Characterization of Amorphous Silicon by Secondary Ion Mass Spectrometry

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INTRODUCTION

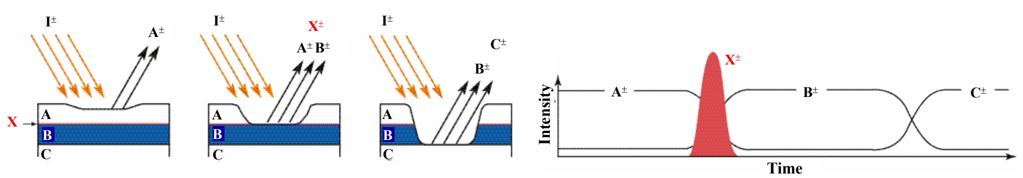
- Impurities and dopant level and distribution in amorphous silicon (a-Si) are important aspects for a-Si(H) solar cell materials [1] and a-Si TFT (Thin Film Transistor) for flat panel display applications [2].
- One way to reduce the cost of solar electricity is to reduce the thickness of the films that form a solar cell [1]. It has also been reported that by switching a-Si TFT to poly-Si TFT, the higher mobility can result in smaller TFT, higher image resolution, lower power consumption, and better performance. However, the production of low hydrogen content a-Si is essential for laser-induced crystallization of a-Si for poly-Si TFT [2].

Why use SIMS and what is new?

- Thinner films, sharp transitions, and varying H content provide new challenges for SIMS analysis.
- Our results have shown that the SIMS calibration curve for H in Si is a straight line over a large H concentration range (up to 32 at.%).
- Using magnetic sector SIMS tool, a P-doped a-Si thin layer (50nm thick) was analyzed using 3keV O2 beam with oxygen leak. Good depth resolution and detection limit have been obtained.
- We have used a low energy (Cs2M)+ detection mode to analyze atmospheric species (C,N and O) in thin a-Si layers. By this mode, higher sputter rate and lower primary beam mixing effects [3] can be obtained.
- We will show various examples of SIMS to monitor other elements such as Li,Na,K,Cl, Al,Cr,Fe,Ni,Cu.

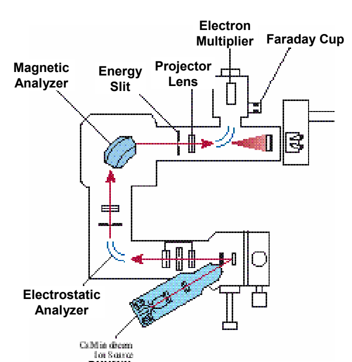
EXPERIMENTAL DETAILS

Dynamic SIMS for Depth Profiling

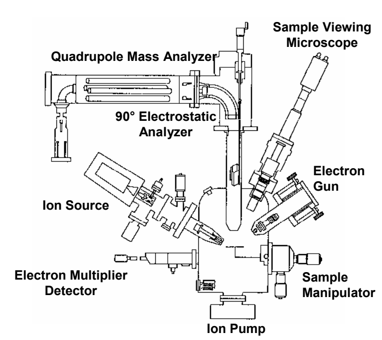


Two kinds of SIMS Instruments (two kinds of mass analyzers)

Magnetic Sector (Cameca)



Quadrupole Mass Filter (PHI)



Instrumentation and Capabilities

Mass Separation	Manufacturer	Strengths	Weaknesses
Magnetic sector	Cameca	· High transmission(~40%) · **High mass resolution** (M/ΔM ~10,000)	· Primary beam incidence angle is dependent on beam energy (21°-65°)
Quadrupole mass filter	PHI	· Low primary beam energy (down to 100 eV) · Primary beam incidence angle (0°-90°) independent of beam energy	· **Low mass resolution** (M/ΔM ~200) · Low transmission (~1%)

Table 1. Instrument Conditions Used for the Current Work

Condition Number	1	2	3	4
Instrument	Cameca Magnetic sector	Cameca Magnetic sector	PHI Quadrupole	PHI Quadrupole
Elements Monitored	H, C, N,O, F, S, Cl	P, Al, Cr, Fe, Cu	H, C, N, O, F, S, Cl	Li, Na, K
Primary Ion Beam	Cs^+	O_2^+	Cs^+	O_2^+
Primary Ion Energy	2.5keV to 14.5keV	2.5keV to 5.5keV	2.5keV to 5keV	2.5keV to 5keV
Positive or Negative Secondary Ions Monitored	$(Cs_2M)^+$: M=H,C,N,O etc or H^-, C^-, $(Si+N)^-$, O^-, F^-, P^-, S^-,Cl^-	P^+, Al^+, Cr^+, Fe^+, Cu^+	H^-, C^-, $(Si+N)^-O^-$, F^-, S^-,Cl^-	Li^+, Na^+, K^+
Oxygen Leak to main chamber	No	Yes for P, No for others	No	No

EXPERIMENTAL DETAILS

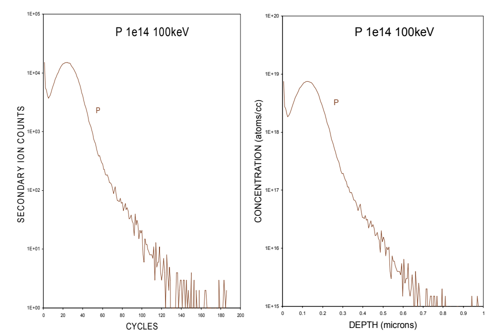
High Mass Resolving Power for magnetic sector SIMS tools

- Mass resolution is defined as: M/ΔM
  (M is mass of interest, DM is mass separation to interfering species)
  For example, P (Phosphorus), mass=31.9738
  (^{30}Si+H), mass=31.9816, ΔM=0.0078 mass units, therefore, a mass resolution of M/ΔM>3956 is needed to follow P in a-Si thin films with a high level of H.

  In order to separate Al and C_2H_3, we need M/ΔM>645
  to separate Al and CNH, we need M/ΔM> 920

SIMS Quantification

- Or how do we go from Raw data (counts / cycle) to Processed data (concentration / depth)?



- With a STANDARD of known composition:

$$RSF = \frac{C_a}{I_a} \times I_m$$

  C_a - is the known concentration of element "a"
  I_a - is the measured intensity of element "a"
  I_m - is the measured intensity of matrix element "m"

- CONCENTRATION:

$$C_a = I_a \times \frac{RSF}{I_m}$$

  C_a = concentration of element "a"
  I_a = intensity of element "a"
  RSF = relative sensitivity factor [3,4,5]
  I_m = intensity of matrix element "m"

SIMS Detection Limits (at/cm^3)

- Selected Impurities in Si under typical depth profiling conditions. Please note that a higher sputter rate typically produces better detection limit. For thin films (~50nm thick), the detection limits may be worse if we cannot sputter the material so fast .

Element	Cs^+ primary beam Negative ions	Cs^+ primary beam Positive ions $(Cs_2M)^+$	O_2^+ primary beam Positive ions
H	1e17	5e17	1E+17
Li			<1e13
C	1E16	2e16	
N	2e15	1e16	
O	5e16	1e17	
F	5e15		
Al			2E+13
P	5e14		1e16 (with O-leak)
S	1e15		
Cl	5e15		
K			2e13
Cr			4e13
Fe			2e14 –4e15
Ni			4e15
Cu			4e14

RESULTS AND DISCUSSION

3.1. Analysis of Hydrogen in a-Si films

Table 2. Comparison of the H-dose on typical samples measured by SIMS and HFS

Sample ID	Total dose by SIMS (atoms/cm^2)	Total Dose by HFS (atoms/cm^2)
#1: H implanted Si Nominal dose: 2.0e15 atoms/cm^2, 30keV	(2.0±0.2)e15 (line 1 in Figure 1) (as SIMS standard)	Below the detection limit of the HFS
#2: H implanted Si Nominal dose: 5.0e16 atoms/cm^2, 170keV	(4.97±0.5)e16	The implanted H peak is deeper (1.58 μm), and the average H is near the detection limit of HFS (approx. 0.2 at.%)
#3: H implanted Si Nominal dose: 1.0e17 atoms/cm^2, 30keV	(9.81±0.98)e16 (line 3 in Figure 1)	1.05e17
#4: H implanted Si Nominal dose: 2.0e17 atoms/cm^2, 30keV	(2.01±0.2)e17 (line 4 in Figure 1)	(2.0±0.2)e17 (line 7 in Figure 1)
#5: 195nm a-Si film	(9.86±1)e16	(8.63+0.9)e16
#6: 300 nm a-Si film	(3.96±0.4)e17	3.62e17

RESULTS & DISCUSSION

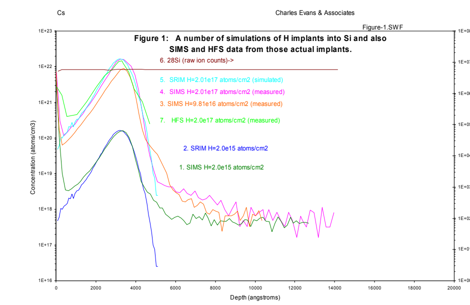


Figure 1: A number of simulations of H implants into Si and also SIMS and HFS data from those actual implants.

Discussion regarding H in a-Si:

- It is clear the agreement between the dose measured by SIMS and the doses measured by HFS are very good. The measured H depth profiles by SIMS and simulated H depth profiles by SRIM code [6] are also good.
- From the results, it can be seen that the implanted H peak increased linearly with increasing the dose and no correction on the RSF value [3,4,5] was needed when moving from the low to high hydrogen content sample.
- The results clearly show that the yield of H secondary ions increases linearly with increasing H content and the SIMS calibration curve [3] for H in Si is straight line from the low to the high H concentration range.

3.2 Analysis of Phosphorus doped n$^+$ a-Si films with high H content

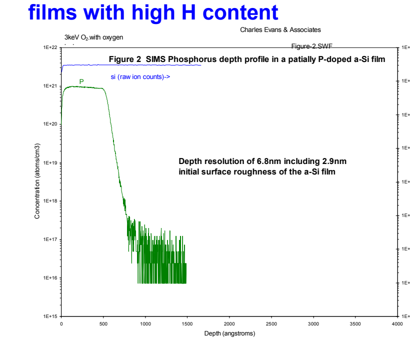


Figure 2. SIMS Phosphorus depth profile in a patially P-doped a-Si film

3.3 Analysis of C,N,O in a-Si thin films

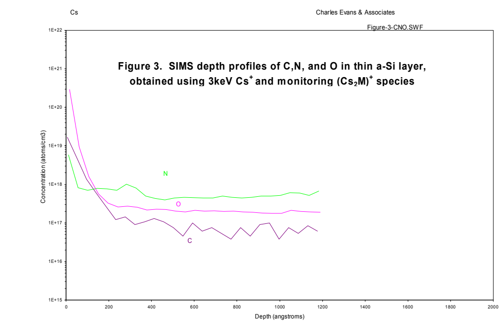


Figure 3. SIMS depth profiles of C,N, and O in thin a-Si layer, obtained using 3keV Cs^+ and monitoring $(Cs_2M)^+$ species

High levels of C, N, and O can affect the mobility of electrons in a-Si films. SIMS depth profiling of trace levels of these species in a-Si needs a good vacuum within the analytical chamber. A higher sputter rate also typically produces better detection limit. Using magnetic sector SIMS with 3keV Cs^+ and monitoring $(Cs_2M)^+$ (M=C,N,O) mode, good depth resolution and good detection limit were obtained.

3.4 Analysis of F and S in a-Si thin films

We have found that if the measured O and H levels are high in an a-Si film, then S and F must be analyzed by magnetic sector SIMS in order to eliminate mass interferences of ^{16}O+^{16}O for ^{32}S or ^{18}O+H for ^{19}F. In this case, a mass resolution of M/ΔM= 2220 is needed for analysis of S and F. If oxygen and hydrogen level are low, F and S can also be analyzed by quadrupole SIMS tool.

3.5 Analysis of Li, Na, K and Cl in a-Si

As possible contaminants, these species can be sources of mobile ionic charge at the a-Si/SiO_2 interface. We have used 3 to 5keV O_2 on a quadrupole SIMS tool to measure Li, Na, and K, and used 3keV Cs^+ tool on a quadrupole SIMS tool to profile Cl.

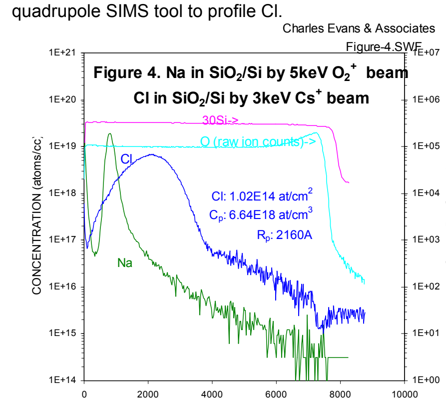


Figure 4. Na in SiO_2/Si by 5keV O_2^+ beam Cl in SiO_2/Si by 3keV Cs^+ beam

3.6 Analysis of Al, Cr, Fe, Ni, and Cu

These species are possible metallic contaminants during a-Si thin film preparation. In practical applications, the a-Si layer is normally followed by an oxide or nitride layer. The metallic contaminants are either fast or slow diffusers within the oxide layer, and will likely lower the breakdown voltage of the oxide layer, therefore, they have to be monitored and controlled. SIMS analysis of these metallic contaminants needs to be done on a magnetic sector SIMS instrument operating at either medium (1000< M/Δ M <3000) or high mass resolution (M/Δ M >3000).

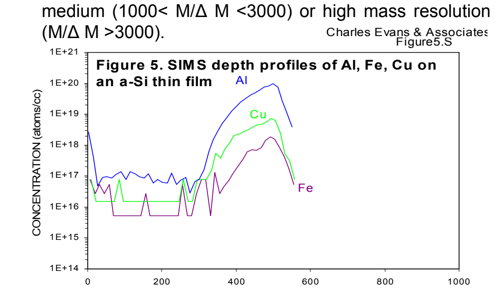


Figure 5. SIMS depth profiles of Al, Fe, Cu in an a-Si thin film

SUMMARY

1. SIMS and HFS have been used to successfully characterize a-Si thin films. The results have shown that the yield of H secondary ions increases linearly with increasing H content and the SIMS calibration curve [3] for H in Si is a straight line over a large H concentration range.
2. Using magnetic sector SIMS, a P-doped a-Si thin layer (50nm thick) was analyzed using 3keV O_2 beam with an oxygen leak. Good depth resolution and detection limit have been obtained.
3. 3keV Cs^+ with $(Cs_2M)^+$ detection mode were used to analyze C, N, and O in a-Si thin films.
4. The results also show that SIMS is a very useful and unique technique to monitor ionic contaminants (such as Li, Na, K, and Cl) and metallic contaminants (such as Al, Cr, Fe, Ni, and Cu) in a-Si, with good detection limits and high depth resolution.

ACKNOWLEDGEMENTS

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