Optical Analysis of II-VI Alloys and Structures for Tandem PV

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ABSTRACT

This project focuses on the optical analysis of II-VI alloy materials for tandem PV devices, including CdMnTe and CdMgTe for the top cells, and HgCdTe for the bottom cells. These thin film ternary alloy materials are being explored for use in both two-terminal and four-terminal device configurations. With complete optical properties for the alloys as well as for the other device components, e.g., transparent back contacts for top cells and interconnect junctions between cells, tandem designs can be developed that minimize not only optical losses but also thicknesses of the components to ensure high performance.

1. Objectives

The overall project objective is to develop the science and technology base of a polycrystalline thin-film technology leading to tandem cells reaching 25% efficiency at AM1.5. The University of Toledo CdTe group is developing II-VI ternary wide-band-gap alloys of $Cd_{1-x}Mn_xTe$ and $Cd_{1-x}Mg_xTe$, as well as thin CdTe in the high performance configuration, e.g., with appropriate current matching to bottom cells of the low-band-gap II-VI ternary $Hg_xCd_{1-x}Te$. Sputtered films of In_2O_3:Sn (ITO), ZnO:Al, ZnTe:N, and ZnTe:Cu are being explored to meet the need for transparent back contacts and low resistance interconnects in monolithic two-terminal structures. Additional key objectives involve the application of spectroscopic ellipsometry as a rapid evaluation tool for electronic structure that facilitates rational materials optimization, but also for the development of an optical property database that facilitates rational device optimization. Using the determined optical functions of the individual components, optical modeling is to be performed with thicknesses and compositions as variables to establish optimum collection. This report focuses on the objectives in the area of spectroscopic ellipsometry.

2. Technical Approach

Three separate technical approaches have been adopted for application of spectroscopic ellipsometry to alloy materials and device development.

(1) Ex situ ellipsometric spectra are obtained on as-deposited films to determine the band gap and critical point structure (i.e., the higher energy band gaps). Such measurements are repeated after $CdCl_2$ treatment and the energy shifts and changes in width of the band gap and critical point structures provide information on the survivability of the alloy and possible desirable increases in grain size.

(2) Accurate dielectric functions are determined for those alloys that have been deposited and treated successfully under $CdCl_2$ vapor while retaining the appropriate alloy composition and band gap. Dielectric functions are also determined for all other components of the device, including the glass and TEC coatings, CdS, transparent back contact, recombination junction materials, and metallic back contact.

(3) The dielectric function database is used in the optical design of tandems, focusing on the two terminal configuration that requires current matching. In such studies, the maximum possible current is determined, based on incident AM1.5 irradiance.

3. Results and Accomplishments

Figure 1 shows the raw optical spectra and the deduced dielectric function for a magnetron sputtered $Cd_{1-x}Mg_xTe$ thin film deposited from a target formed from 80/20 wt.% CdTe/MgTe. The substrate was soda lime glass held at ~200°C. The pressure was 2.5 mTorr, and the plasma power was 40 W. Table 1 demonstrates the success of the $CdCl_2$ treatment of this film through measurements of the band gap before and after the treatment, as well as the energies and widths of the higher energy critical points. The critical point narrowing that occurs with $CdCl_2$ treatment of the $Cd_{1-x}Mg_xTe$ alloy is significant, an indication of a large increase in grain size as occurs in CdTe.

Figures 2-4 show the results of optical calculations of short circuit current, optical quantum efficiency, and reflectance and absorption losses in the non-active layers. The calculations were performed using the dielectric function database developed through this work. Dielectric functions for the best $Cd_{1-x}Mg_xTe$ with a band gap of 1.6 eV were used, as were those for single crystal $Hg_xCd_{1-x}Te$ with a band gap of 1.1 eV. For $Hg_xCd_{1-x}Te$, development of a dielectric function for the optimum treated films is in progress.

Figure 2 shows the total current under current-matched conditions as a function of total active layer thickness. (Individual layer thicknesses are shown in parentheses in the figure.) The results of Figs. 3-4 depict the quantum efficiency, the reflectance, and the absorption losses for the pair of current-matched thicknesses of 0.61 μm for $Cd_{1-x}Mg_xTe$ and 1.5 μm for $Hg_xCd_{1-x}Te$ in a realistic model that forms a starting point for our studies. The losses include (i) reflection from the full structure (1.9 mA/cm^2 for E>1.6 eV and 3.7 mA/cm^2 for 1.1<E<1.6 eV); (ii) absorption in the glass and TCO layers assuming TEC-15 (2.3 mA/cm^2 for E>1.6 eV and 4.1 mA/cm^2 for 1.1<E<1.6 eV); (iii) absorption in the top 1300 Å CdS layer (4.9 mA/cm^2 for E>1.6 eV); and (iv) absorption in the heavily doped 1000 Å ZnTe top cell back contact (1.0 mA/cm^2). If these losses could be overcome the matched current could reach ~22 mA/cm^2. Such modeling gives insights into the steps needed to reach the 25% efficiency threshold in thin film PV technology.

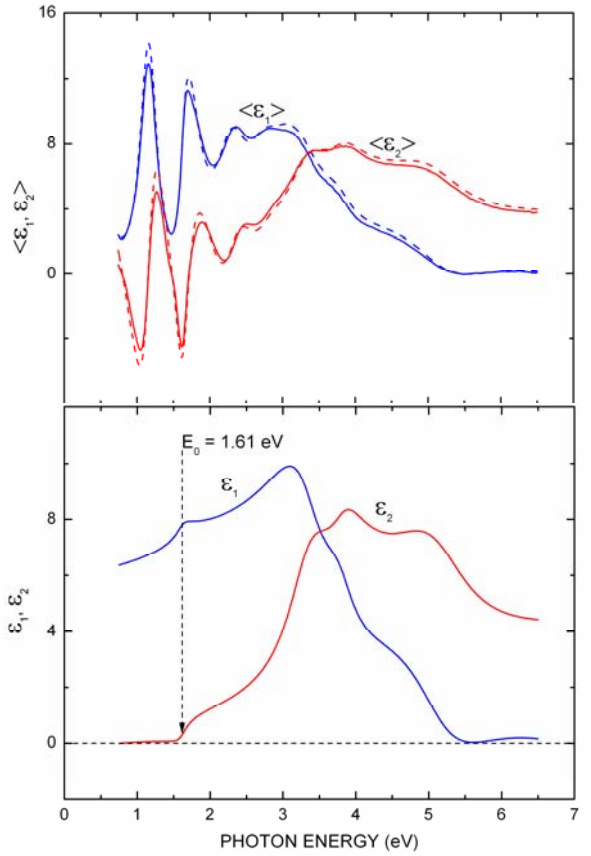

Fig. 1 Unprocessed optical spectra (top) and deduced dielectric function for an as-deposited $Cd_{1-x}Mg_xTe$ alloy.

	CdTe as-dep.	CdTe $CdCl_2$-treat.	CdMgTe as-dep.	CdMgTe $CdCl_2$-treat.
E_0 (eV)	1.497	1.499	1.615	1.633
E_1 (eV)	3.274	3.331	3.354	3.303
$\Gamma(E_1)$ (eV)	0.411	0.200	0.480	0.216
$E_1+\Delta_1$ (eV)	3.844	3.883	3.901	3.878
$\Gamma(E_1+\Delta_1)$ (eV)	0.484	0.368	0.520	0.309
E_2 (eV)	5.193	5.208	5.179	5.197
$\Gamma(E_2)$ (eV)	0.993	0.796	1.252	0.879

Table 1 Band gap and critical point energies and widths for the as-deposited and $CdCl_2$-treated $Cd_{1-x}Mg_xTe$ of Fig. 1 in comparison with CdTe results.

Conclusion

The utility of optical studies based on spectroscopic ellipsometry for development of thin film II-VI ternary alloys for tandem PV has been demonstrated. The dielectric function of the film in as-deposited and $CdCl_2$ treated states provide immediate feedback into the success of the treatment. Also, the dielectric functions serve as a database for tandem cell design.

Acknowledgments

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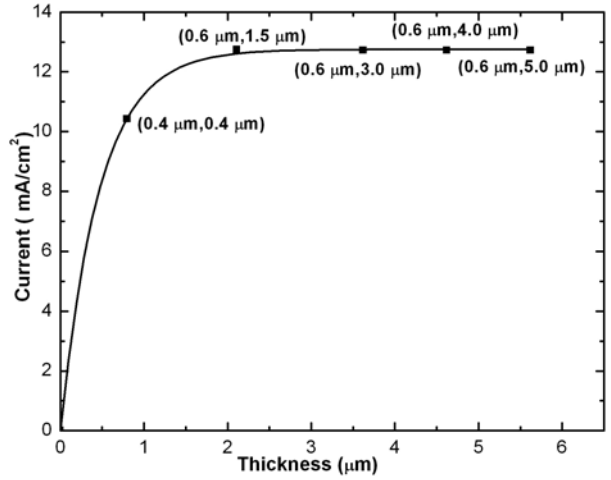

Fig. 2 Predicted maximum current versus total active layer thickness for realistic $Cd_{1-x}Mg_xTe$ - $Hg_xCd_{1-x}Te$ tandems.

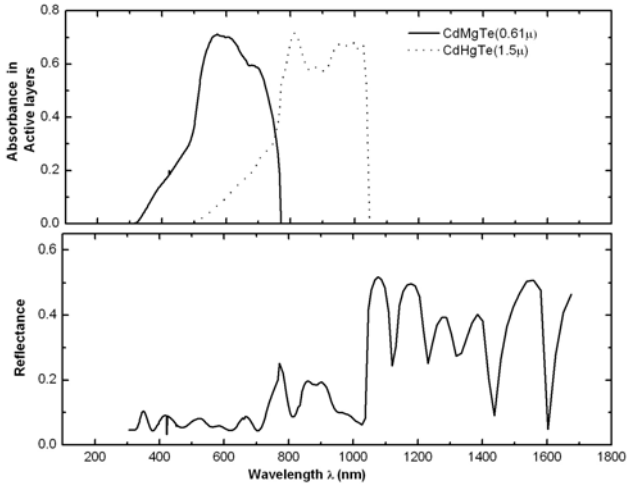

Fig. 3 Predicted maximum QE and the reflectance for a $Cd_{1-x}Mg_xTe$ (0.61 μm) - $Hg_xCd_{1-x}Te$(1.5 μm) tandem.

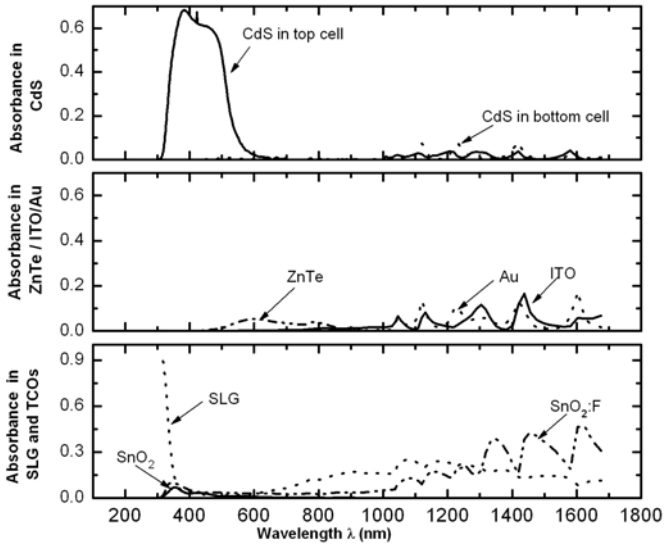

Fig. 4 Predicted absorption losses for a $Cd_{1-x}Mg_xTe$ (0.61 μm) - $Hg_xCd_{1-x}Te$(1.5 μm) tandem.