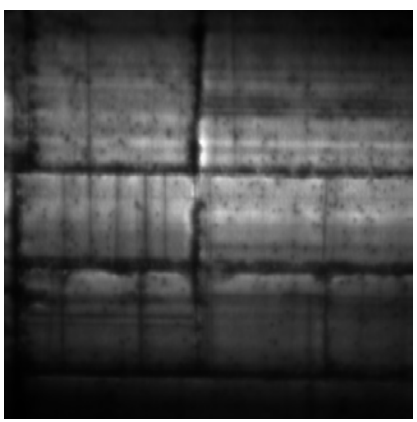
Task 4, Ultrafast imaging of defects (Angelo Mascarenhas)

Accomplishments

Metamorphic GaInP solar cell junctions are single-crystal despite having a very large lattice-mismatch with underlying layers. The spatial pattern of lattice dislocations directly reveals the success or failure of growing the necessary stepped grade layers.



PL imaging at the bandgap emission energy reveals fine dark points that are the surface intersection of lattice dislocations. The counted density of these points reproduces other industry-accepted measurements of defect densities.



At the same time, the real-time nature of this data acquisition allows an entire sample to be rapidly surveyed. It is quickly found that the relatively homogeneous regions shown above occur rarely. The majority of the sample is actually dominated by “cross-hatching”, i.e., surface striations due to residual strain.

Task 4, Ultrafast imaging of defects (Angelo Mascarenhas)

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

Budget Status and Potential for Expansion

Budget is on target (for 3 months starting Feb/2010).

Collaborations and Technology Transfer

NREL's III-V group (Myles Steiner)

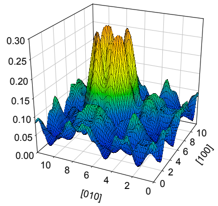
NREL's CdTe group (Ramesh Dhere)

Future Plans

- Continue defect density measurements on metamophic GaInP as growth designs are changed through refinements to grading profile, gallium concentration and growth temperature.
- Cleaved-edge measurements on a CdTe solar cell under bias.

Summary

- The fundamental researches in this PV Agreement focus on improving understanding of existing materials, address barriers facing current PV technologies, develop novel new materials, and accelerate the process of moving technologies from theoretical or early stage research into applied technologies.



- The synergy between experimental studies which have greatly improved their ability to grow high quality materials and optimize device design and the theoretical studies which have provided understanding of fundamental materials properties using state-of-the-art quantum-mechanical computational theories and tools will greatly accelerate scientific discovery of new PV materials and the research and development program of SETP

- Support of this program also represent recognition of the critical role that theory, modeling, numerical simulation, and scientific data management and mining play in the PV research and development process

- Scientific underpinning, modeling, and predictions pertaining to PV materials and phenomena via theory is indispensable to steer experimental efforts in emerging technologies and concepts into fruitful directions.