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Record breaking solar cells: $\text{Zn}_x\text{Cd}_{(1-x)}\text{Te}$ graded bandgap nanoarrays

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Record breaking solar cells: $\text{Zn}_x\text{Cd}_{(1-x)}\text{Te}$ graded bandgap nanoarrays

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Abstract

CdTe is the leading material for thin-film solar cells due to ease of processing and reduced cost. However, low conversion efficiencies due to defects in the material are still a problem in these devices. We propose implementing micro and nano-enabled pseudomorphic growth of ZnCdTe to dramatically increase the efficiency of CdTe solar cells. Simulations predict that defect-free films are possible in graded ZnCdTe nanoislands below 90 nm as well as 24 % efficient solar cells with the use of ZnCdTe grading. Selective growth of CdTe showed single grains when the island sizes decreased below 300 nm. The simulation and experimental results demonstrate for the first time the ability to use nanopatterned substrates to enhance uniformity and efficiency in CdTe thin film solar cells. More than 20 reports, presentations, and papers were produced as part of this work and the results from this project enabled UTEP and Sandia to secure to grants.

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1. INTRODUCTION

CdTe thin film solar cells have the lowest module cost in the market ($\sim 75\phi$), making them the most desirable thin film technology. CdTe has an ideal direct bandgap of 1.5 eV providing a theoretical conversion efficiency of $\sim 30\%$. However, laboratory cell efficiencies of CdTe based solar cells have not improved significantly for the last 17 years and the current world record efficiency is 17.3%. Low efficiencies are attributed to the low minority carrier lifetime caused by the high defect density that results from the lattice-mismatch between CdS and CdTe [1]. These defects trap carriers, reduce the voltage, fill-factor (FF), and efficiency of CdTe PV modules. Up to 4% of the losses can be attributed to low voltage and low FF, which is directly related to defects [2].

2. PROPOSED CONCEPT

We propose implementing nano-enabled pseudomorphic growth of ZnCdTe to dramatically reduce defects and increase the efficiency of CdTe modules. Figure 1 shows a cross-section schematic of the structure we proposed. The graded colors from green to red represent different composition and graded bandgap of the ZnCdTe alloy, and the 100 nm scale bar tells the dimensions of the nano-pattern in which we will deposit the ZnCdTe alloy. Varying the composition of $\text{Zn}_x\text{Cd}_{1-x}\text{Te}$ causes favorable variation in the lattice parameter and bandgap. When combined with nanoscale crystal growth, increasing Zn content improves the lattice matching between ZnCdTe and CdS. Moreover, a graded bandgap creates an internal built-in field, which enhances the collection of minority carriers [3], reduces recombination [4], and leads to higher efficiencies by localizing absorption [5]. Molecular dynamics (MD) with an analytical bond order potential (BOP) [6] was also proposed to simulate the growth of compound semiconductors and understand the fundamental physics of defect formation on mismatched substrates.

Figure 1. A graded bandgap and a nanopatterned substrate help the reduction of defects.

3. RESULTS

3.1 Simulations

3.1.1 Crystal Growth

In order to model our concept, we studied the growth of CdTe and $\text{Zn}_x\text{Cd}_{1-x}\text{Te}$ using molecular dynamics (MD) simulations based upon bond-order potentials (BOP). One advantage of MD simulations is that they solve the positions of atoms as a function of time using the fundamental Newton's equation of motion and therefore can reliably track the defect evolution at an atomic-scale resolution. The BOP is a novel potential based on quantum mechanics that can accurately predict defect type and density in heterostructures[7,8].

High-resolution transmission electron microscopy (HRTEM) experiments have been performed to examine defects in CdTe/GaAs multilayers with a lattice mismatch of $\epsilon_0 \approx 12.78\%$ [10]. To directly compare the accuracy of our simulations with the experiments, we performed an MD simulation of CdTe overlayer growth using the same lattice mismatch. The computational system, shown in Fig. 2(a), is periodic in the x and z directions containing 100 (10.1) and 8 (101) planes, respectively. To incorporate the lattice mismatch with only the CdTe BOP, a substrate containing 35 (040) planes in the y (thickness) direction was compressed by 12.78 % in the x dimension to match the size of GaAs. To prevent the dimension from relaxing back to that of CdTe, the atomic positions of the bottom 25 (040) planes were fixed during a constant volume MD vapor deposition simulation. The configuration obtained after about 4 ns of deposition is shown in Fig. 2(a) with comparison to a modified HRTEM image [9] shown in Fig. 2(b). Figure 2(a) indicates seven misfit dislocations near the interface. These dislocations are clearly the edge type of Lomer dislocations with two extra planes about 144.7° from the y axis. Both the dislocation configurations and average dislocation spacing are in remarkably good agreement with the experimental results shown in Fig. 2(b).

Figure 2. BOP simulation and HRTEM image of atomic structure of CdTe-on-GaAs multilayers

MD simulation using the high-fidelity BOP was applied for the first time to thin-film CdTe-based solar cells to explore formation of misfit dislocations as a function of island sizes. The geometry used in the simulations is shown in Fig. 3, where the substrate and the islands are shown in yellow and blue, respectively. The growth direction is in the [010] direction. Using the experimental lattice mismatch strain of 0.10 between CdTe and CdS, molecular statics (i.e., energy minimization) simulations were performed, and the results are shown in Fig. 3 for an island size of approximately 15 nm and an island height of about 6 nm. Fig. 3 clearly shows 3D strain relaxation of the CdTe islands along the growth direction. This strain relaxation helps reduce misfit dislocations. BOP-MD leads to an analytical expression of energy as a function of dislocation density, mismatch strain, and island size. The energy-minimizing dislocation density can then be solved as a function of island width and lattice mismatch, as shown in Fig. 4. The results indicate that the dislocation density can be reduced from a $\sim 0.04 \text{ \AA}^{-1}$ in planar CdTe/CdS solar cells (red point) to zero (blue point) in ZnTe/CdS if the island width is $\leq 90 \text{ nm}$.

Figure 3. Simulated CdTe island growth on top of CdS. 3D relaxation of stress processes occur in the growth processes

Figure 4. Dislocation density vs. island width for different island-substrate mismatches

3.1.2 Electrical Performance

A way to reduce defects in the interface is to use a graded composition material $\text{Zn}_{(x)}\text{Cd}_{(1-x)}\text{Te}$ where X changes as the growth happens. This graded composition will have a threefold purpose 1) It will reduce the amount of defects in the interface due to the reduced lattice mismatch; 2) it will also enhance absorption due to internal electric fields created by the graded bandgap [5]; and 3) it will enhance the ohmic response of the back contact. In order to prove the concept, several simulations using the software wxAMPS [10] were done. Figure 5 shows a simulated bandgap diagram (no bias) illustrating the position of the gradings. The grading used in contact with the CdS will be referred as the front grading and the one used for the ohmic contact will be referred as the back grading. The incorporation of zinc could reduce lattice

mismatch and thus defects. The lattice mismatch between wurtzite CdS:CdTe is 10.1% and only 4.6% between wurtzite CdS:ZnTe. However, there is a tradeoff between the level of defects released due to the use of Zn and the electrical degradation due to the incorporation of Zn.

Figure 5. Band energy diagram of proposed front and back gradings incorporating zinc. The gradings will reduce defect density at the front interface and enhance the contact in the back

It is well known that CdTe with its high electron affinity of 4.5eV is hard to contact, either due to effects caused by the diffusion of the metal or because of the rarity of metals with high work functions. In order to overcome the high work function of CdTe, we add zinc to the structure to form a graded structure in the back. The back grading consists of a $\text{Zn}_{0.1}\text{Cd}_{0.9}\text{Te}$ layer. Figure 6 shows the simulated current density vs. voltage curves (J-V curves) of three devices for different grading conditions in the front together with an enhanced back contact. The back grading acts as a reflector layer that reduces recombination, improves the voltage, and enhances the ohmic contact. As a result, the performance of the cell goes up dramatically. According to simulations, if both reduced defects and graded structures at the front and back are used, the overall performance of the cell will be enhanced. Figure 7 shows the simulation results of using the graded structure in the front and back. It's important to mention that Zn compositions less than 30% are not shown because they do not relieve the stress in the junction and thus do not make a difference in the defect density. From Figure 7 it can be seen that it is desirable to obtain less defects and use a small amount of Zn in the matrix

Figure 6. Effect of different gradings in the front of the cell together with a back grading reflector layer.

Figure 7. Solar cell efficiency vs. the zinc composition X in the CdTe solar cells for two different defect densities.

3.2 Material Characterization

Glass/ITO/CdS substrates were micro and nano-patterned using the following patterning techniques: Optical lithography (OL), Nano Imprint lithography (NIL), Interferometry lithography (IL), electron beam lithography (eBeam) and step and flash imprint lithography-reversed tone (SFIL/R). CdTe was subsequently selective grown in these samples and the microstructure was analyzed with SEM/FIB and EBSD. From SEM/FIB analysis, it can be seen that positive selective growth of CdTe was achieved at the micro and nano scale level. Also, as it

is shown from figure 8b, uniform and single nano-CdTe grains were obtained in nano-patterned substrates, compared to multigrain structures obtained in the micro patterned substrates (Figure 8a). EBSD in figure 8a shows that multiple CdTe grains corresponding to different colors were obtained in each micro-window. On the other hand, EBSD shows only one color representative to one CdTe orientation per nano-window when CdTe was grown on a no-patterned glass/ITO/CdS substrates.

Figure 8. FIB/SEM cross-section and EBSD analysis confirms multi-grain CdTe structures on micro-patterned substrates a) vs. single-grain CdTe structures on nano-patterned substrates b)

Separate from development of the selective-area growth, initial experiments were conducted to achieve compositional variation. Initial growths incorporate ZnTe as a buffer layer between CdTe and CdS. Fig. 9 shows cross section transmission electron microscope (TEM) images of two samples taken at a 2,100X magnification: 9a) CdTe and 9b) ZnTe grown on planar CdS/ITO/glass substrates. Fig. 9 indicates that even though higher temperatures usually yield bigger grains, the grain sizes of the CdTe/ZnTe/CdS films grown at the lower temperature resulted in bigger grains than the ones obtained for the CdTe/CdS films grown at a higher temperature (our best condition). This indicates that ZnTe can be used as a buffer layer to reduce grain boundaries due to the smaller lattice mismatch between ZnTe and CdS.

Figure 9. Cross sectional TEM image of a) CdTe deposition on top of CdS; and b) CdTe/ZnTe on top of CdS. Bigger grain sizes and fewer defects are apparently visible in the ZnTe deposition than in the CdTe deposition.

3.3 Electrical Characterization

Electrical performance of the selectively grown CdTe on micro-patterned substrates was tested by making solar cell devices of 0.5cm in diameter and also by using a nano-manipulator to probe individual micro-islands and test their J-V responses. A 10 μm-thick CdTe film was grown on top of the selectively grown micro-CdTe islands to fabricate solar cell devices. Prior the back contact formation, samples received a CdCl_2 treatment and NP etching. Even though the efficiencies of these first devices were not so high, it was proved that solar cells can be fabricated using micro-patterned substrates. A J-V plot of three contacts of a micro-patterned CdTe solar cell is shown in figure 10

Figure 10 JV measurements show that solar cell devices can be fabricated with micro-patterned CdS substrates

Micro-CdTe islands were also tested individually to study their electrical performance as a function of size. In order to improve the electrical contact between the CdTe micro-islands and the nano-probes of the nanomanipulator, selective growth of Copper was made on top of the micro-islands and J-V measurements were made on them as shown in figure 11

Figure 11. JV measurements with a zyvex nanomanipulator station on micro-CdTe islands will be used to study the effect of feature size on the electrical performance of micro and nano cells

4. PROJECT IMPACT

The outcomes of the project presented in this report are the result of the collaboration among 4 campuses: SNL-CA, SNL-NM, UTEP and CINT. 14 sandians from 3 different divisions were directly involved in this project plus 2 professors and 7 students from UTEP: 3 PhD's, 3 Master's and 5 undergraduates. By the end of the NINE funding, 2 Master's students defended their theses, 4 journal articles and 2 conference papers were published, 1 was submitted, 2 additional papers are in preparation, 1 Technical Advanced and 1 patent are being processed. In addition to supporting sandians on this project, 5 students were directly supported at UTEP and 3 students were supported for summer internships for 2 years in Sandia. The results of this project were presented at 9 conferences. Finally, this project help Funding through one NSF awarded to UTEP, and one DOE gran granted to the Sandia/CINT/UTEP team.

5. CONCLUSIONS

We presented a summary of simulations and experiments using graded composition and nano-island growth to reduce misfit defects in CdTe/CdS solar cell devices. For a complete description, refer to the published work. Defects are the major reason for the low current, voltage, and efficiency of the CdTe photovoltaic modules because they trap and recombine carriers. A significant reduction in defects is therefore expected to significantly enhance the efficiency of CdTe based solar cells, which may enable the cost of the PV module to reach the \$0.50/W target value. Our high-fidelity molecular dynamics simulations predicted that defect-free films are possible if the CdTe film is graded with Zn and is constructed as nano-islands with island sizes below 90 nm. Our experiments showed that it is feasible to achieve selective deposition and that smaller window sizes are desirable to create single crystal growths. Also, the grain sizes are larger when using a CdTe/ZnTe stack than when using only a single layer CdTe. The simulation and experimental results demonstrate for the first time that nanopatterned substrates can be used to enhance uniformity in thin film solar cells.

6. MANUSCRIPTS, PRESENTATIONS, POSTERS AND INTELLECTUAL PROPERTY GENERATED THROUGH THIS WORK

Oral presentations and posters without proceedings

Jose L. Cruz-Campa, David Zubia, Xiaowang Zhou, Donald Ward, Carlos A. Sanchez, Jose J. Chavez, Brandon A. Aguirre, Farhana Anwar, Damian Marrufo, Erik D. Spörke, Calvin Chan, Ping Lu, Michael J. Rye, Heber Prieto, John C. McClure, and Gregory N. Nielson, Path to increase efficiency in thin film CdTe solar cells, New Mexico Chapter of AVS. The Science & Technology Society Symposium, May 22, 2012- Albuquerque, NM

Jose L. Cruz-Campa and David Zubia, Record breaking solar cells, 4th Thin Film Solar Summit USA, December 1-2, 2011, San Francisco, CA

Aguirre et. al., Selective Growth of CdTe on Nano-Patterned CdS, Southwest Energy Science and Engineering Symposium, El Paso, TX, March 2012

J Chavez et. al., Molecular Dynamics Simulation of Strained, Nanoscale CdTe Crystal Growth using Bond-Order Potentials, Southwest Energy Science and Engineering Symposium, El Paso, TX, March 2012

F Anwar et. al., Novel Control Technique For Cadmium Sulfide Chemical Bath Deposition Using Real Time Monitoring of Cadmium Ion Molarity, Southwest Energy Science and Engineering Symposium, El Paso, TX, March 2012

D Marrufo et. al., Growth of Thin Film Cadmium Telluride and Zinc Telluride Films Using Novel Close Space Sublimation Depositor, Southwest Energy Science and Engineering Symposium, El Paso, TX, March 2012

Aguirre et. al., CdTe Growth Control Using Patterned CdS Substrates for CdTe Solar Cells, CINT symposium, Albuquerque, NM, September 2012

J Chavez et. al, Nanostructure-Boost of Energy Conversion Efficiency of CdTe/CdS-Based Solar Cells: New Predictions and Experimental Studies, ASME 6th Conference on Energy Sustainability, San Diego, CA, July 2012

Aguirre et. al, Poster presentation, Micro & Nano Technology Forum of the ASME conference in Houston, November 2012

J Chavez et. al, Poster presentation, Micro & Nano Technology Forum of the ASME conference in Houston, November 2012

J Chavez et. al. Poster presentation, Simulations on CdTe growth, MAES symposium, Las Vegas NV, 2011

Journal papers

J. Chavez, D. K. Ward, B. M. Wong, F. P. Doty, J. L. Cruz-Campa, G. N. Nielson, V. P. Gupta, D. Zubia, J. McClure, and X. W. Zhou, Defect formation dynamics during CdTe overlayer growth, Physical Review B, in press (2012)

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CdTe vapor deposition from a bond-order potential-based molecular dynamics method, Physical Review B 85, 245302 (2012)

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X. W. Zhou, D. K. Ward, B. M. Wong, F. P. Doty, J. A. Zimmermann, Molecular Dynamics Studies of Dislocations in CdTe Crystals from a New Bond Order Potential, The Journal of Physical Chemistry C, 116, 17563 (2012)

Conference papers

Jose L. Cruz-Campa, David Zubia, Xiaowang Zhou, Donald Ward, Carlos A. Sanchez, Jose J. Chavez, Brandon A. Aguirre, Farhana Anwar, Damian Marrufo, Erik D. Spörke, Calvin Chan, Ping Lu, Michael J. Rye, Heber Prieto, John C. McClure, and Gregory N. Nielson, Towards Dislocation-Free ZnCdTe Solar Cells Through Nanoscale Crystal Growth And Compositional Grading, Proceedings of EU PVSEC 2012, in press

Jose L. Cruz-Campa, David Zubia, Xiaowang Zhou, Donald Ward, Carlos A. Sanchez, Jose J. Chavez, Brandon A. Aguirre, Farhana Anwar, Damian Marrufo, Ping Lu, Michael J. Rye, John C. McClure, and Gregory N. Nielson, Nanopatterning And Bandgap Grading To Reduce Defects In CdTe Solar Cells, Proc. 38th IEEE PVSC, In Press (2012).

Master Thesis

Farhana Anwar NUMERICAL MODELING OF CdS/Zn_xCd_{1-x}Te SOLAR CELL, University of Texas at El Paso, Summer 2012

Heber Prieto NANOPROBE I-V CHARACTERIZATION OF CdTe/CdS MICRO AND NANO-PATTERNED SOLAR CELLS, University of Texas at El Paso, Summer 2012

Technical advances

SD-12202 PHOTOVOLTAIC CELL WITH NANO-PATTERNED SUBSTRATE

Patents

PHOTOVOLTAIC CELL WITH NANO-PATTERNED SUBSTRATE. Prepared in September by the legal department of Sandia National Labs. Filing in process

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