

K-edge EXAFS and XANES Studies of Cu in CdS/CdTe Solar Cells

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Introduction

Copper is an important dopant element in CdTe thin-film solar cells. It is a deep acceptor in CdTe and is commonly used to obtain a heavily doped, low-resistance back-contact. However, Cu is also a fast diffuser in CdTe and can accumulate at the CdS/CdTe junction. It is suspected of leading to cell performance degradation in some cases. A substantial, thermally restorable “aging” behavior was also found in Cu-doped CdTe. The present study is designed to help identify the lattice location and amount of Cu in CdTe.

Methods and Materials

Experiments were performed at the APS MR-CAT beamline sector 10-ID (Fig. 1). Cu K-edge x-ray absorption (XAS) and Cu *K* fluorescence measurements were conducted on thin films of CdTe and on thin-film solar cells based on CdTe. XAS spectra and full fluorescence spectra with 9.5-keV beam energy were collected in a fluorescence geometry with a 13-element Ge detector. A monochromatic x-ray beam is available by tuning the cryogenic Si-111 double-crystal monochromator in Hutch A. Defining slits were set to 400 μm .

Two methods were used to obtain the absorption of the samples. By comparing the transmitted intensity and the incident x-ray beam intensity, sensitive absorption coefficient spectra from Cu-abundant samples (Cu_2Te

powder, CuO powder, Cu foil, and so on) can be easily obtained. However, most CdTe-based solar cells contain only less than 1% Cu. Thus, a much more sensitive method is required. Cu *K* fluorescence (at 8048 eV) intensity, proportional and sensitive to the absorption in the samples, provides a promising method for low-Cu-level XAS spectra measurement. The 13-element Ge detector is designed not only for this purpose but also for obtaining the full fluorescence spectra. Since the Cu *K* fluorescence intensity is also proportional to the Cu concentration in the materials exposed to the x-ray beam, the amount of Cu in CdTe relative to a reference sample with a known concentration of Cu is obtainable. Two samples were prepared as references for these experiments. Layers of 100 \AA and 200 \AA Cu were evaporated on 3- μm polycrystalline CdTe, then diffused at 150°C and 250°C, respectively, for 45 min.

Results

Cu Concentrations by Fluorescence

Cu concentrations in sputtered films, sputtered thin-film solar cells, and sputter targets were found to be much higher than specified by several different manufacturers. Specified concentrations from atomic absorption spectroscopy ranged from 1 to 9 ppm in either CdTe targets or as-received powders. The deposited films, cells, and sputter targets yielded significantly higher apparent concentrations of Cu; however, there is evidence that some of the fluorescence signal is arising from Cu in the sample holder and detector structures. This discrepancy is under further investigation. (See Fig. 2.)

XAS Studies

Figure 3 shows a typical XANES spectrum for a sputtered, polycrystalline film of CdTe 3- μm thick. The film received 20 nm of evaporated copper that was diffused at 250°C. Comparison with reference spectra shown in Fig. 4 indicates that much Cu is located in a local environment similar to Cu_2Te . Complete analysis is still in progress.

Stability of CdTe under Irradiation

CdTe thin-film solar cells, particularly those utilizing Cu in the back contacts, often exhibit changes in

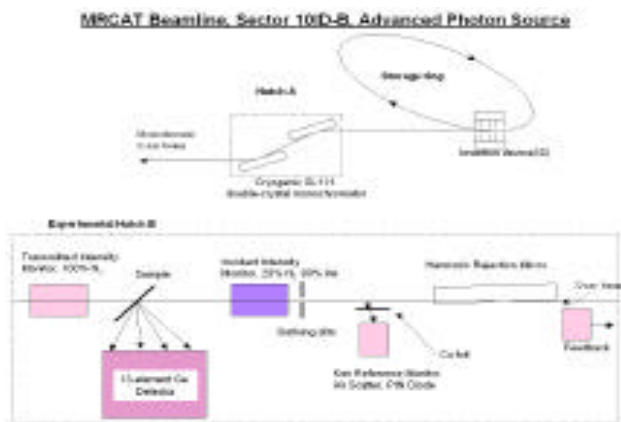


FIG. 1. Experiment apparatus.

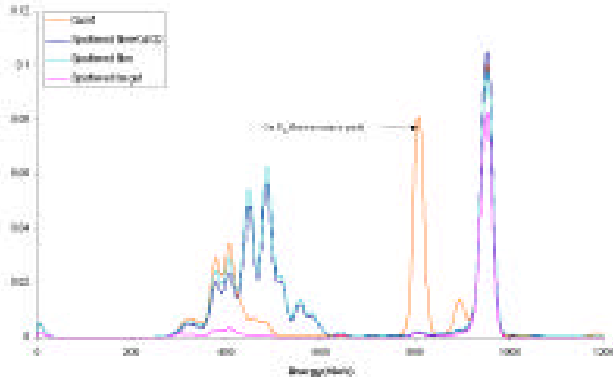


FIG. 2. $\text{Cu K}\alpha$ fluorescence from a sputtered film, a film after treatment with CdCl_2 , Cu foil, and CdTe sputter target.

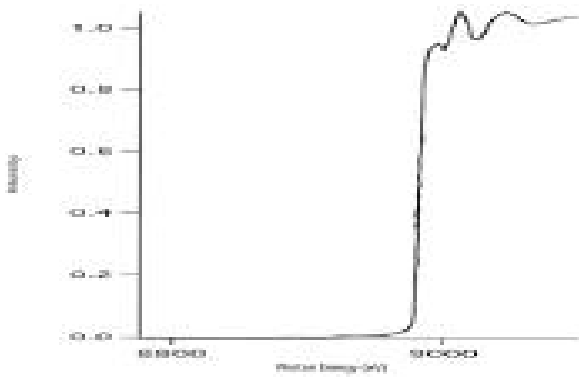


FIG. 3. K-edge x-ray absorption spectrum of 3 mm of CdTe film with 200 μm of diffused Cu.

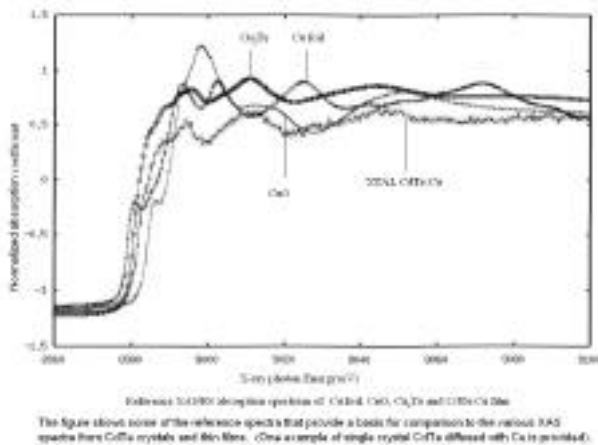


FIG. 4. Reference XANES absorption spectrum of Cu foil, CuO, Cu_2Te , and CdTe:Cu film.

performance under one-sun light soak conditions. It is therefore to be expected that the high-intensity x-ray beam could produce defects in CdTe and perhaps even change the Cu-related chemical bonds in CdTe. We found that spots irradiated by the x-ray beam for only 10 s are visible to the naked eye. We have found that band-to-band photoluminescence (PL) is very sensitive to defects in CdTe and have used this to study the effects of the x-ray beam.

PL mapping was used to study spots on samples exposed to the x-ray beam for about 8 h. The PL mapping is shown in Fig. 5, where the vertical axis represents the total PL intensity observed by the charged-coupled device (CCD) detector in the region from about 770 to 850 nm. The intensity decreased to one-tenth at the center of the x-ray beam irradiated spots.

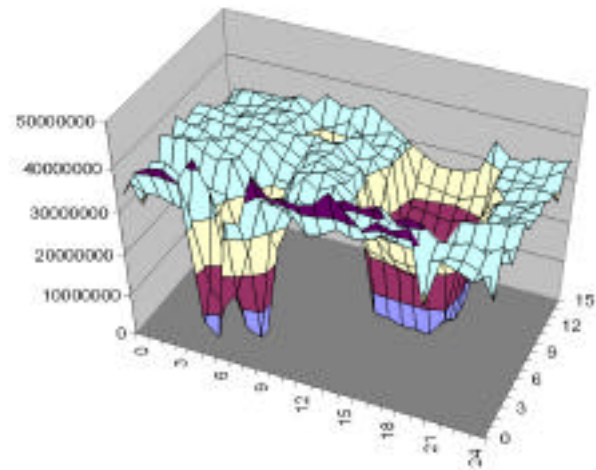


FIG. 5. PL mapping on CdTe cell after 8 h of exposure to x-ray beam.

These x-ray-beam-induced changes observed by PL raise the question of whether the XAS spectra are stable during the data acquisition period of up to 8 h. Therefore we obtained Cu K near edge XANES spectra while rastering a virgin sample under the beam. By comparing it with the XANES spectra from unrastered films after 8 h of exposure, a difference is observed in a pre-edge feature. Fig. 6 illustrates that this pre-edge feature just above 8980 eV is more pronounced in the sample that was moved after each datum point (10-s dwell time).

We are continuing to use a combination of XAS studies and PL studies together with light soaking and other stress conditions to elucidate the mechanisms for these observed changes.

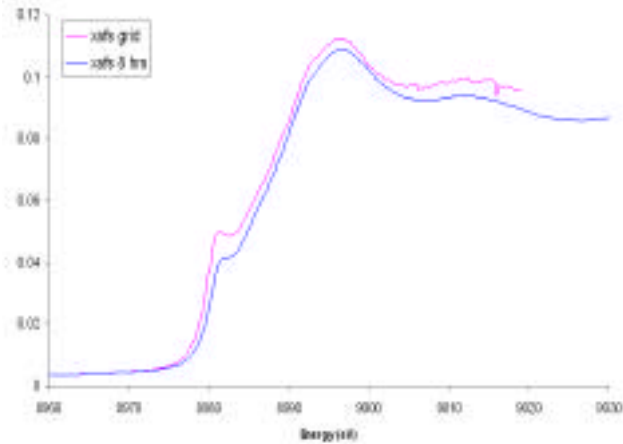


FIG. 6. XANES spectra of rastered virgin cell and a cell exposed for 8 h during data acquisition.

Acknowledgments

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