X-RAY ABSORPTION FINE STRUCTURE STUDY OF AGING BEHAVIOR OF OXIDIZED COPPER IN CdTe FILMS

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ABSTRACT

We have used the MR-CAT beamline of the Advanced Photon Source at Argonne National Laboratory to study the fine structure in the Cu K-edge x-ray absorption in 2 µm thick polycrystalline films of CdTe on fused silica. 4 nm of evaporated Cu is diffused either with or without prior vapor $CdCl_2$ treatments in dry air. The phase-uncorrected radial distribution function inferred from the absorption fine structure indicates predominantly Cu_2Te when Cu is diffused into the as-deposited CdTe film but indicates a Cu_2O environment when Cu is diffused *after* the vapor $CdCl_2$ treatment. We believe most of the diffused Cu decorates grain boundaries as oxides, consistent with the low doping densities typically observed in CdTe solar cells. This Cu_2O likely plays a role in grain-boundary passivation. We also found that the chemical environment around Cu atoms in both CdTe and real cells can change with light soaking. This instability of Cu_2O in sputtered CdTe could contribute to cell degradation.

INTRODUCTION

High performance CdS/CdTe thin film solar cells are usually completed with a low resistance back contact containing Cu. Most successful stable back contacts to CdTe have involved the use of copper to create a heavily doped layer next to the metal. In our relatively thin (2-2.5 µm CdTe) sputtered cells, we have successfully used very thin evaporated Cu (3 nm) followed by evaporated Au (10-20 nm) to achieve 14% efficiency cells at AM 1.5.[1] If all of the Cu were evenly diffused through the CdTe, one could expect a Cu density of $\sim 10^{20}$ cm^{-3}. However, C-V measurements of CdTe cells from several laboratories indicate maximum acceptor densities in CdTe of $\sim 5 \times 10^{14}$ cm^{-3}.[2] Thus most of the Cu is electrically inactive. The goal of our measurements was to identify the lattice location of most of the Cu in CdTe.

X-ray absorption fine structure (XAFS) is a powerful technique for understanding the lattice environment around selected elements. The periodic oscillatory structure, known as extended x-ray absorption fine structure (EXAFS), in the absorption spectrum above the edge due to the phase difference between back-scattered and out-going electron waves is the key to this technique. The lattice environments are derivable from the Fourier transform of the EXAFS spectrum.[3,4] Fitting with theoretical standards derived from the *ab initio* multiple-scattering code FEFF[5] is used to obtain more detailed information about the near-neighbor distance and the coordination numbers of the environment surrounding the atoms of interest.

By using the fine structure in the Cu K-edge x-ray absorption spectrum, we can elucidate the predominant lattice location of Cu in polycrystalline, thin-film CdTe solar cells. In particular, we have studied how the typical $CdCl_2$ vapor treatment in dry air changes the local environment of the Cu subsequently diffused into CdTe.

High-temperature $CdCl_2$ treatment in the presence of oxygen is a critical step needed to improve the performance of CdTe thin-film cells, which can improve the cell efficiency a factor of two or more.[6,7] However the process is not yet well understood. The oxygen in the air or He/O_2 or Ar/O_2 atmospheres during the chloride process is probably active in passivating the grain boundaries although some may also be active in forming doping complexes.

In the case of CdTe, the present XAFS measurements suggest that in sputtered films prepared without post-deposition $CdCl_2$ treatment and with typical amounts of Cu at the back contact, Cu resides in a Cu_2Te environment; however, in films prepared with chloride treatment, most of the Cu ends up bound with oxygen.[4] Details are given below. Also our XAFS of HCl-etched films show this Cu_2O is quickly removed, which suggests that this Cu_2O forms a very thin layer at the grain boundaries and may play an important role in grain boundary passivation. Here we report measurements of CdTe layers peeled off from cells, both unstressed and light-soaked. The Cu_2O is also found in completed cells and exhibits bonding changes with light-soak condition.

EXPERIMENTAL DETAILS

The 2-3 micron CdTe layers were magnetron sputtered at ~ 250 °C[8] onto either fused silica or Kapton polyimide sheet substrates.[9] All the samples were prepared with 4 to 20 nm evaporated Cu layers which were diffused in N_2 at 150 or 200 °C for at least 45 minutes. Some of the samples were annealed at 387 °C in $CdCl_2$ vapor in a dry air environment for 30 minutes before Cu deposition, diffusion and etching. Among these $CdCl_2$ treated films, some received 200 Å of evaporated Au and were diffused without vacuum break to prevent oxidization by air, except

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