

Basic Research Opportunities in CU-Chalcopyrite Photovoltaics

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BASIC RESEARCH OPPORTUNITIES IN CU-CHALCOPYRITE PHOTOVOLTAICS

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ABSTRACT

A brief review is presented of fundamental research topics of primary importance to the development of improved solar cells based on chalcopyrite-structure materials. The opinions presented are a consensus opinion of the authors of the paper, with input from members of the chalcopyrite solar cells research community in the United States. Major topical areas identified included, in order of importance, are 1) development of an integrated predictive understanding of CIGS(S) materials and devices, 2) development of novel deposition techniques and characterization of the mechanisms of growth in existing and novel processes, 3) novel materials, especially with wide-energy gaps (≥ 1.7 eV) other than Cu-based chalcopyrites, 4) development of real-time material characterizations for process control, and 5) alternative front- and rear-contact materials. Although the five topics identified are quite broad, they do not include all topics of interest. Also discussed briefly are some other potential research areas not in the highest priority topics, in particular, areas identified as primarily "engineering" rather than "science."

I. INTRODUCTION

This paper presents the results of a discussion of basic science research topics of primary importance in developing improved solar cells based on chalcopyrite-structure materials. Participants in the discussion were the authors of this paper, with input from a number of other experts in the field. The discussion was held May 3, 1999, in Seattle, Washington, as part of the Basic Research Opportunities in PV Workshop.

I.A. Significance of Chalcopyrite-Structure Solar Cells

Solar cells based on chalcopyrite materials are produced from thin-film layers on inexpensive soda-lime glass substrates. The specific materials used in the best devices are Cu(In_{1-x}Ga_x)Se [CIGS] alloys, although other highly efficient devices have been produced with some selenium replaced with sulfur [CIGSS] and with pure CuInSe₂ (CIS). Significant advantages of these alloys include: they span the energy-gap range needed to make the highest efficiency single- and

multijunction solar cells, they work well in the form of small-grained ($\sim 1 \mu\text{m}$) polycrystals, and they are not strongly sensitive to impurities and crystalline defects. It is important that the materials function well in thin-film form, as thin-film manufacturing processes are well known to be scalable and capable of coating very large areas of glass at practical costs. It will be necessary to produce thousands of square kilometers of solar cells to make a major contribution to world energy needs.

CIGS(S) [$\text{Cu}(\text{In}_{1-x}\text{Ga}_x)\text{Se}_2$ or $\text{Cu}(\text{In}_{1-x}\text{Ga}_x)(\text{Se}_{1-y}\text{S}_y)_2$]-based solar cells have the highest verified efficiencies in both small-area devices and large-area (4000 cm^2) modules, 18.8% and 12.1%, respectively, of any thin-film photovoltaic technology. Performances exceeding 16% conversion efficiency are achieved routinely in a number of laboratories worldwide. Test modules and arrays based on CIGS(S) alloys have been operating outdoors for over 10 years with little degradation. Furthermore, no increase in degradation has been found as overall performance of devices and modules has improved. The prospects for CIGS(S) solar cell technology changed significantly in the past year when Siemens Solar Industries began selling modules based on CIGS(S). Several other manufacturers are making exciting progress, and they appear poised to enter the market with products of their own in the future.

Not only do CIGS(S) solar cells hold the current thin-film performance records, but these records have also been achieved in single-junction devices with energy gaps that are not optimized to the solar spectrum. Significant further advances can be anticipated with either tandem-structure devices or with larger energy gaps in the absorber layers. By contrast, competing technologies have either nearly fully exploited the potential of multijunction devices (as in the case of amorphous Si) or lack the broad range of alloys needed to make a multijunction device (as for CdTe).

In spite of the many advantages of CIGS(S), major hurdles exist before it can achieve its optimal performance and lowest cost of manufacturing. The most significant hurdle is the lack of a sufficient understanding of the materials, processing methods, and devices. A number of senior members of the CIGS(S) community producing high-performance devices have been heard to make comments that can be paraphrased as, "We do it, but we do not fully understand why it works." Optimization of current devices and the planning and design of new devices are often done empirically, based on experience with what worked before or based on "conventional wisdom." As the scientific understanding of CIGS(S) materials has gradually progressed, many of these assumptions have been proven wrong or misguided. Unfortunately, most major questions remain unsatisfactorily understood, or serious disagreements exist about the validity of the conclusions. Consequently, the research topics needing immediate attention include some relatively elementary questions.

These problems are magnified by the fact that there is hardly any research on chalcopyrites outside the photovoltaics (PV) community. Thus, while the PV community working on Si or III-Vs can benefit from the tremendous investment that has existed outside PV in basic materials science of Si and III-Vs, the PV community working on CIGS(S) has to carry out its own materials science research.

In addition to basic science issues directly addressing the problems of current-generation CIGS(S) devices, future-generation devices require major scientific research. Questions can be divided into a clearer set addressing specific needs of next-generation devices that will evolve predictably from current devices, and more speculative questions such as whether some undiscovered material exists that can radically improve all devices. In other words, both evolutionary and revolutionary scientific approaches to next-generation technologies are worthy of effort. The recommendations presented here include research addressing both current and future-generation devices through both evolutionary and revolutionary pathways.

In summary, the potential benefits to basic science research in CIGS(S) materials, processes, and device physics are large, and the problems needing attention are fairly clear.

I.B. Objectives of Basic Science for Chalcopyrite Devices

When laying out recommended areas of research, it is important to state in advance the objectives of that research. We considered the time scale of application of any potential research recommended and concluded that dramatic benefits can be expected on all time frames. However, such significant benefits can be anticipated from research in support of current technologies that the highest-priority recommendations address these topics. The results will also be fundamental to planning future generations of devices and even to design of cost-effective and well-organized scientific research exploring the possibility of future device designs. We believe that scientific research on CIGS(S) will yield conclusions that will reach beyond solar cells. With this in mind, we suggest that the scientific objectives of a basic research program in CIGS(S) should be as follows.

- To conduct fundamental experiments leading to broadly applicable physical and chemical principles specifically addressing the material properties and processing of CIGS(S).
- To develop from these results novel materials and processes and quantitative and predictive models of materials and devices.
- To develop the science required for methodical design and manufacture of next-generation chalcopyrite-based solar cells.
- To explore potential revolutionary advances in chalcopyrite materials and processes.

I.C. Current Understanding of Chalcopyrite Materials and Solar Cells

Recent experiments have yielded extremely encouraging results in small and module-sized devices based on CIGS(S) alloys. The best devices generally have alloys containing a majority of CuInSe_2 , with additions of CuGaSe_2 and CuInS_2 at the back and front surfaces in some devices and at constant concentrations in other cases. In general, the performance of the devices falls when the $\text{Ga}/(\text{In}+\text{Ga})$ contents exceed ~ 0.50 , which is not understood. A comparison of the performance of the best small-area CIGS solar cell (18.8%) with that of the best Si solar cell (24%) is shown in Figure 1. It can be seen from the quantum efficiency data that the majority of the difference in performance is in the blue end of the spectrum. Further refinements of the device and development of novel materials for the front contact could potentially reduce or eliminate this difference, further enhancing the CIGS cell performance. One important consideration in making this comparison is that the Si cells are made by a photolithography process that is difficult to scale to large volumes; in contrast, the CIGS(S) cell is made by standard thin-film deposition methods that are currently being expanded to larger areas. In spite of this remarkable performance, factors limiting reproducibility in production of the best devices remain poorly understood.

Some of the major outstanding issues in the materials science and electrical engineering of CIGS(S) devices include the following.

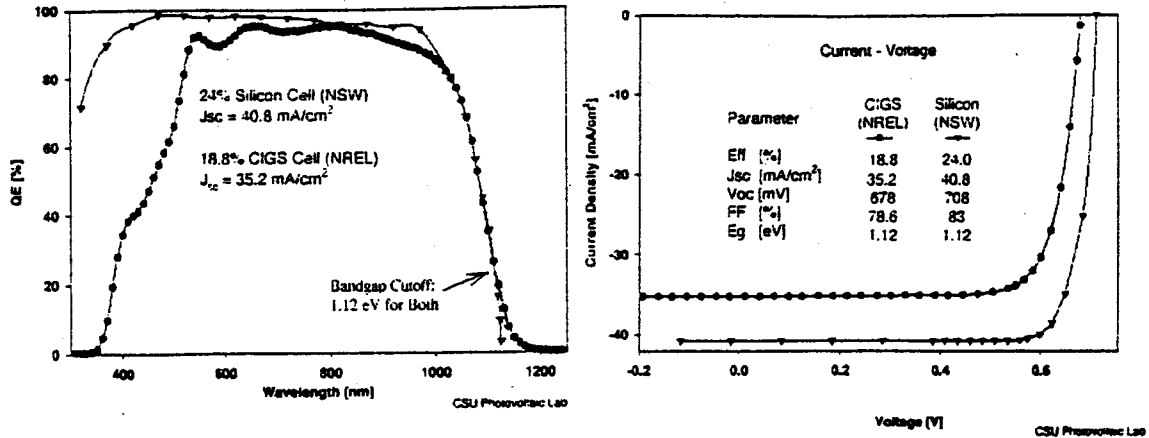


Figure 1: Compares the spectral response (left) and current/voltage (right) curves for the best CIGS solar cell with the best single-crystal Si cell.

- The primary materials factors (phases present, defects, impurities, surfaces, alloy, etc.) that limit the performance of both record and standard devices are not known.
- The nature of the current-collecting barrier (homojunction-like or heterojunction-like) is not known.
- A detailed and predictive model of even general aspects of device performance is not available.
- All materials in the device show a clear need for improvement. This includes the front contact, the rear contact, the heterojunction-forming material, and the absorber layer itself.
- The materials and processes currently available are not compatible with fabrication of top-junction devices in tandem- structure CIGS(S) solar cells.

In addition to these areas where science can provide a more systematic procedure for improving the technology of the devices, the limits to performance of existing devices are currently set by a lack of control of the manufacturing processes. Thus, the performance of large-area devices falls significantly below the average performance of small areas of the same units. This reflects problems with yield and is closely coupled to the lack of diagnostic tools that could assist in manufacturing. Although the design and implementation of these tools for individual processes is considered by some to be "engineering" rather than "science," the development of the basic methods used in the characterization of the material and the proof of the concept to be used in process control requires significant true science to be done.

II. BASIC RESEARCH CHALLENGES IN CIGS(S)

II.A. Major Topical Areas for Basic Research

A prioritized list of research topical areas was developed during the course of the workshop. Each topic was assigned a consensus priority for research effort representing the fraction of total effort that the team felt should be devoted to that topic. It was assumed that all topics would be studied in parallel, and all were considered important to the ultimate success of chalcopyrite-based devices. The topical areas, in order of importance and assigned priorities, were:

Topic	Priority
I Development of an integrated predictive understanding of CIGS(S) materials and devices.	30%
II Development of novel deposition techniques and characterization of the mechanisms of growth in existing and novel processes.	30%
III Novel materials, especially with wide energy gaps (≥ 1.7 eV) other than CIGS(S) alloys.	15%
IV Development of real-time material characterizations for process control.	15%
V Alternative front- and rear-contact materials.	10%

As can be seen from the priorities assigned, these topical areas fell into three ranges of importance. The first two were considered the highest priority and vital to effective engineering of advanced materials and devices. In particular, Topic I encompasses a set of detailed theoretical and experimental studies needed to resolve long-standing debates over how the materials and devices function (see discussion below).

Although tandem-junction devices are not specifically mentioned in the above list, it was clear from the discussion that these represent an important area of research. Specific issues needed to produce a working tandem-junction device based on chalcopyrite absorbers fall into Topics I, II, III, and V.

It should be noted that while the five topics identified are quite broad, they do not include all topics of interest. Section II.C. discusses some of the potential research areas that were considered interesting and potentially worthy of funding, but that did not fall into the highest-priority areas. Areas identified as primarily "engineering" rather than "science" topics were not included in the list above, but also represent important areas of research.

II.B. Discussion of Topics of Research Recommended

II.B.1. Development of an integrated predictive understanding of CIGS(S) materials and devices.

The most pressing problems in the design of CIGS(S) solar cells and processes result from the lack of a detailed understanding and models of the materials and cells. Experimental and theoretical work is needed to determine assumptions to be built into device models. The objective of modeling should be to build a three-tier structure. First, basic theoretical studies using first-principles calculations are needed as a foundation for device models. Second, detailed models of the devices need to be shown to predict as many aspects of device behavior as possible. Several versions of such models exist, but they themselves, their input assumptions, and their parameters still require refinement. Finally, a simple device model providing predictiveness without intensive calculations is needed for application at the manufacturing design stage.

First-principles theoretical studies are useful primarily for two reasons: (1) Theory can isolate one factor at a time (e.g., study one particular defect, or one particular surface), whereas this is difficult experimentally. [The inability to separate experimental variables has proven a major problem in characterization of CIGS(S).] (2) Theory can consider geometries or structures that are conceivable, but currently difficult to make in the laboratory. First-principles electronic structure calculations (such as density functional theory) are important tools. In the past, most of the calculations were performed for pure chalcopyrite compounds and simple chalcopyrite alloys and interfaces. Past accomplishments include the analysis of band structures and interband optical transitions of chalcopyrites and their ordered defect compounds (ODC), order-disorder transitions of chalcopyrites and chalcopyrite/II-VI alloys, X-ray structure factors, charge density maps, band offsets between chalcopyrites and between chalcopyrites and II-VI compounds, and band-gap bowing of chalcopyrite alloys. However, only recently, due to a series of theoretical

and computational developments, it has become possible to apply first-principles quantum theory to predict the defect properties of ternary chalcopyrite compounds. This has provided new insights into defect physics in CIGS(S). For example, these calculations investigated the effects of Ga and Na doping in CuInSe₂, and, along with experimental results, have begun to explain the unusual defect properties in CuInSe₂.

Despite recent advances in understanding of the material properties of CuInSe₂ and related compounds, there are still many fundamental questions that need to be answered. It will be important in future work to examine materials from as broad a range of laboratories as possible, produced under as wide a range of conditions as possible.

Although not a complete list by any means, some of the important topics needing more work include the following:

- Understanding the relationship among surface energies and structures, the formation, structure, chemistry and growth of grain boundaries in CIGS(S), and how these affect electronic properties CIGS(S). In particular, debates concerning segregation of any of the constituent elements to the heterojunction or grain boundaries must be settled.
- Developing effective strategies for doping of CIGS(S) by extrinsic impurities including determination of solubility, level-depth, whether co-doping can improve the dopability in CIGS(S), and which intrinsic defect limits the maximum doping in CuInSe₂. It will also be useful to determine the defects controlling the lifetime of minority carriers and the trapping and detrapping rates for these.
- Developing improved alloys, defect phases, and polytypes of CuInSe₂ that can improve the PV properties.
- Determining whether the solar cells should be viewed as homojunction or heterojunction devices, and determine the role of the window/heterojunction materials.
- Establishing a data base for all chalcopyrite compounds, and use it to select the best materials for absorbers, multijunction partners and window materials.
- Developing a user-friendly device model using the first-principles model results, as well as experimental data, as input to predict the efficiency of the solar cells.

II.B.2. Characterization of film growth mechanisms and development of novel deposition techniques. The development of photovoltaic device structures based on CIGS(S) has advanced rapidly during the last few years. The direct energy gap of CIGS(S) results in a large optical absorption coefficient, which permits the use of thin layers (1 - 2 μm) of active material, and allows high-device performances in spite of the modest carrier diffusion lengths. The highest-efficiency CIGS(S) device was prepared based on a multi-step physical vapor deposition (PVD) process in which elements are simultaneously co-deposited onto the substrate. Unfortunately, PVD is challenging to scale up in both deposited area and throughput. Process temperatures also tend to be high, which complicates use of polymer substrates and permits interdiffusion of layers in superstrate device geometries. Thus, there is a need to develop novel low-cost and low-temperature methods to form CIGS(S) films. A related high-priority issue in CIS PV technology is improving the understanding of thin-film growth mechanisms in both traditional and novel processes. It is good news that the quality of the CIGS(S) films and devices is becoming increasingly decoupled from the method of film delivery because of improved understanding of growth. However, much work remains to be done.

Vapor-phase co-deposition of elements deposits the chalcopyrite film atom-by-atom with great precision. There are a number of unresolved questions about how PVD co-deposition parameters (e.g., substrate temperature, total- and differential-atomic fluxes, background ambient, and pressure) might be optimized to further improve CIGS(S) film quality. Multi-step sequential

vapor-phase processes are arguably better suited than vapor-phase co-deposition to large-scale, low-cost manufacturing. However, much remains to be understood about them. For example, the mechanisms through which Group I-III metal alloy layers react with Group VI elements to form dense, large-grain CIGS(S) films that adhere well to an underlying electrode are incompletely studied. The mechanisms by which the substrate and electrodes affect the characteristics of resulting CIGS(S) films, and how one might optimally select substrates/electrodes and/or tailor CIGS(S) film deposition processes to surrounding materials need work. Optimal use of alkali metals to improve film properties and achieving desired composition grading in multi-step processes would also benefit process designs. Given the industrial importance of vapor-phase co-deposition and multi-step processes, there is great leverage in their better understanding.

Vapor-phase co-deposition and multi-step processes have in common the use of vacuum deposition methods, which have numerous advantages, including precision composition control, a broad base of processing know-how, and a knowledge base for design of research and production-scale equipment. However, vacuum deposition suffers from high up-front capital equipment costs. A variety of novel film-deposition methods promise to replace capital-intensive physical vapor deposition with non-vacuum deposition of constituent layers and/or complete CIGS(S) films.

Currently, a great deal of effort is being made to develop such low-cost technologies. Processes based on electrodeposition (ED), electroless-deposition (EL), and nanoparticle-based processes have the potential for: (a) a low-cost, high-rate synthesis of CIGS(S); (b) large-area, continuous, multi-component, low-temperature depositions; (c) non-vacuum, low-capital-cost processes; and (d) efficient material use. The devices fabricated using ED, EL, and nanoparticle precursors resulted in efficiencies of 15.4%, 13.4%, and 12.4%, respectively. Such novel techniques offer a variety of potential advantages, but in general they are much less mature -- both from the standpoint of basic science understanding and from the standpoint of empirically developed standard recipes. For example, the mechanisms of nanoparticle layer densification and grain growth are not yet clear. As with studies of vacuum processes, there is significant leverage in exploring non-vacuum processes in more detail.

II.B.3. Novel materials. Novel materials based on ternary CuInSe_2 hold promise for further increasing device efficiencies and lowering product costs. Of particular interest are wider-band-gap materials suitable as absorber films in multijunction devices. Isovalent alloys with gallium and sulfur are useful in this regard, and improved understanding of these materials is a research priority. To date, modest additions of Ga and S in CuInSe_2 have been shown to increase single-junction device efficiencies. However, considerable work is needed to make wide-band-gap materials work as well as currently employed narrow-gap compounds. Furthermore, novel materials, including non-isovalent, non-isostructural alloys such as CIS-ZnSe and nanocrystalline and multi-phase materials may provide advantages relative to the CIGS(S) alloys explored to date. Of particular value would be wide-bandgap materials that can yield efficient superstrate cells that can be mechanically stacked with existing substrate cells to form tandem junctions. Materials that can be processed at low temperatures would facilitate the fabrication of monolithic tandem structures. Further work in characterizing such new materials and exploring which materials might be useful in very high-efficiency multijunction structures should be a priority.

II.B.4. Development of real-time material characterizations for process control. A major issue in any manufacturing environment is the ability to assess the product performance non-destructively during processing. The goals of any such analyses are first to produce material within given tolerances reproducibly. Second, it is necessary to control uniformity and defects in the devices to increase product yield and performance. To be most effective, the test should be non-destructive so that it can be used on all devices. It should not be performed on occasional

test structures. Rather, it should take place at many points during product formation on the normal production material to reduce continued manufacturing on already unsatisfactory devices. Finally, an *in-situ* analysis should permit feedback control of the process to correct problems as quickly and effectively as possible.

The first problem in designing process control systems is knowing what to test. As described above, major questions remain concerning what is characteristic of a good device. General composition ranges can be specified, but many other issues such as the best surface morphology, crystalline orientation, and microstructure are matters of intense debate. Thus, achievements in this category of basic research will be aided by progress in the other topical areas listed here. Nonetheless, some general recommendations can be made.

It is generally agreed that the optimal composition of CIGS(S) films is near stoichiometry, but slightly to moderately rich in the group III elements. The exact amount by which the film should be III-rich is still controversial. Some *in-situ*, non-destructive, non-contact strategies for composition control have been reported. In addition, uniformity and defect density in devices have been studied using optical-beam-induced current (OBIC) measurements. Although this is not a non-contact method and is used at the end of the process, it has been useful in quickly characterizing defects in large areas of devices. A number of other process control strategies have been considered. However, there is clearly a need for much more sophisticated techniques. Examples of such methods could include applications of X-ray fluorescence spectroscopy, photoluminescence, ellipsometry, resistivity, laser scattering, and dual-beam optical modulation (DBOM). Results have been reported with all of these methods characterizing the CIGS(S) materials and devices. However, none have been effectively exploited for process control.

Successful development of effective process control strategies requires detailed scientific analysis of CIGS(S) materials using the techniques and a careful quantitative study of the results to show how specific conditions can be detected and maintained. To control processes effectively, it is necessary to understand the physics of the analysis methods. Relatively little effort has thus far been devoted to understanding the methods outside of manufacturing environments. What has been done has been largely empirical and generally does not produce the basic understanding needed to truly design new methods of process control.

II.B.5. Alternative front- and rear-contact materials. Current CIGS(S) devices use Mo for the back contact and CdS combined with ZnO as the front contact. It is widely agreed that none of these materials is satisfactory. Mo retains large amounts of stress under typical deposition conditions. This is particularly awkward when using flexible substrates. Adhesion of Mo both to the glass substrate and to the CIGS(S) film can be a problem and can lead to localized or general failures. The surface chemistry and reactivity of Mo with Se can influence the characteristics of the absorber and the performance of the device. For example, the presence of a Mo_xSe interlayer between the absorber and the Mo can reduce the penetration of Na from the substrate glass into the absorber. This, in turn, can decrease the acceptor concentration and voltage output of the device. Furthermore, Mo is opaque and consequently will be unacceptable for the back contact of the top device in any tandem-junction device.

The current heterojunction partner material, CdS, is unattractive because of the environmental hazards associated with Cd. Furthermore, although efficient CIGS(S)-based devices are routinely fabricated using a very thin CdS "buffer layer," uncertainty remains as to why solution-deposited CdS. There is also the question of whether alternative materials (e.g., ones that don't contain Cd lowers the efficiency of the device) and alternative processes (e.g., those compatible with in-line vacuum processing) might provide equal or better performance. Consequently, new contact technologies are needed for both single and multijunction CIGS(S) devices.

The next-generation CIGS(S)-based thin-film device will ideally have the following characteristics. The back-contact and substrate combination will offer superior reproducibility to the present soda-lime glass/Mo or stainless-steel/Mo systems. This will expand the list of potential substrates and back-contact metals to those more optimally suited to CIGS(S) thin-film processing and will reduce the cost of manufacturing. Considerable research will be required to understand the details of the interaction of contacts with the absorber layers and how to improve the contact designs.

II.C. Other Issues

Although the most pressing issues in the science of chalcopyrite-based solar cells are covered above, other areas are also worthy of research support. For example, even though CIGS(S)-based devices are well-known for their stability and CIGS(S)-based prototype products have impressive durability, CIGS(S) devices can show transient effects related to electrical bias, light exposure, encapsulation, etc., that require explanation. Although CIGS(S)-based PV devices are relatively impervious to environmental exposure, long-term product performance in a wide range of demanding applications requires a durable, low-cost package. CIGS(S)-based PV shares with other PV technologies a common need for better, more-stable potent materials and less-expensive transparent cover materials. Many other issues could be listed here and are omitted only for brevity. CIGS(S) remains the solar cell technology most in need of studies of a broad range of issues both in science and engineering.

III. SUMMARY AND CONCLUSIONS

The team concludes that a well-planned program of basic scientific research can have a major impact on both the viability of the current-generation CIGS(S)-based solar cells and on the design and implementation of future-generation chalcopyrite devices. We have identified five topical areas of major importance to this process and have attempted to outline some of the specific experiments that could be performed and models that should be developed to have the maximum impact in this field. We have recommended a mixture of approaches aimed at both evolutionary and revolutionary progress. The purpose of the scientific research should be to develop quantitative deposition process/device performance relationships that can be used for process design optimization and control, as well as in the practical possibility of non-empirical engineering of future-generation devices.

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