Friday, October 29, 2021 – CdTe Photovoltaics Workshop Breakout Session

The 5th Annual CdTe PV Workshop was held in Chicago, IL on October 28-29, 2021 with primarily in-person but also some virtual/remote attendees. Following the series of 24 presentations on Thursday, a Friday brainstorming session was held to gather ideas, input, and (possibly) consensus regarding priority R&D, technology, and industry topics for the accelerated success of CdTe PV. Four topics were discussed by breakout groups:

Topic 1: How can and should the CdTe PV community broaden and seize new market PV applications?

Topic 2: How can should the CdTe PV community improve and enhance the supply chain, market share, and deployment?

Topic 3: What are key directions for near-term technology development?

Topic 4: Describe the technology roadmap for blue sky research

The output of the topic discussions is detailed in the following pages. Note that this is still largely "raw" input, without editorial or organizational refinements. Some groups added names to their notes; these have been removed here to be consistent with the notion that these are in many cases shared ideas intended to support and guide the CdTe PV community. These notes are intended to eventually provide input into an updated publicly-available CdTe PV Technology Roadmap published under the auspices of the U.S. DOE.

Topic 1: How can & should we broaden new market applications?

Potential Markets: Agricultural PV (AgriPV), Rooftop PV/Building Applied PV (BAPV), Solar Windows/Building Integrated PV (BIPV), Vehicle-integrated PV, Person-portable, Aerospace/Space-integrated PV

Policy/Outreach changes that could be critical
- Investment tax credit (ITC) for solar windows
- Education of architects/installers vs making products/installation as similar as possible to pre-existing processes to facilitate adoption
    - Engage soft cost work with DOE
    - Code development for BIPV

Standards changes that could be critical for solar windows
- Local code concerns → goal to develop state/federal standards
- Plug and play standard? How to integrate to a bus?
- Voltage standards
- UV stability testing (encapsulant stability becomes more critical for window lifetime of semi-transparent modules)

Getting good data sets to establish CdTe as a legitimate player and examine potential value propositions
- AgriPV includes
    - Looking at the effects of tuning transparency as a tradeoff in efficiency and crop yield. Might need to balance with irrigation if it blocks precipitation (runoff concerns?)
    - Compare to Si (studies to date have controlled transparency with spacing of modules, bifacial Si)
    - Different climates, crops, optimizations
    - Spectral effects from transparent conductive oxides (TCOs)/coatings?
- Is there BIPV data that is needed?
- Reliability data in specialty applications and broad conditions
- Update PV Watts at NREL (it is using very old CdTe data, 2012 data(?))
    - How to account for thermal coefficient and spectral efficiency and energy yield

Technical needs to enable markets
- High quality transparent back contacts (enables bifacial, solar windows, AgriPV, higher energy density applications like vehicle/aerospace with tandems)
- Lightweight/flexible – more investigations with alternate substrates/carrier process, liftoff process, high efficiency substrate design on opaque foil
- Partial shading strategies – modeling, experimental sensitivity and solutions
- May need to design module structures into ways to mount and integrate windows/spandrel glass – should we be emulating what the window industry does rather than what is done by the PV industry
    - Is there a concern with oxygen in the package? If necessary, can consider getters in the package

- Ways to fabricate different sizes for windows (**<u>customization</u>**) – are there process modifications that are needed, should it be done on different glass sizes to start or something else? (agility with downstream processing, laser processing, bussing, etc)
    - How to get way from single SKU (single size)
    - Lamination vs air gap vs hot-melt
- UV stability of encapsulants (encapsulant stability becomes more critical for window lifetime of semi-transparent modules, AgriPV)
    - Could consider UV blocking layers

Topic 2: How can the community improve/enhance the supply chain, market share, and deployment?

Action items:

- Develop a plan to educate congress (US-MAC)
  - Develop a plan: What is needed for 50 GW manufacturing in 2030?
  - It could be shared with people who are not necessarily in the solar industry through smaller organizations. For example, we have a "Progress Now Colorado"
  - Use power purchase agreement (PPA) as incentive: a fixed PPA would secure profit margin hence to encourage investment and growth
  - A delegate group to visit congresspeople
- White paper and 3 slides ppt: including fact sheet, roadmap, and talking points
  - Span the entire value chain
  - CdTe is still underfunded at $22M
  - Be persistent/patient
  - Need the roadmap including R&D priorities
  - Broader/continuous R&D beyond US-MAC
  - Mandatory module recycling policy
  - PV module with lowest carbon footprint label
- Start dialog between CdTe community and USGS on strategic minerals:
  - Invite them to the next workshop. Focus on Te and other key materials of balance of system (BOS) components; Ask NREL first
  - 5Nplus, First Solar (FS), Toledo Solar (TS) [Goldfarb, Richard, 2015, Tellurium—The bright future of solar energy: U.S. Geological Survey Fact Sheet 2014–3077, 2 p., https://dx.doi.org/10.3133/fs20143077]
- Glass:
  - Research on low-iron glass raw materials sourcing
  - Lower the manufacturing cost of thinner glass
- Alternative racking materials or design (NREL+Univ))
- Solar roof panels (No shingles - Industry)
- Follow up at some monthly meetings (sub-groups)
- Determine appropriate references to address "toxicity"/carcinogenic bioavailability concerns of CdTe – ensure this is carefully handled with an minimize chance for miscommunication

- Additional Notes:
- what level of incentive is required to drive production at targeted volume
- Bring back Cu processing in NA. what is the business case? May need incentives
- Te was never a focus of mining. It is a question of price.
- Government officials get interested if there is a way to bring $$ to their state.
- Te is a strategic mineral on US government list. We should put out a policy statement, contact our congress representative.
- Add incentive if US can manufacture. Remove tariff (Te) if can't be sourced domestically

- Extend product lifetime, reduce absorber thickness, improve Te extraction efficiency, increase module energy density
- Low iron glass may not be challenge, but probably worth a survey
- Labor (make products lighter)
- Aluminum as another example. Can substitute with stainless steel (SS), polymer (Samsung), or improved rail design. How about concrete, or wood, or bamboo?
- Thin film PV is more suitable for light weight or flexible application: but thin glass is too expensive
- Glass-based full scale module on roof
- Market share
    - Incentives must be set to last for decades. But how? Using PPA
    - PV people are farmers. If farmers receive incentives, we should as well (book "A contract with earth")
    - Would market share be increased through different "marketing"? Do people with purchasing power have negative thoughts of Cd in CdTe?
- Mandatory module recycling policy
- Bipartisan act: add more installation by de-regulating the solar industry, simply/streamline the process

Topic 3: Near-term technology development

Main points

- Where is the missing Voc given the high lifetimes? Getting better at quantifying losses
  - Need to understand the j_0, selectivity metrics, identifying locations in the device where it happens, understanding the interaction between As and Cl
  - Find the contacts that are going to give us high selectivity
- More access to samples for exploratory work on contacts for people who don't make their own absorbers to reduce the entry barrier in the community ➔ ad-hoc or formally organized? Who is the quarterback? Need for research coordinators? Should be part of the consortium
- Need for well-defined "test structures" for contact development + well-defined suite of characterization "multi-modal" + modeling
  - Systematic approach: How to bridge the gap between high-throughput and detailed time-consuming characterization techniques and simulations
- More intimate relation between simulations and experimental (see Marco's work)
  - Standard samples to be used
  - Standard characterization needed in every lab (J-V, C-V, EQE, ERE, PL, what more?)
  - Identify "tiers" of characterization techniques to be used
    - Systematic high-throughput
    - Medium in-depth
    - In-depth expensive techniques and equipment
    - Improving network of shared instrumentation to increase the rate of learning
- Are impurities important? Using high-purity material and incorporating select impurities will be key to figure that out, some impurities may be beneficial.
- Need for a database of results to benefit from "the power of big data"
  - What is the meta-data needed for each sample?
- Shall we keep the journal of bad/negative results?

Key unfiltered ideas from participants:

- Breach the 1 V mark. Why haven't we broken that yet? Great lifetimes but poor voltages. Single-crystal is able to get close to detailed-balance (SQ) limit in c-Si, GaAs, CdTe but not in polycrystalline material. Are grain boundaries the issue?
- Impurities in source material at 10^{15}-10^{16} cm^{-3}: is that an issue? One could use a single-crystal surface to study grain boundary effect in a very controlled manner.
- Get more impurities to know if they have an effect. Or introduce new defects in a controllable manner like using radiation bombardments.
- What about the interaction Cl and As?
- Contacts to CdSeTe because the internal voltage is there. The back surface is very complex.

- There is more than band alignment, you need to understand the defects at the interfaces, inside the device and between the metal contact and the cladding/passivation/barrier layer. So-called surface Fermi level pinning needs to be carefully examined.
- Need to find process to understand the back of the device
- Absorber may not be the issue
- We may be stuck in a local minimum and maybe a lot of things need to be fixed at once.
- Cl n-type dopant, As p-type dopant. Is Cl an issue and can we get rid of it?
- Does the community have access to fast-turnaround test structures that allow for rapid characterization of back contact quality? Or do we need to develop some?
- No Cl in 1 V devices
- Performance drops when we take chlorine out.
- Can't discount 20 years of work with Cl. But I will work towards supplying large-grain CdTe thin films that don't have Cl so that people can study the effect of Cl better. MBE single-crystal sample can be an ideal candidate.
- Chlorine treatment twice seems to work
- Hydrogen plasma treatment worked together with Cl
- CST devices have iVoc >1 V and ERE > 4% with Cl treatment
- Issue with sub-bandgap features need to be investigated
- What test structure are needed?
- Absorbers are good enough. Evidence points to the back contact as being the issue
- Do round-robin on the most promising devices
- I think we need to carefully characterize test structures to ensure that when we process them for high ERE and lifetime that we know chemically and electronically what the interfaces look like. Is it the absorber that is good; or is it the interface(s).
- Spread of performance/parameters across samples may be an issue
- Sub bandgap absorption - what is SQ limit for these materials? What is Voc nrad?
- What about Auger?
- Shouldn't be an issue, especially with the density of impurities in CdTe.
- Impurities from everywhere
- I think we need to carefully characterize test structures to ensure that when we process them for high ERE and lifetime that we know chemically and electronically what the interfaces look like. Is it the absorber that is good; or is it the interface(s).
- Systematic voltage loss analysis needed. Using a single-crystal high performance device and add different defects to it one at a time to pinpoint the specific impact of that particular kind of defects.
- Impurities in starting materials, impurities introduced during fabrication
- How do we limit degradation? Is it just a question of encapsulation.
- The benefit of their new GrV process is really the improved stability I believe.
- To find the right back contact you need to test the whole book and throw pasta at the whole because you cannot predict what is interface will be like

- Can we control orientation to test back contacts in a controlled way? One can use MBE samples grown on different oriented substrates to study this particular defect.
- What is the optimal order of doing experiments? What problem is to be focused on first.
- How much work is needed on heavily doped emitters and window layers?
- The general idea being that we need higher emitter doping to realize the benefits of increased p-type doping.
- Doping control in emitter and back buffer
- Work function is important beyond doping
- Conductivity of layers themselves is important
- What happens with anneals? Do we mess up interfaces? Residues left on?
- Do we need to do de-scumming of samples?
- I would be interested in seeing very gentle processes like ALD used to deposit back contacts that maybe don't mess up sensitive rear surface passivation.
- Understanding and tracking what are the accidental things that happen that can be detrimental or beneficial (e.g., oxidation)
- Tracking elements throughout devices
- SIMS can help
- More systematic characterization needed
- Need high-throughput characterization techniques
- Need to be able to figure out the band diagram
- Happy to contribute samples

Topic 4: Blue sky research

Novel Absorbers

- CST-only absorbers with direct contacts (if possible) to reach higher single junction optimization
  - Has high ERE/lifetime as opposed to CST/CdTe + Cu
  - How to flesh out fluctuations in inhomogeneity of CST?
  - What is the origin of long lifetime?
  - CST/Te does not work well, could it be Se-rich surface around each CST grain that prevents the charge from coming out? We could punch holes through it by laser scribing to allow it to come out.
  - Selective contact (ion implantation, laser opening)
- Elimination of $CdCl_2$ treatment
  - Why is $ZnCl_2$ not doing as well as $CdCl_2$?
  - Isothermal $CdCl_2$ treatment
  - Cost issue, safety issue, etc.; Thus beneficial in many ways to not have (except for efficiency of course)
  - Elimination of Cl?
- N-type CdTe, CST
- Continue work towards high-lifetime absorbers

Device Architectures

- Substrate design
  - Enabled by n-type absorber?
  - Enabled by long-lifetime CST-only absorbers
- Flexible substrates
  - Flexible glass used is not cheap
  - YZO
  - Stainless steel
  - Lower temperature deposition

Contacts, Interconnects, Transparency

- Bifaciality
  - Intrinsic to understand and achieving passivation
  - If you can passivate, then you should be able to make the back surface bifacial as well
- Passivation
  - Native oxides (necessary for bifaciality, CdO_x, TeO_x, SeO_x)?
  - Investigate negative fixed charge
    - Alumina has defects that cause passivation (electrical field developed with SiO_2/Alumina)

        - Chemical passivation kills the dangling bonds by reconstruction

- Tandem cells
    - Development of high-efficiency wide gap top cell (CZT, CMT, CdSe)
    - Want CST to be just two contacts and then additional layers
    - Pushing materials envelope within metal chalcogenides (making the best CST or CZT) for potential tandem applications
    - SbSe is tunable, but indirect bandgap along with 1D transport, thus requiring preferential orientation
    - CdTe/CdTe tandem to demonstrate and study interconnection layers; start with bifacial single junction design?
    - CdTe/ZnTe was tried many years ago, but it behaved poorly
    - CdTe/Perovskite tandem possibility (Perovskite can be deposited at ~100˚C)
    - For tunnel junction, ITO has worked, but could use 2D materials such as graphene or nanowires, quantum dots, any materials that could serve as contacts
    - Nanocontacts would be good for nanoprobing within SEM for a greater understanding of passivation and contact resistance

Other Blue Sky Topics

- Centralized Facility for CdTe-Based PV Devices
    - Centralized facility which focus on various areas
    - Possibly create a standardized tool that can be set up in 4 or more areas?
    - Easier for Si to develop a design package since they are close to their theoretical maximum efficiency and optimization of devices
    - Somehow integrate a strong simulation
    - PDIL (Process and Development Integration)?
    - Have highly characterized films
- Library of Heterojunctions
    - Modeling and experimental research offering GB/surface recombination velocities, band profile with high degree of certainty (Scanning Kelvin Probe)
    - Library of single crystal studies that can be used to determine the differences in recombination velocity, interaction with $CdCl_2$ chemical species
- Space applications
    - Possible to have an impact as the III-V materials are not cheap; may be attractive to smaller companies who want to use in satellites. CdTe material has been demonstrated to be radiation hard.
    - W/kg is the standard, so a less efficient module would require more material, size issues to think about. Liftoff technology can be very attractive.
    - Radiation conditions are another great consideration.