Characterisation of thin film chalcogenide PV materials using MeV ion beam analysis

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Abstract-- There are many technical challenges in the fabrication of devices from novel materials. The characterization of these materials is critical in the development of efficient photovoltaic systems. We show how the application of recent advances in MeV IBA, providing the self-consistent treatment of RBS (Rutherford backscattering) and PIXE (particle induced X-ray emission) spectra, makes a new set of powerful complementary depth profiling techniques available for all thin film technologies, including the chalcopyrite compound semiconductors. We will give and discuss a detailed analysis of a CuInAl metallic precursor film, showing how similar methods are also applicable to other films of interest.

Index Terms-- Photovoltaic cell materials, Materials science and technology, Semiconductor films, Thin film devices, Ion beam applications.

I. NOMENCLATURE

IBA: ion beam analysis; RBS: Rutherford backscattering spectrometry; EBS: elastic (non-Rutherford) backscattering spectrometry; ERD: elastic recoil detection; PIXE: particle induced X-ray emission; PIGE: particle induced gamma-ray emission; SEM: scanning electron microscopy; EDS: energy dispersive (X-ray) spectrometry (usually used of electron stimulated emission in the SEM, but equally applicable to PIXE); XRD: X-ray diffraction; SIMS: secondary ion mass spectrometry;

CIS: Copper-indium-diselenide (CuInSe_2); CIGS: copper-indium-gallium-diselenide ($\text{CuIn}_{1-x}\text{Ga}_x\text{Se}_2$); CIAS: copper-indium-aluminium-diselenide ($\text{CuIn}_{1-x}\text{Al}_x\text{Se}_2$); CIA: copper-indium-aluminium precursor film.

TFU ("thin film units"): 10^{15}atoms/cm^2 . Thin films often have densities significantly different from bulk materials, and for accurate work absolute units of thickness are used equivalent to mass per unit area.

NDF: acronym for the DataFurnace code (see text below) used to extract depth profiles from IBA data.

II. INTRODUCTION

Chalcopyrite-based $\text{CuIn}_{1-x}\text{Ga}_x\text{Se}_2$ (CIGS) solar cells have achieved the highest level of performance to date for single junction polycrystalline thin film technology. Current state-of-the-art CIGS solar devices exhibit efficiencies up to 19.9% [1]. However this material has a relatively low bandgap ($E_g = 1.2\text{ eV}$ for $x = 0.3$) compared to the 1.5 eV required for optimum solar energy conversion. CIGS devices fabricated with higher bandgap are found to have substantially reduced efficiencies [2]. This is attributed to fill factor and open circuit voltage losses arising from increased defect density and stronger interfacial recombination when the Ga content is increased. Substituting Ga by Al makes it possible to produce a material, $\text{CuIn}_{1-x}\text{Al}_x\text{Se}_2$ (CIAS), with the same bandgap as CIGS but with a smaller value of x . This is because the variation of E_g with Al content is up to 2.7 eV for CuAlSe_2 compared to 1.7 eV for CuGaSe_2 . Indeed CIAS solar cells with $E_g = 1.16\text{ eV}$ and $x = 0.13$ have been produced with efficiencies of 16.9% [3]. This compares to 16.5% for CIGS deposited under similar conditions but with $x = 0.26$ ($E_g = 1.16\text{ eV}$) [3].

While the most efficient devices so far have been deposited using the co-evaporation method, we have investigated the production of CIAS thin films by a two-stage process: the sputter deposition of Cu/In/Al metallic precursor layers followed by annealing in a selenium environment to synthesize the compound [4]. In principle this method promises improved scalability for commercial production compared to other deposition methods. But on the other hand the selenisation technique can yield unwanted elemental depth profiles due to the binary selenides having different reaction temperatures. This work is part of our ongoing effort to understand this phenomenon including in-depth analysis of the metallic precursors.

These materials are complex, and can be troublesome to fabricate, with many possible fabrication routes, so that characterization methods are important for establishing the processes. This paper will describe very novel methods of accurate thin film depth profiling using a self-consistent analysis of simultaneously collected spectra from MeV ion backscattering together with the stimulated photon emission.

III. DEPTH PROFILING USING ION BEAM ANALYSIS

These high-Z materials have very strong absorption, and an effective photovoltaic (PV) absorber film is a fraction of a micron thick. But such thin films are not easy to profile: the

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sputtering techniques (Auger electron or X-ray photo-electron spectroscopy, or SIMS - secondary ion mass spectrometry) are plagued by artefacts including those of interfaces, and SIMS is not quantitative because of the large matrix effects. Analytical methods such as SEM-EDS (energy dispersive X-ray spectrometry on the scanning electron microscope) have little or no depth resolution and do not work well for these thin films.

However, Rutherford backscattering (RBS) is a well-established non-destructive depth profiling technique [5] where the depth resolution comes from the energy loss of the probing beam (such as 1.5MeV $^4\text{He}^+$) detected after elastic scattering at backward angles from the atomic nuclei of the target; films of this sort of thickness have very convenient energy loss of the primary beam, so that the depth resolution is good. Because the RBS elastic scattering cross-section is derived simply from the Coulomb potential [6], and the energy losses of light ion beams in materials are well known [7]-[9], RBS is an accurate technique suitable for standards work [10], [11]. Depth profiles can now be extracted from RBS spectra (or other related particle scattering spectra) with codes validated by an IAEA-sponsored inter-comparison exercise [12], including the DataFurnace code [13] used here.

On the other hand, RBS using MeV ion beams does not have good mass resolution for these chalcogenide compounds, and RBS also has low sensitivity for light elements in a heavy matrix (such as the Al in CIA) since the yield goes with Z^2 , although non-Rutherford elastic backscattering (EBS) cross-sections can greatly enhance the light element sensitivity [14] (but not for Al).

The ion beam technique comparable to SEM-EDS is PIXE (particle-induced X-ray emission), which has a similarly poor depth resolution, although it has orders of magnitude better sensitivity since there is effectively no bremsstrahlung from the primary beam. However, the self-consistent analysis of RBS/EBS/PIXE data has recently been introduced, where the resulting analysis has the mass-sensitivity of PIXE combined with the depth-sensitivity of RBS [15]-[19]. We apply these methods here for the first time to PV materials (but see [20]).

IV. ANALYSIS

A CuInAl precursor film of about $\frac{1}{3}$ μm was sputter deposited on a soda-lime glass substrate coated with a $\frac{3}{4}$ μm Mo electrode layer (sample N109G). The unheated substrates are rotated above the high purity targets to produce a structure of several hundred layers. The CIA film had a Cu seed and an In cap, both $\sim 7\text{nm}$ thick. The PV absorber layer is subsequently made from this precursor film by selenisation of the CIA film in a tube furnace with an Ar atmosphere and vaporized selenium from a solid source.

The analysis was carried out on the 2MV Tandatron accelerator at Surrey [21] using 1.5MeV $^4\text{He}^+$, two particle detectors with solid angles of 1.2msr and 6.4msr at scattering angles of 172° and 148° , and for PIXE a 3mm thick Si(Li) crystal (Gresham, now known as e2v - "English Electric Vehicles") with solid angle 0.25msr at a backward angle to the beam of 60° , with an 8 μm Kapton filter to stop backscattered particles.

The beam current was $\sim 30\text{nA}$ into a nominally 1mm diameter beam spot giving a counting rate of 33kHz in the large particle detector, but only 500Hz in the X-ray detector since the He-PIXE cross-sections are low. The particle detectors have pulse shaping amplifiers implementing pulse pileup rejection with a time resolution of about 500ns, and the remaining pileup for the large detector was about 3% of the detected count-rate. We will also comment on other analyses carried out under different conditions which are not reported here.

The DataFurnace computation engine was NDFv9.2b [22]. This has a very good (but not perfect) pulse pileup calculation, which enables the use of high counting rates in accurate work. Errors in the algorithm are mostly in the treatment of the high energy tails of pronounced edges: see [23] for a worked example. Moderate layer roughness in a layer structure is calculated through its equivalent excess energy straggling [24], [25]. This is not valid for the severe roughness often designed into PV films for maximum light absorption, but IBA spectra from such rough films can also be calculated [26], although NDF does not yet implement this algorithm. NDF has a double scattering calculation [22], and this was included here.

Fig.1 1.5MeV He-PIXE spectrum from sample N109G at normal beam incidence, dots are data, line is GUPIX fit (without background). Note the log scale of the ordinate. Visible lines are: CuL, AlK, MoL, InL, CuK, MoK.

The PIXE data were analyzed using the DATPIXE code of Reis [15] as implemented in NDF by the LibCPIXE module [16]. LibCPIXE interprets characteristic X-ray line areas (specifically: of $K\alpha_1+K\alpha_2$ or $L\alpha_1+L\alpha_2$) extracted from the raw data, in this case using GUPIX ([27], [28]; with the output giving $2*\text{FWHM}$ centred on the main peak) which is also a validated code [29] (see Fig.1). GUPIX cannot be used for a complete analysis of the profiles since it is not designed as a depth profiling code and cannot handle any but the simplest layer structures. However, at present LibCPIXE does not implement either He-PIXE or the fluorescence correction (neither does it calculate the Cu L lines), so we use an analysis assuming an equivalent velocity proton beam (with similar ionization cross-sections, when scaled with Z^2). At present this calculation device also has the major problem that NDF does not currently permit stopping power corrections for PIXE, so that the probe beam velocity at underlying layers is calculated incorrectly, leading to incorrect ionization cross-sections deeper in the sample. We use a manual procedure as a temporary fix in this present work, where we apply cross-section corrections obtained by comparison to X-ray yields calculated (for simplified structures) from GUPIX, using its GUYLS utility (which also gives the fluorescence correction: $<1\%$ in these structures).

V. RESULTS

Fig. 2 shows the particle spectra (for two detectors) collected from an as-deposited CuInAl metallic precursor on Mo/glass (before selenisation). The Al content of the film significantly affects the spectral shape but has no detectable direct signal since the scattering cross-sections are small. The spectra have been fitted with the three-layer structure shown in Fig. 3, where the first layer has excess In to account for the excess yield in channel 245 (for the large detector), and the third layer has no Cu, to account for the spectral dip at channel 166. This dip cannot be fitted unless the second layer has a thickness variation ("roughness") of 11%.

Fig. 2. Fitted 1.5 MeV He RBS spectra collected simultaneously from two detectors (data – symbols, fits – lines), assuming the 3-layer structure of Fig. 3, and only metals present with 95% of the SRIM 2003 Mo stopping power. The large detector has scattering angle 148° and the small one 172° . Partial spectra (calculated before pileup correction) for Mo, Cu, In are shown for the large detector. Note: signals from the surface are at high energy (high channel number: the In signal is at the highest energy) and the substrate (Mo) signal is at low energy.

Even though these spectra show no direct Al signal, the Al content is actually determined from the energy loss, which gives the observed heights of the signals. In this case the total collected charge is determined through the Mo energy loss by the Mo "substrate" signal (the He beam does not have sufficient energy to penetrate to the glass substrate). The problem is that the Mo energy loss is not known sufficiently accurately to determine the Al content with any precision. In this case 1at% Al in the bulk of the CIA film requires 95% of the tabulated Mo stopping power. A comparable fit using an unmodified Mo stopping power gives 6.6at% Al in the bulk of the CIA film (see Figs. 4-6).

Also, the layers both at the surface and the interface are ambiguously determined in this analysis. To account for the interface signal (at ch. 166 for the large detector) we have to introduce an invisible element, but it doesn't have to be Al (as it is in Fig. 2): we can also assume that both layers are oxidized.

By themselves the RBS spectra are multiply-ambiguous. How much Al is in the bulk of the CIA film? How much oxidation is happening at the surface and the interface? To identify the Al profile directly we use the (simultaneously collected) He-PIXE spectra, and to get some depth information from the PIXE data we also collect spectra with the sample tilted normal to the X-ray detector so that the take-off angle is quite different, leading both to very different relative absorptions for the different colour X-rays and also to different ioni-

zation cross-sections near the interface. By itself, PIXE at two angles only permits distinguishing the front from the back of the CIA film. But the RBS already tells us a great deal about the CIA film, in particular that it is essentially only three layers with excess In at both the surface and the interface. We shall show that the joint RBS/PIXE data gives an unambiguous depth profile of the major and minor elements.

Fig. 3. Fitted three-layer structure for the RBS spectra of Fig. 1, with 11% roughness of the 2nd layer, assuming only metals present and 95% of the tabulated Mo stopping power. The Al has no significant direct signal in Fig. 1 and is fitted here from its energy loss: half of the fitted Al is in the interfacial layer. The depth scale is given in absolute thin film unit equivalent to g/cm^2 , since the film density is not known. With reasonable assumptions (linear combination of metal densities) this three-layer film is 370nm thick.

Figs. 4 & 5 show respectively the RBS spectra for two detectors at normal incidence (as in Fig. 2) and PIXE data for the sample normal to the beam and normal to the detector, all self-consistently fitted. Only the characteristic line areas (data and fits) are shown for the PIXE. Theoretical X-ray cross-sections are used [28], except that the In L line cross-section is increased by 22%. Note that both sets of PIXE data are well fitted, consistent at better than 3%, indicating the relative correctness of the solution (including the Al signal) in view of the calculation errors we have listed.

Fig. 6 shows the derived depth profile. This has assumed a two-layer structure for the main CIA thin film in which the Al concentration (6.6at% on average) increases towards the interface. It also assumes a two-layer structure for the surface In-rich layer: it is probable that this is an artefact of surface roughness, since the proposed O profile is surprising, and roughness would give the same behaviour with a more plausible profile.

VI. DISCUSSION

We have demonstrated that PIXE/RBS, for the particular sample analysed, could determine not only the Al content but also its depth profile in a heavy metal matrix.

In the analysis conditions used, the absorption of the Al X-rays for this film thickness (at normal incidence) is 75%, and the cross-section reduction for Al at the interface due to the energy loss of the incident beam in the layer is 20%. There are a total of 129 TFU ($129.10^{15}\text{Al}/\text{cm}^2$) in the structure of Fig. 6, and 60 TFU are needed to fit the interface signal in Fig. 2 (assuming that the "invisible element" is Al), which

would increase the detected Al signal by over 8%. Therefore to determine whether the interfacial layer has a significant Al content we would need an analysis with a precision better than about 2%. This is normal practice for EDS analysis, but would require the calculations to be correct, that is, without the approximations used in this work.

For this work it is essential to have a direct Al signal. For this the range foil must be thin enough to have transmission above, say, 10% for the 1.49 keV Al K line. This effectively excludes H-PIXE, and limits the energy for He-PIXE to about 2.4 MeV. On the other hand, to get the heavy metal K line signals, much higher beam energies must be used for usable cross-sections. Thus, a complete analysis may require the use of various conditions, in which case a code which facilitates the self-consistent analysis of all of the data is clearly indispensable.

Fig.4. 1.5 MeV RBS data with fits as in Fig.2. The fitting was done self-consistently on the RBS and PIXE data (shown in Fig.4) assuming the five-layer structure of Fig.5, and unmodified SRIM 2003 stopping powers. Al was assumed to be absent from both the surface layers and from the interfacial layer.

There is the question of the applicability of these methods to selenised and sulphidised films, and to new alternative compound systems (such as $\text{Cu}_2\text{ZnSn}(\text{S,Se})_4$ [30] where Zn and Sn are easily analyzed with the present methods). Se is very visible by RBS, but because the Se ($L\alpha=1.38\text{keV}$) is an extremely good absorber for Al ($K\alpha=1.49\text{keV}$), and hard to resolve from it, the Al content of CIAS films needs complementary PIGE analysis, which we will report separately. Depth profiling Al by PIGE is a well established technique [31], also now implemented in NDF. The sulphidised films have the problem that the S K line (2.31keV) overlaps the Mo L group (with the $L\alpha$ at 2.29keV). However, using the methods of this work (a low energy beam and various geometries to minimize and modulate the signal from the substrate) should be completely successful.

Na is also important for the chalcopyrite absorber films that need it for passivation. It diffuses through the Mo electrode from the soda-lime glass substrate during the selenisation process. We will report separately the analysis of Na in the Mo electrode using the forward recoils induced by the elastic scattering of heavy ions (HI-ERD), and it may also be detectable in the CIAS films. The Na K X-rays are too soft for detection by PIXE when a range foil to stop the scattered particles is used, especially since they are within 75 eV of the Cu L. If the

detection system is insensitive to distortion introduced by the scattered particles or if they are excluded magnetically then these methods may work for Na, with a good and well qualified detector. Otherwise SIMS calibrated with implantation standards should be used.

Fig.5. PIXE line areas and fits from normal beam incidence (above) and normal exit to PIXE detector (below). The line areas were extracted from the spectra using GUPIX. The inward and outward pathlengths differ by a factor of 2 ($\sec 60^\circ$) in both cases. NDF simulates He-PIXE with equivalent velocity proton-PIXE, with cross-section corrections calculated by the GUYLS utility of GUPIX and an enhancement of the In L line cross-section by 22%. The Cu L line cross section is not well known, and the Mo lines are ignored since they are calculated incorrectly: velocity equivalence cannot be maintained at depth without appropriate stopping power corrections, not implemented by this version of NDF. The detector resolution is 163 eV.

Fig.6. Depth profile fitted from RBS/PIXE data shown in Figs. 4 & 5. The double surface layer is probably a roughness artefact. The main CIA layer is split into two with Al steadily increasing to the interface and with 5% roughness on the first layer and 18% roughness on the second (closest to the interface). This layer structure is real and gives a better fit both to the RBS and to the PIXE data. More than two layers would give an even better fit, as can be seen from the fitting artefact for the large detector at channel 206 in Fig.4. The interfacial layer has an equivalent In thickness of 41 nm and there is the equivalent of a 7 nm layer of excess In spread through the two surface layers.

At a trivial level, the present analysis was complicated by the current version of the DataFurnace code working incorrectly for He-PIXE (no stopping power corrections, so that He-PIXE could not validly be approximated by an equal velocity proton beam), forcing us to make various otherwise unnecessary manual calculations. For a correctly working code the depth profiles for all of the metals (including Al) would

have come automatically out of the fitting. But the manual calculation also highlights the fact that in principle it is very inconvenient to correctly invert these spectra to obtain depth profiles by manual methods in the general case since extensive iteration is required. Because automatic fitting could not be used in this case we also could not use the Bayesian methods [13], [22] promised before the Conference to determine the analysis uncertainty (and spectral ambiguity). These shortcomings are temporary.

VII. CONCLUSIONS

We have demonstrated in a trial manual analysis that CIA metallic precursor films can be unambiguously depth profiled by IBA, except for any Al at the bottom interface of the film. We have shown that an automatic code is available which, with some minor extensions, can readily do an equivalent analysis at the high precision that is usually associated with these methods, which will allow the Al to be accurately profiled up to the interface.

We have demonstrated both that neither RBS by itself nor PIXE by itself is capable of solving these samples, and also that this can be done by the self-consistent RBS/PIXE analysis that has recently become available.

We have shown that a complete analysis of the selenided CIAS films, with a direct profile for Al, cannot be done by IBA methods unless PIGE is used. A self-consistent RBS/PIXE/PIGE analysis is now also available and will be reported separately.

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applications. He was awarded his PhD in 1993 by the University of Northumbria. His research interests include thermo-photovoltaics, device characterisation and thin film PV materials and devices based on the chalcopyrite materials system. He is currently the Operations Manager of the PV Cell Test Facility and is the principal investigator on the PV21 SUPERGEN programme at Northumbria.

X. BIOGRAPHIES

Nianhua Peng was born in 1962 in Hanyang, Hubei, China. He graduated from Wuhan University with BSc degree in Semiconductor Physics, MSc degree in Solid State Physics and from Cambridge University with PhD degree in Solid State Physics. His previous employment experience included Wuhan University, Leeds University and St Andrews University. He joined Surrey Ion Beam Centre in 1998. Now he is a Liaison Fellow with a particular interest on the applications of energetic ion beams to materials research.

Christopher Jeynes was born in 1951 in Kent, England. He graduated from Bristol University in 1972 with a BSc (Hons) in Maths & Physics, in 1975 with an MSc in the Science of Materials and in 1981 with a PhD "Carbonado and the diamond polishing process". He immediately joined the Surrey Ion Beam Centre (IBC) and developed a strong interest in accurate ion beam analysis (IBA). He has been the Senior Liaison Fellow at the IBC since 1989 and has worked on a large number of implantation and analysis projects for many collaborators in the UK and internationally. Since 1997 he has, with Dr. Nuno Barradas in Lisbon, developed the internationally recognized Data-Furnace code for the self-consistent and accurate treatment of IBA data.

Melanie Bailey (née Webb) was born in 1980 in Manchester, United Kingdom. She graduated from the University of Manchester with a 1st Class Honours Degree in Physics in 2001. In 2005, she graduated from the University of Surrey with a PhD entitled "Blistering and Exfoliation of GaAs". Her previous employment provided a background in patent law, technology transfer and marketing. In her current position as Ion Beam Analysis Liaison Fellow at the University of Surrey Ion Beam Centre, Dr Bailey works with collaborators from a host of different fields. Her areas of special interest are accurate ion beam analysis and the application of ion beam analysis to forensic samples.

Guillaume Zoppi was born in Annecy, France in 1978. He received a degree in physics in 1998 from the IUT Annecy, Université de Savoie, France and graduated from Northumbria University with a BSc (Hons) in Applied Physics in 1999 and with an MSc in Optoelectronics and Communication Systems in 2001. In March 2002 he joined the physics department at Durham University to work on CdTe thin film solar cells grown by Metal-Organic Chemical Vapour Deposition (MOCVD) in close collaboration with Bangor University. After completing a PhD, he joined a team of experienced researchers at Northumbria Photovoltaics Applications Centre (NPAC) to work on thin film solar cells based on CIGS absorber layers as part of the PV21 SUPERGEN programme.

Ian Forbes was born in Devon in 1959. He gained an honours degree in Materials Technology from the University of Surrey in 1983. After working on optical fibres for GEC during the mid eighties he obtained a post graduate diploma in optoelectronics from Newcastle Polytechnic. He then worked at the Northumbria Photovoltaics Applications Centre (NPAC) on MOD and EPSRC-LINK funded research projects into ITO/InP solar cells for space