

Probing the Interface Morphology and Atomic Distribution in Photovoltaic Materials Using Synchrotron Radiation

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ABSTRACT

Interface morphology and atomic density profile are important factors for controlling the physical properties of layer-structured photovoltaic materials. High intensity x-rays from synchrotron radiation now can afford many useful techniques to be used for non-destructive characterization of buried interfaces and density profile of specific elements, in many cases that cannot be achieved by the other conventional characterization methods. Examples of recent applications of three methods (i) Grazing Incidence X-ray Scattering (GIXS), (ii) Angular Dependence of X-ray Fluorescence (ADXRF), and (iii) X-ray Absorption Fine Structures (XAFS) to the studies of CdS/CdTe, $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$, CdS/Cu(In,Ga)Se₂, and CdS/Zn₂SnO₄ systems are presented.

X-rays from synchrotron radiation provide many useful approaches for probing the atomic density depth profiles, the morphology of *buried* interfaces, as well as the local structure around defects in layer-structured materials. In comparison with other known method such as STEM, the x-ray techniques show many advantages, for example: *nondestructive* characterization of buried interfaces, no need for vacuum, suitable for large-scale on-line evaluation of as-made thin film PV materials, capability of obtaining depth profile of specific atomic species in complex materials. Structural information obtained from these techniques are not only important prerequisites for understanding the physical properties of these photovoltaic materials but also can provide valuable feedback for modifying the material preparation processes to improve the performance of photovoltaic devices.

Three methods are especially useful for probing the microstructure in thin film PV materials: (i) Grazing Incidence X-ray Scattering (GIXS), (ii) Angular Dependence of X-ray Fluorescence (ADXRF), and (iii) X-ray Absorption Fine Structures (XAFS). The GIXS method includes measurements of specular and diffuse scattering of x-rays as a function of grazing incidence angle. Due to the angular dependence of the x-ray penetration depth, the GIXS method affords a *nondestructive* tool to obtain important *global* microstructural information about the *buried* interfaces such as the layer thickness, interfacial roughness, and correlation lengths of interface height fluctuations in layered structures. The ADXRF spectrum is obtained by measuring x-ray fluorescence of a selected

element as a function of x-ray incidence angle, it can provide useful information about the compositional depth profile of a selected atomic species in complex material. The XAFS techniques include extended x-ray absorption fine structures (EXAFS) and near-edge x-ray absorption fine structures (NEXAFS). EXAFS generally refers to the modulation of x-ray absorption coefficient about 40-1000 eV above an absorption edge of a specific element, it provides *local* structural information on the interatomic distance, coordination number, and disorder about a selected atomic species. The NEXAFS features are directly related to the transition of core electrons to unoccupied states near the Fermi level, from which the chemical valency, signatures of specific chemical bonding environment can be identified. Details of these techniques can be found in some previous publications: Phys. Rev. **B38**, 8579 (1988); Phys. Rev. **B47**, 16373 (1993); J. Appl. Phys. **83**, 4173 (1998); Appl. Phys. Lett. **74**, 218 (1999); J. Appl. Phys. **86**, 6052 (1999); Appl. Phys. Lett. **76**, 3729 (2000); Phys. Rev. **B63**, 195209 (2001).

In Figs. 1-4, we show examples of GIXS, EXAFS, and ADXRF techniques applied to the studies of different photovoltaic materials. For a CdS/CdTe/glass system, semi-quantitative analysis of the ADXRF data (Fig. 1) shows that Te atoms in the buried CdTe layer were driven into the top CdS layer as the annealing temperature increases. Further

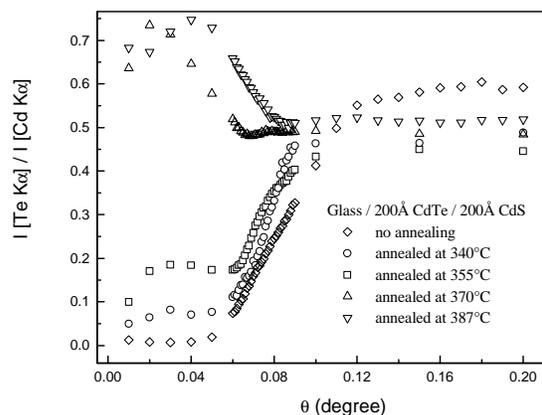


Fig. 1. ADXRF of CdS/CdTe samples.

detailed analysis about the depth distribution of the Te atoms is in progress. Figure 2 shows GIXS data used to characterize the $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ system with various

concentrations of Ge. Layer thickness, interfacial roughness, and exact Ge content of $\text{Si}_{1-x}\text{Ge}_x$ thin films grown on Si substrates by MBE were obtained. Figure 3 shows the EXAFS data used to determine the local structure around Cu atoms in CdTe photovoltaic materials prepared with Cu back contacts. The results indicate that Cu atoms can migrate from the back contact into the CdTe matrix, occupying some interstitial sites, forming Cd-Te complexes around Te or substituting for the Cd sites in CdTe. More recently, an improved data analysis procedure of ADXRF has been employed to obtain the concentration depth profile of constituent elements in a $\text{Zn}_2\text{SnO}_4/\text{CdS}/\text{glass}$ system. An example is given in Fig. 4, where the depth profile of Cd obtained by this new method shows that Cd atoms in the buried CdS layer can migrate into the Zn_2SnO_4 top layer as a result of annealing in Ar, He at $600^\circ - 625^\circ\text{C}$ or in CdCl_2 at $400^\circ - 420^\circ\text{C}$. Annealing in CdCl_2 at a relatively low temperature is of particular interest. It can induce more drastic changes in the Cd density distribution around the $\text{Zn}_2\text{SnO}_4/\text{CdS}$ interface, as clearly revealed by our ADXRF data.

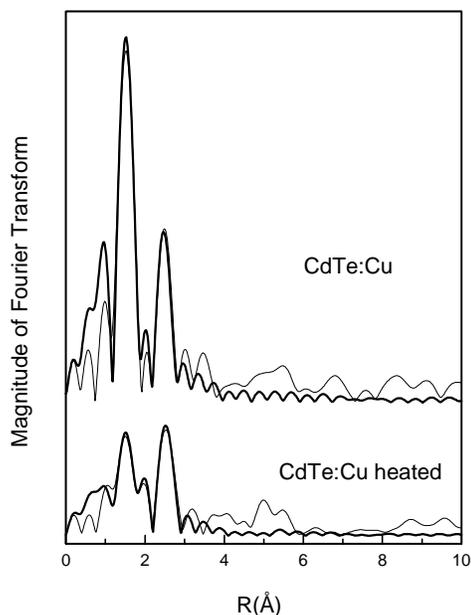


Fig. 3. EXAFS of Cu-doped single crystal of CdTe. Fine lines: experimental. Coarse lines: calculated.

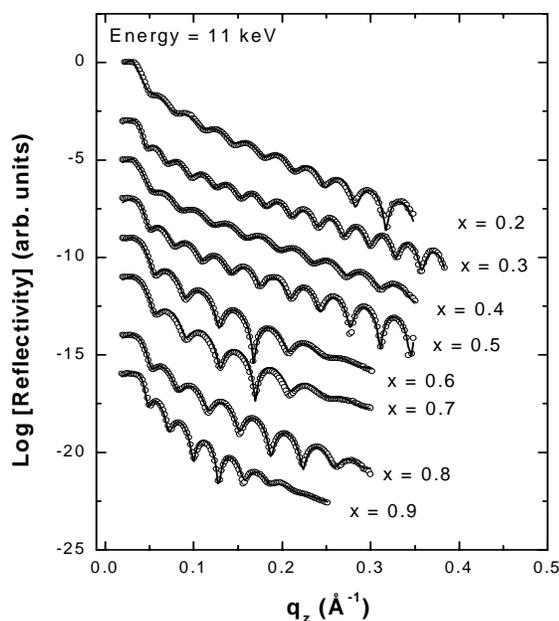


Fig. 2. GIXS of $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ samples. Circles: experimental. Lines: calculated.

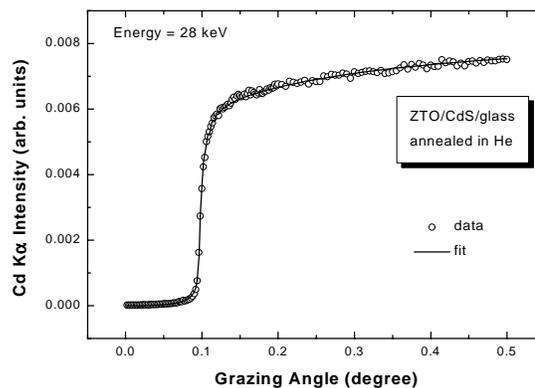


Fig. 4. ADXRF of $\text{CdS}/\text{Zn}_2\text{SnO}_4$ samples.

These results have demonstrated that by using the non-destructive x-ray probing techniques, much detailed microstructure of various photovoltaic materials and interfaces can be characterized without altering the integrity of the cell/device structure.

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