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Determination of Cu Concentrations in CdTe/CdS Devices by High Mass Resolution Secondary Ion Mass Spectrometry

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ABSTRACT

We have used secondary ion mass spectrometry (SIMS) to quantitatively determine the concentration of Cu in CdTe/CdS devices. Empirical standards were fabricated by ion implantation of Cu into single-crystal and polycrystalline CdTe and single-crystal CdS. Relative sensitivity factors were then generated from the measured implant profiles. Quantified profiles show that the apparent increase in Cu in the CdS is genuine, and not a sputtering artifact. This is the first quantified profile of Cu through CdTe/CdS device structures.

1. Introduction

Despite the technological significance of Cu in CdTe/CdS thin-film photovoltaic devices, little is known about the actual concentration of Cu in the devices. SIMS is a sensitive method for the analysis of trace elements in materials. However, SIMS is subject to artifacts caused by changes in secondary ion yield when profiling through different materials. It is possible to correct for these changes by preparing empirical standards of the element or matrix of interest. The simplest method to prepare standards is by ion implantation.

2. Experimental

SIMS depth profiles were obtained on a Cameca IMS-5F using an O_2^+ primary ion beam at 12.5 kV (8 kV impact energy) and detection of positive secondary ions. The mass spectrometer was tuned for mass resolution $m/\Delta m \approx 4000$ to separate the $^{63}Cu^+$ signal from mass interference from $^{126}Te^{2+}$. Device quality CdTe/CdS was supplied by First Solar Inc (FSI), as part of a back-contact study for the National Thin Film Partnership CdTe team. The CdTe was wet $CdCl_2$ processed at FSI. Contacts were applied by the National Renewable Energy Laboratory and the University of South Florida (HgTe:Cu graphite paste) and a ZnTe:Cu contact, also at NREL. Standards were fabricated by ion implantation of $^{63}Cu^{2+}$ at 400 kV, with a nominal dose of $1e15$ at/cm² (actual measured dose was $9.68e14$ at/cm²). Multiple materials were implanted including polished single crystal CdTe and CdS, and polycrystalline CdTe (vapor $CdCl_2$ treated).

3. Results and Discussion

Figure 1 shows a typical high-mass-resolution (HMR) depth profile from a ZnTe/CdTe/CdS thin-film device

structure. Each of the layers is clearly identified, although some broadening is observed due to topography. The profile also shows a substantial increase in the Cu signal in the CdS layer relative to the CdTe layer. To fully understand whether this increase represents a real change in concentration, it is necessary to correct for changes in ion yield between the CdTe and CdS matrices. To perform the correction, first a relative sensitivity factor (RSF) is generated from the implant standard. Then, the RSF is applied to the Cu signal in the unknown referenced to the matrix signal in the unknown.

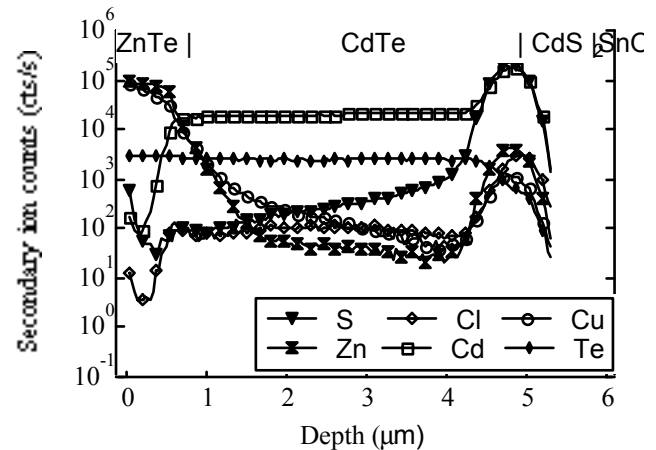


Figure 1. Unquantified depth profile from CdTe/CdS device.

The depth profiles shown in Figures 2-4 were obtained from the implant standards. Each standard was analyzed under low-mass resolution and again under high-mass resolution. For the case of CdTe, the dynamic range is significantly reduced for low-mass resolution. This shows the loss of sensitivity to Cu if low-mass resolution is used instead of HMR. No interference exists in the case of CdS, and the dynamic range is equal for the low- and high-mass resolution cases.

The Cu RSF's are referenced to the Cd matrix signals in the CdTe and CdS and to the Te signal in the ZnTe layer. The values of the RSF's must also be corrected for the isotopic abundance of ^{63}Cu to give the elemental concentrations of Cu in CdTe and CdS [1]. The RSF's generated in this study are shown in Table 1.

Table 1.

Matrix	RSF
CdTe	1.7e21
CdS	1.4e21

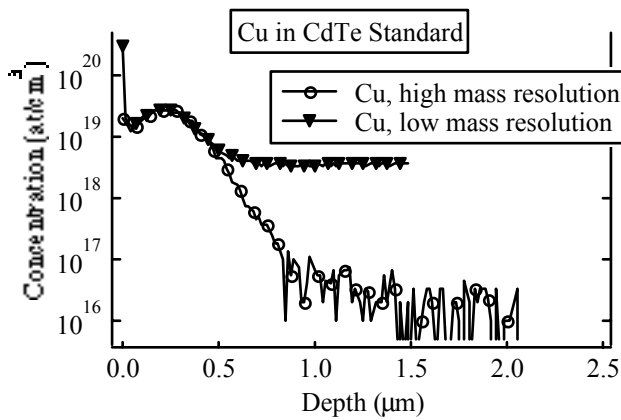


Figure 2. Depth profile of Cu in single crystal CdTe implant standard profiled with low- and high-mass resolution.

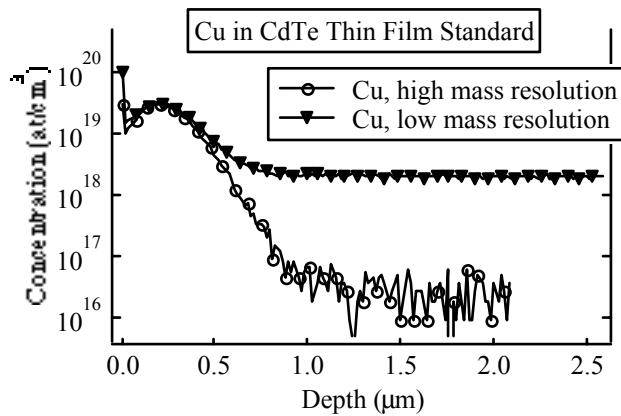


Figure 3. Depth profile of Cu in polycrystalline CdTe implant standard profiled with low- and high-mass resolution.

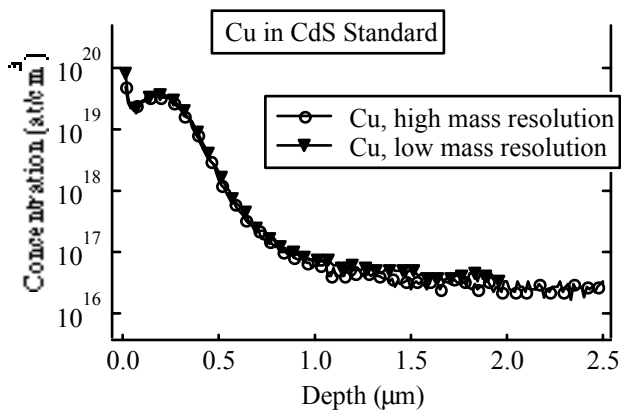


Figure 4. Depth profile of Cu in single crystal CdS implant standard profiled with low- and high-mass resolution.

Shown in Figure 5 are the raw Cu counts from depth profiles of one control device with no contact and three devices with different Cu-containing back contacts. Again, the increase in the Cu signal in the CdS is observed. Applying the RSF's shown in Table 1 to the profiles in Figure 5 yields the quantified data shown in Figure 6. It is now clear that the increase in Cu signal corresponds to a real increase in the Cu concentration in the CdS layer. Although the SIMS measurement does not distinguish between Cu at grains and Cu at grain boundaries, SIMS does show that

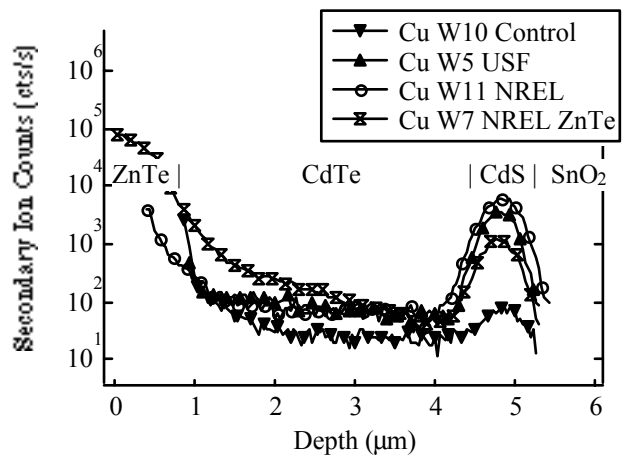


Figure 5. Raw Cu depth profiles from one un-contacted control device and three devices with different back contacts.

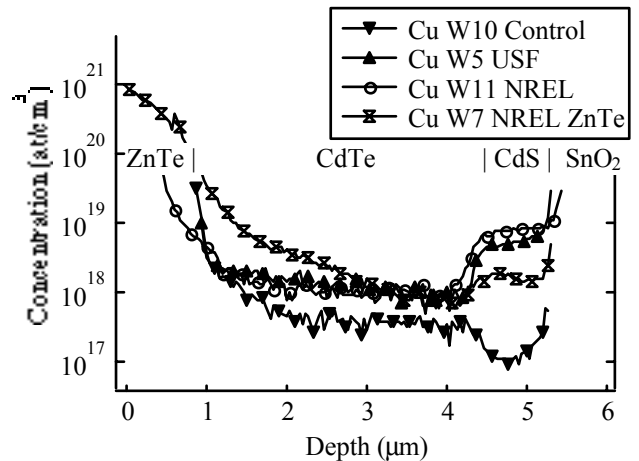


Figure 6. Quantified Cu depth profiles from four devices shown in Fig. 5.

there is still a real increase in the overall Cu concentration in the CdS layer.

4. Summary

High-mass-resolution depth profiling by SIMS has been used to study the distribution of Cu in CdTe/CdS. Ion implant standards have been fabricated to correct for changes in ion yield between the different matrices. Relative sensitivity factors have been calculated for Cu in CdTe and CdS. Quantified profiles of Cu through CdTe/CdS devices are shown for the first time.

REFERENCES

[1] R.G. Wilson, F.A. Stevie, C.W. Magee, "Secondary Ion Mass Spectrometry", John Wiley and Sons, New York, p. 3.1-1, NY,(1989).

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