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Quantitative Elemental Analytics of Photovoltaic CIGS Thin Films by the use of ToF-SIMS and ICP-MS

K. Kaufmann[1], S. Meyer[2], S. Wahl[2], E. Jarzembowski[3], C. Hagendorf[2]

[1] Hochschule Anhalt (FH), Anhalt University for Applied Sciences, Bernburger Str. 55, 06366 Köthen, kai.kaufmann@csp.fraunhofer.de

[2] Fraunhofer-Center for Silicon Photovoltaics CSP, Walter-Hülse-Straße 1, 06120 Halle (Saale)

[3] Martin Luther University Halle-Wittenberg, Halle-Wittenberg, Universitätsplatz 10, 06108 Halle, Germany

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Motivation

- The depth dependent composition of the absorber layer in CIGS solar cells is a key parameter for high efficiencies
- The spatial distribution of sodium influences the efficiency as well [1]
- Also the sodium content at layer interfaces has impact on layer adhesion
- Quantitative depth profiles can be obtained by XPS but due to the low concentration the sodium distribution is not measurable
- In this study ToF-SIMS is used for depth profiling the CIGS matrix elements and also sodium

Samples and preparation

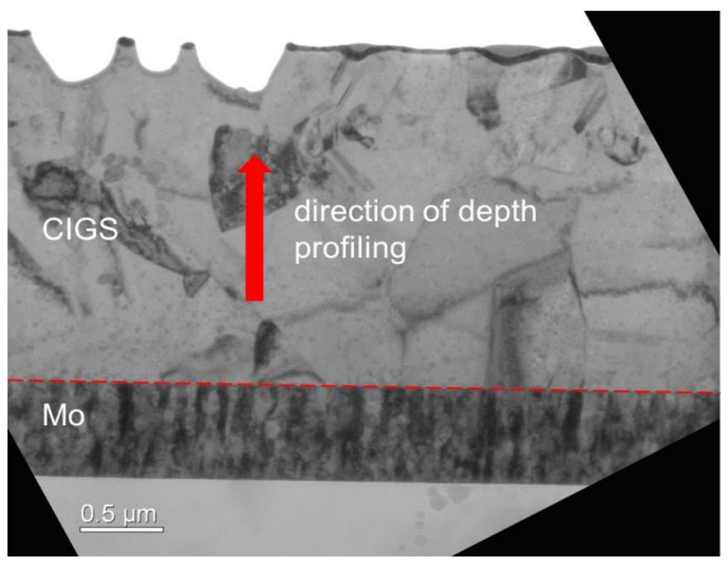

Fig. 1, TEM crosssection of the Mo/CIGS layer stack

- CIGS was deposited by a three stage coevaporation process
- For ToF-SIMS depth profiling the CIGS layer was removed from the Mo substrate by a lift-off process to provide a clean surface with a low surface roughness

Results — Quantitative ToF-SIMS of CIGS matrix elements

- After diluting the the CIGS layer in HNO_3 the composition was measured with ICP-MS (Table 1)

Table 1, CIGS comosition as measured by ICP-MS

Element	Cu	In	Ga	Se	Na
Atomic Fraction	0.25 ±0.03	0.17 ±0.02	0.07 ±0.01	0.51 ±0.05	0.001 ±0.0005

- For quantitative ToF-SIMS depth profiling MCs+-clusters were detected ($CuCs^+$, $InCs^+$, $GaCs^+$ ans $SeCs^+$) (see Fig.2)
- Quantification was done with the ICP-MS results using the equation

$$c(z) = I_{ToF}(z) c_{ICPMS} / I_{Tofmean}$$

$c(z)$ depth dependent concentration
$I_{ToF}(z)$ depth dependent ToF-SIMS intensity
c_{ICPMS} mean concentration determined by ICP-MS
$I_{Tofmean}$ mean ToF-SIMS intensity for one given element

- Fig. 3 shows the quantified ToF-SIMS depth profile in comparison with a XPS depth profile of the same sample

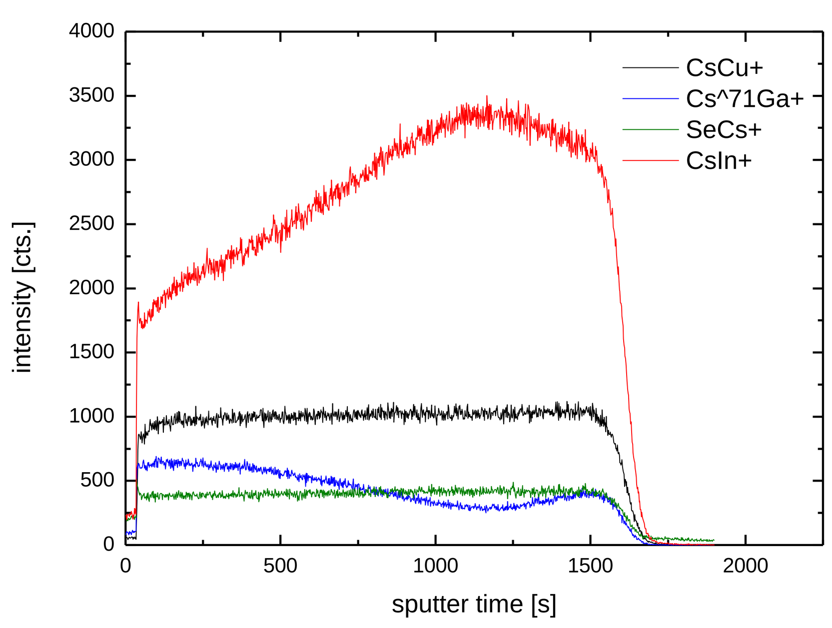

Fig. 2, depth profile MCs+ clusters prior to quantification

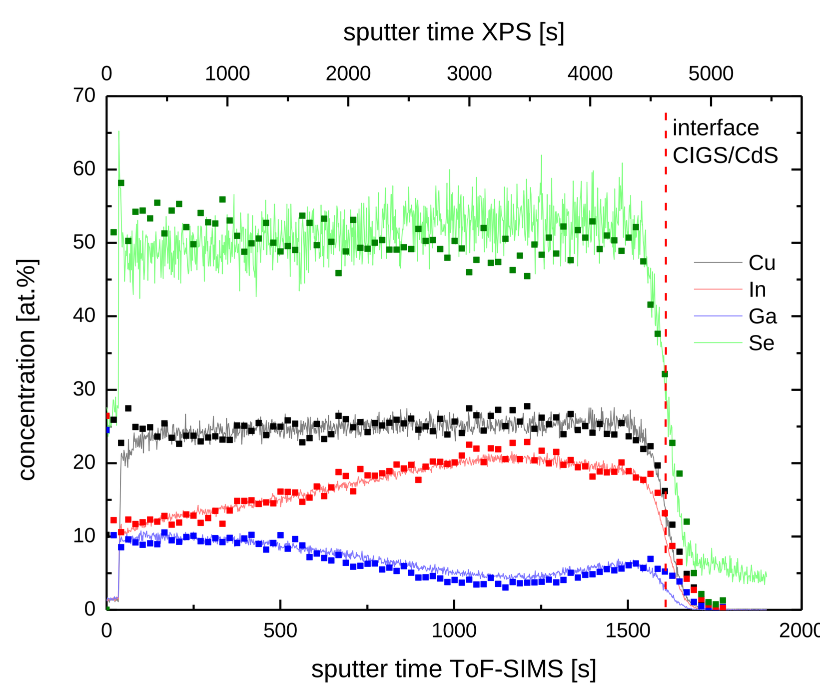

Fig. 3, quantified ToF-SIMS depth profile (lines), XPS for comparison (dotted)

Results — Distribution of Sodium

- For Na analysis depth profiling was carried out using O_2^+ ions and Cs^+ ions as well
- Depth profiles were obtained from the top of the CIGS layer and also from the bottom after lift off
- Fig. 4 shows the depth profiles for the two sputter ion species and for detection of the $NaCs^+$ clusters
- The depth profiles were normalized to the mean bulk intensity
- Matrix effects caused by stoichiometry changes should be weak, the RSF changes less than 5% [2]
- Uncertainties at the CIGS/Mo interface may be caused by changing ionization probabilities
- This assumption is supported by the fact that matrix effects are expected to be reduced in the case of Cs sputtering and smallest when detecting MCs^+ clusters

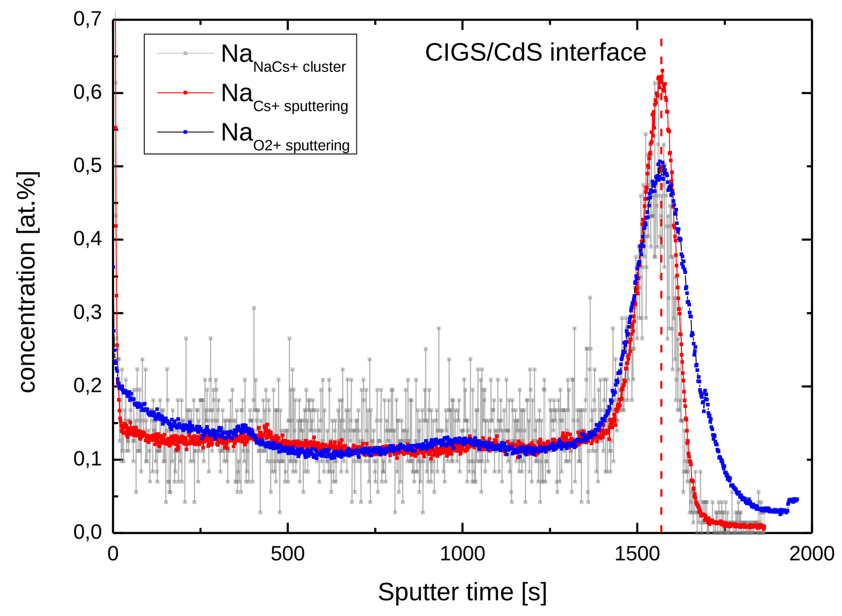

Fig. 4, Na depth profile for Cs sputtering, O2 sputtering and Cs sputtering while detecting NaCs+ ions

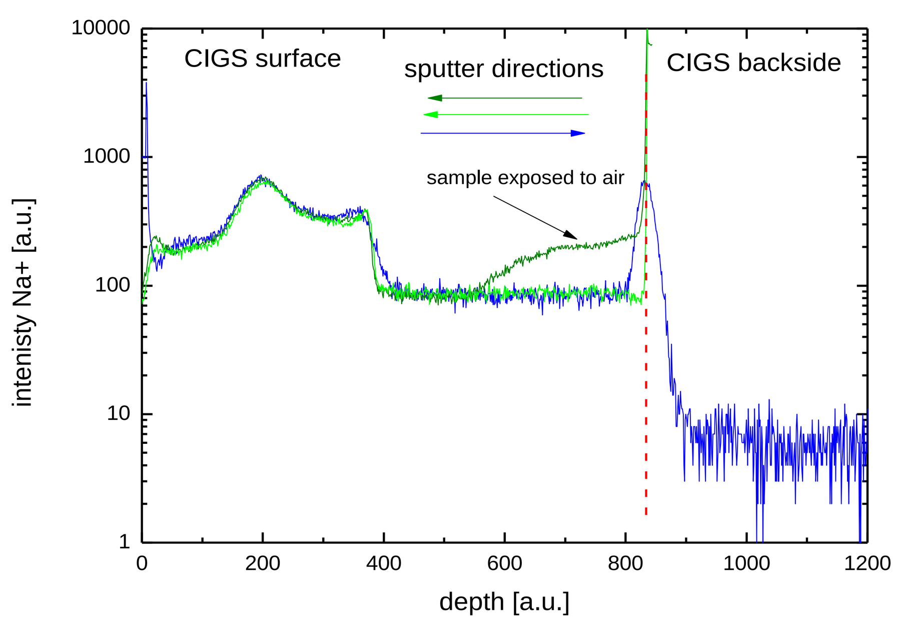

Fig. 5, Na depth profiles obtained from different sputter directions. The shape of the sodium feature is not affected by the different sputter directions

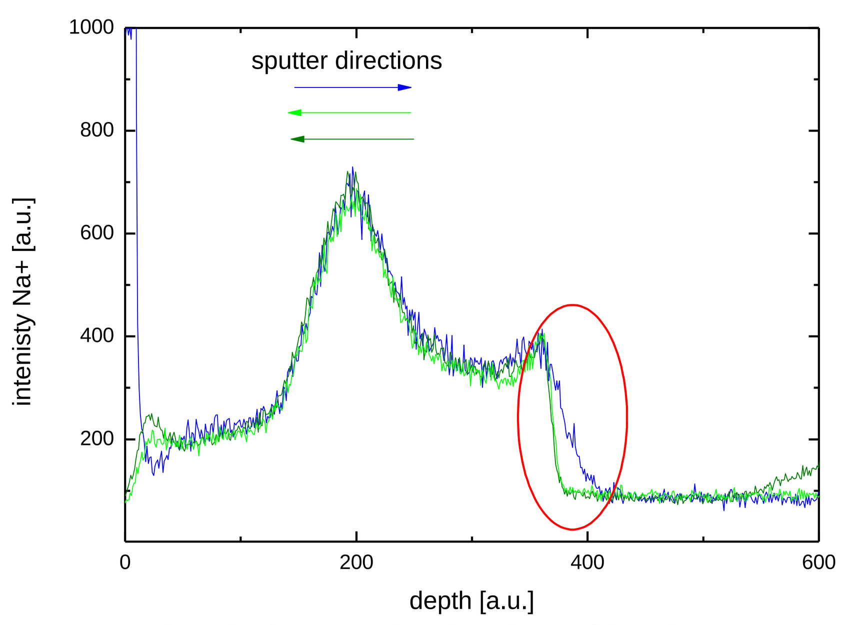

Fig. 6, detail of Fig. 5, the depth profiles show some differences at the steep slope of the feature. This can be attributed to ion beam induced intermixing.

- Na depth profiles for two different sputter directions indicated by the arrows are shown in Fig. 5.
- A depth profile of a sample exposed to air after lift-off for two weeks is represented by the darker green line.
- Since the Na depth profile is only little affected by changing the sputter direction, it can be concluded that sputter beam induced segregation effects are low in these type of samples
- The difference between the depth profiles can be attributed to sputter beam induced intermixing effects or effects due to different surface roughness

Summary

- With MCs^+ cluster ToF-SIMS both the CIGS matrix elements and also Na can be analyzed quantitatively
- The sodium depth profile is nearly unaffected by beam induced effects which may lead to an unwanted Na migration, therefore the Na distribution can be measured spatially
- Exposition of the CIGS surface to air lead to diffusion of sodium into the CIGS layer

References

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[2] Larry Wang1, Alice Wang and R.S. Hockett, SIMS study of Na in CIGS and impurities in CdTe/CdS, Photovoltaic Specialists Conference (PVSC), 2009 34th IEEE

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