Subject: Re: Update
From: treharne <R.Treharne@liverpool.ac.uk>
Date: 15/05/14 12:47
To: Louis F Piper <lpiper@binghamton.edu>
CC: Keith Butler <ktb22@bath.ac.uk>

Hi Louis,

I've added all the data and correspondence that Rob has sent so far to the dropbox folder "/ZTO-Project/Resuts/combi_XPS_UCL". The powerpoint files give a good summary of the analysis so far.

I'll drop him a line copy you in.

Set for ZTO deposition tomorrow. Will aim for Sn compositions in range 90 - 100%.

Kind regards

Rob

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On 14/05/14 22:42, Louis F Piper wrote:

> Hi Rob,
>
> This is great. We can combine the HAXPES and the XPS together. If Rob wouldn't mind I wouldn't mind attempting principle component analysis on his XPS data set - unless he is already doing data mining? Can you introduce us?
>
> For the Sn-rich, we should try slightly off the SnO2 endpoint because the subgap feature suggests a "black SnO2" result.
>
> ---
> Louis Piper, PhD
> Assistant Professor

> Physics, Applied Physics & Astronomy
> Materials Science and Engineering
> Binghamton University
> State University of New York
> Telephone: 607 777 3086
> http://bingweb.binghamton.edu/~lpiper/
> ---
>
> On Mon, May 12, 2014 at 10:30 AM, Robert <R.Treharne@liverpool.ac.uk> wrote:
>> Hi Louis,
>>
>> Yes - we have good access to a high spec Woollam ellipsometer. Plus we have a lot of experience with the ellipsometric analysis of these films.
>>
>> What composition range would you like me to focus on for the Sn rich ZTO sample?
>>
>> Also, I have just received a huge XPS dataset (768 spectra!) from Rob Palgrave in UCL from his very nice scanning XPS system. Data was taken from a sample identical to one we sent to you Louis. I'll get it into a more presentable form and upload it to the dropbox asap.
>>
>> Rob
>>
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>> On 12/05/14 15:23, Louis F Piper wrote:
>>> Awesome. We can try some in situ studies to induce the su gap states at Binghamton. Meanwhile, if we can get the new Sn richer ZTO samples for the next HAXPES run we should be set. Especially

some more SnO2 endpoint phases with different degrees of crystallinity...ie different post growth annealing....

Do you have ellipsometry measurements at Liverpool?

On Monday, May 12, 2014, <ktb22@bath.ac.uk> wrote:

> Hi,
>
> So all of the DFT PDOS are now in the dropbox. It looks like we have a nice match. The size of the subgap feature increases with increasing Sn content, also the PDOS reveals it to be primarily Sn based.
>
> At least we seem to have a consistent story here!!
>
> Keith
>
> Quoting Keith Tobias Butler <ktb22@bath.ac.uk>:
>
> > Hi All,
> >
> > I have just put one of the pDOS plots in the Dropbox. So far I only have the result for the ZnSnO3 structure. There is some tailing of the valence band, I would say the VBM is really at ~ 3eV, so tgive the correct band gap. The major subgap state however is definitely Sn related, so that fits nicely with your HAXPES. I'll look at the structure later and see what kind of geometry is related to the density.
> > I'm also runnig samples at 3 other Sn/Zn ratios, so we will have 3:1, 2:1, 1:1, 1:2
> >
> > Cheers
> >
> > Keith
> > On 09/05/2014 21:53, Louis F Piper wrote:
> >
> > > Hi,
> > >
> > > Quick update, we are doing the HAXPES on a-ZTO (attached) - we should get every other sample of the set in this run. For SnO2 ref., we are seeing two interesting features in the valence band region that I don't see for highly-crystalline SnO2. The feature labeled 1) subgap and the other 2) band filling.

1) We don't see evidence of Sn2+ from the lineshape. *Rob*, how crystalline the SnO2 was from the XRD? It could be disorder-related instead....? The feature seems to grow with increasing Sn (the rough dSnO2/(dZnO+dSnO2 are given in the legend from the sample map).

2) The band filling is likely CB filling, but UCSB have previously claimed electron accumulation with similar HAXPES... * Rob*, do you have any sense of the carrier concentration for the SnO2?

Keith, can you pass on the PDOS for direct comparison with the spectra?

Thanks

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On Tue, May 6, 2014 at 9:39 AM, Keith Tobias Butler <ktb22@bath.ac.uk <mailto:ktb22@bath.ac.uk>> wrote:

> Hi,
>
> That's great about the incoporation into PV platforms. It makes
> the study really well rounded, great.
>
> At this stage there's probably little point in having a skype, so
> I guess we'll just carry on as we are.
>
> Thanks a lot for the updates,

Cheers,

Keith

On 06/05/2014 14:30, treharne wrote:
> Dear Louis and Keith.
>
> Apologies, I am yet to send glass/conductive-layer/ZTO samples to
> Binghampton.
>
> I will aim to do this this month.
>
> Louis, will it be better for you if I deposit onto thinner glass?
> I can deposit onto 1mm thick borosilicate.
>
> Also, Keith - in future, we could potentially incorporate a ZTO
> into our existing thin-film PV platforms. This would tie in very
> nicely with our current research activities.
>
> Kind Regards
>
> Rob
>
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>
> SI logo
> On 06/05/14 14:15, Louis F Piper wrote:
>> Hi,
>>
>> My progress has been slower. Basically, we have not been able
>> to measure the samples yet because of shipping

problems and then
beam interruptions. We are trying to do HAXPES this week. The
glass is very thick but we will try our best. Hopefully I will
have some good news soon. Otherwise, we can use the lab XPS
here and try to induce and remove subgap features (aka a-IGZO
style).

Rob, did you ever send a second set of samples with a conductive
layer between the glass and a-ZTO? We never received them.

Louis

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On Tue, May 6, 2014 at 2:24 AM, <ktb22@bath.ac.uk
<mailto:ktb22@bath.ac.uk>> wrote:

> Hi Louis & Rob,
>
> Sorry it's been a while since I have been in touch regarding
> the ZTO work. From my end, I have completed the simulations
> of the various stoichs, and looked at work functions. There
> is plenty more analysis I could/should do, I was just

wondering if you had found anything interesting.

As it stands I think that we can definitely do a paper on
the effects on the work function, conductivity and structure, predicting optimal compositions for devices.

We have
i) A series of consistent samples
ii) Characterisation of electrical properties
iii) Characterisation of local environments
iv) Characterisation of electronic structure
v) Simulation of electronic structure

It would be nice if we could put some of it into a device to
do some measurements, if either of you know someone who can.
If not I think there's enough there regardless.

What do you think?

Should we have a Skype meeting to decide how to move this on?

Cheers

Keith

--

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