Post-growth thermal annealing effetcs on the crystal structure of Zinc Sulfide

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Abstract

Zinc Sulfide films were prepared on Silicon and Sapphire substrates and individually doped with different concentrations of Iron or Chromium. The finished samples were then annealed first at 100°C for 12 hours, and then at 600°C for 12 hours. The full width half maximum(FWHM) was measured by X-Ray Diffraction (XRD) and the crystallite size calculated using the Scherrer equation. The results showed that the thermal annealing oxidized the samples to different extents and that the Iron doped samples had an elevated rate of oxidization and a preferred hexagonal wurtzite orientation(hcp-lattice).

1 Introduction

There are many possible changes that can occur when a thin film gets annealed. Some of these include; a reaction with the substrate material, oxidization, delamination, crystal growth, etc. This articles attempts to explain how post-growth annealing affects the crystal structure of Zinc Sulfide in thin films and if any of these processes occur; to what extent do they occur?

2 Materials and Methods

Four different samples were created having different substrates, dopant concentrations, and dopant types:

Sample 1	Sample 2	Sample 3	Sample 4
2.10 % Fe	2.10% Fe	2.00 % Cr	0.32 % Cr Delta doped
Silicon	Sapphire	Sapphire	Silicon (1 Micron SiO_2)

The samples then went through a theta-2theta XRD-scan with the following parameters:

Start	Stop	Rotation	Step Length	Scan Speed
15°	85°	60 rpm	0.038 696 2°	0.5 sec/step

The samples where then annealed for 12 hours at 100°C and rescanned, annealed for another 12 hours at 600°C and then rescanned for a third time with the same parameters. The scans were then analyzed to determine any changes [1].

3 Results

The results showed an increase in crystal size independent of substrate material, but to a larger lesser extent in the Iron doped samples. Perhaps most interesting was how the annealing process seemed to cause an inverse relationship between Zinc Oxide (ZnO) growth and increase in crystal size.[2]

4 Tables and Graphs

From the table we see how the crystal size increases or remains somewhat constant when the smple gets annealed, this can be normalized and confirmed with respect to the substrate peaks that we do not expect to change when annealed.[3]

The graphs clearly show the growth of 3 to 4 peaks that were not present in the original base scan that coincides with the peaks of ZnO. Further it seems that the longer we anneal the sample the more these crystals grow. We can see that this is not a reaction with the substrate material as the behaviour is the same for both Silicon and Sapphire substrates. Finally we can deduce that the change has to be in the Zinc Sulfide and not due to a collection of dopant, as we see this behaviour for both the Chromium and Iron doped samples, but to lesser extents as the dopant perhaps works as a catalyst.

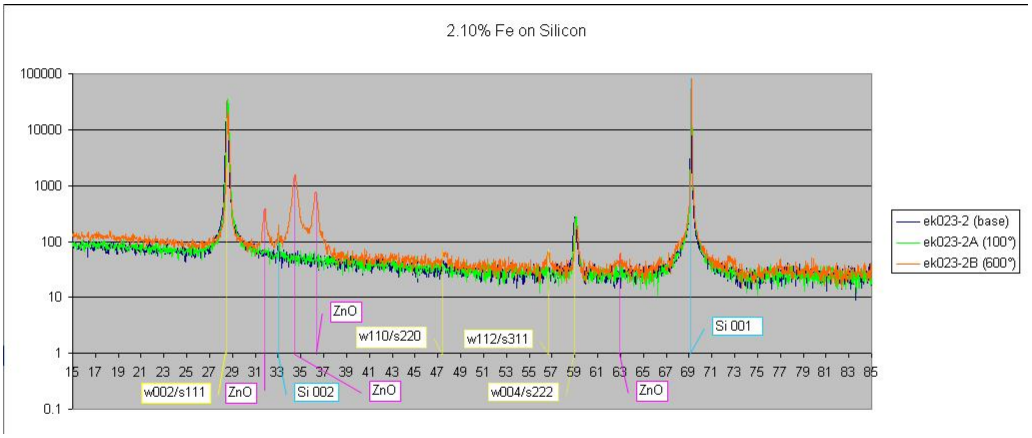

Figure 1: 2.10% Iron doped on Silicone substrate

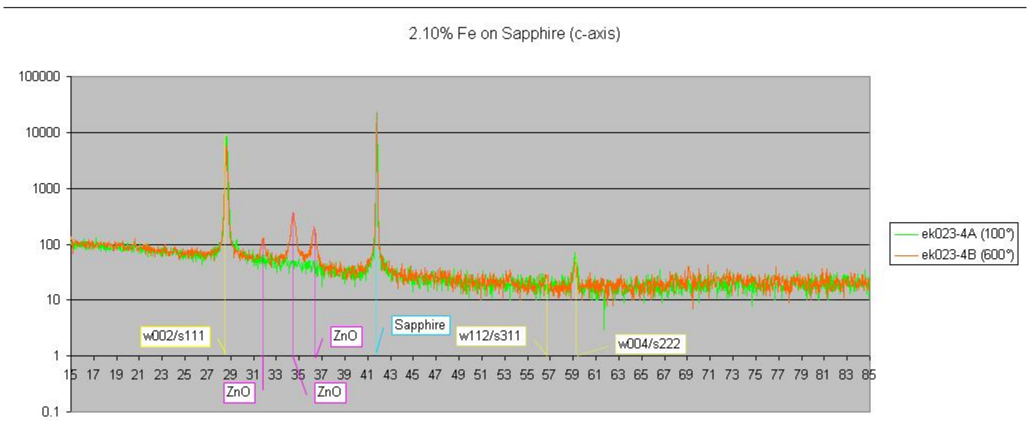

Figure 2: 2.10% Iron doped on Sapphire substrate

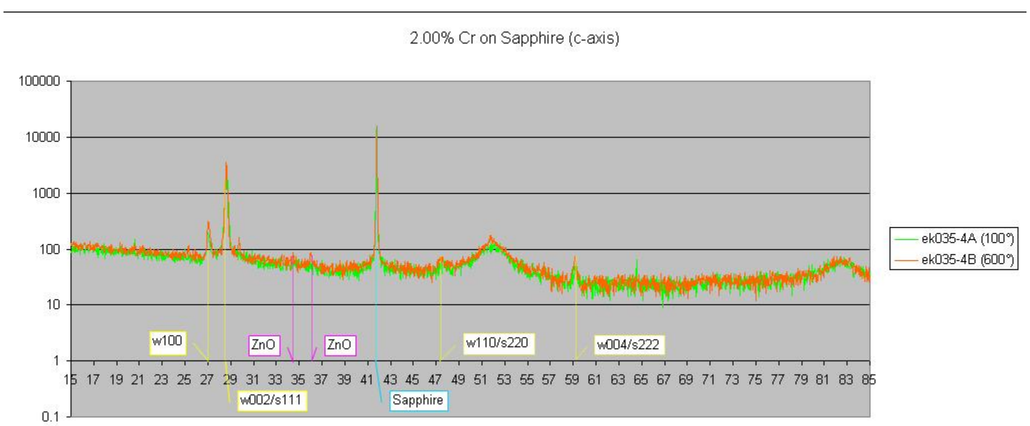

Figure 3: 2.00% Chromium doped on Sapphire substrate

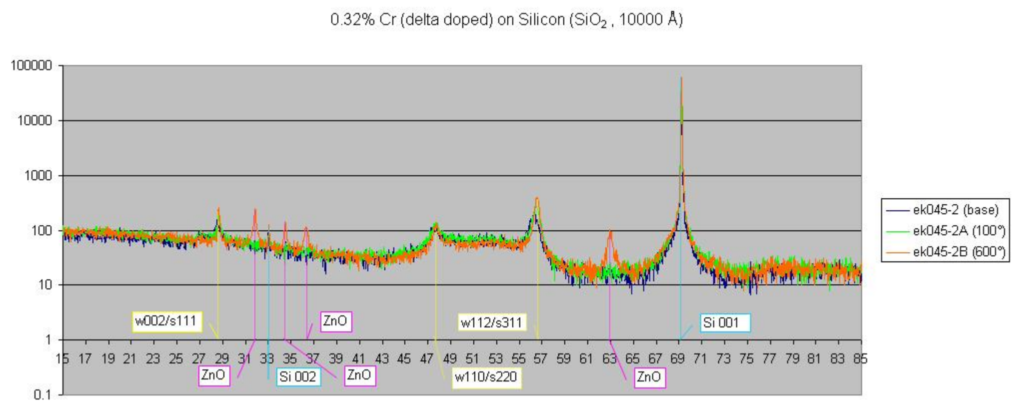

Figure 4: 0.32% Cr delta doped on Silicone substrate

5 Discussion

It appears that the Iron doped samples when annealed cause more oxidation, whilst the chromium doped samples give way for a larger crystal growth of the Wurtzite/Sphalerite crystals.

To continue from here it would be interesting to see what happens to the samples *while* annealed and do scans in a furnace. Another possibility would be to do scans on smaller temperature intervals to get a better global view of what happens to the samples at what temperatures.

6 Acknowledgments

I would like to thank Ursula Gibson and Eric Karhu for giving me the opportunity to complete this project.

References

Notes

[1] Analysis was done using the EVA-software and PDF-2 database for crystal structures

[2] Based on data from the PDF-2 database

[3] see excel table