AN 456

SIMS Analysis of C, O, and N in Solar-Grade Silicon

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Introduction

C, O and N contamination in solar-grade silicon can be detrimental to the performance of silicon solar cells. C can form defects that cause shunts or break wire saws. O can form B-O complexes that degrade solar cell efficiency. N can modify the Si point defect distribution of vacancies and self-interstitials that control diffusion of detrimental metal impurities such as Fe.

These contaminants may originate in many sources, such as the original solid silicon feedstock or the process used to manufacture the rectangular blocks of multi-crystalline silicon (mc-Si) or the cylindrical boules of single crystal silicon (c-Si). Determining the amount of contamination and identifying its source are key to reducing the final contamination levels in the silicon solar cells.

Discussion

Secondary ion mass spectrometry (SIMS) can quantitatively measure C, O and N contamination in silicon feedstock, mc-S blocks, and c-Si boules, as well as in the finished silicon solar wafers and silicon solar cells. This allows an investigation of the sequential sources of C, O and N contamination and their contribution to the final contamination levels in the finished product.

In the following case study, SIMS measurements of C, O and N were made on various silicon materials used in the process of making solar cells. Two sources of Si feedstock were used: (a) polysilicon from a modified Siemens process, referred to as “7N” Si feedstock (99.99999% pure), and (b) upgraded metallurgical grade silicon (UMG-Si) referred to as “5N” Si feedstock (99.999% pure). These two silicon feedstocks represent two ways and costs for manufacturing purified Si. The Si feedstock is fed into direct solidification furnaces that melt and regrow the silicon into very large multi-crystalline blocks. The blocks are then cut into subsections called bricks from which wafers are cut. To save cost, the 7N Si (higher cost and purity) and 5N Si are sometimes mixed in predetermined proportions in the direct solidification furnaces.

In this study the 7N and 5N were mixed in a ratio of 80:20 to form one block while a separate block was made from 100% 7N Si. SIMS was performed on corner, edge, and center wafers from each block and these results compared to the results obtained from the 7N and 5N Si feedstock materials.

Table 1. SIMS Impurity Concentrations (x10^{16} atoms/cm^3)

	Carbon	Oxygen	Nitrogen
7N Si feedstock	<0.5	<1.0	0.03
5N Si feedstock	37	200	0.55
7N corner	55	11	1.3
7N center	71	8.0	1.1
7N edge	54	7.8	0.96
7N:5N corner	41	16	1.1
7N:5N center	49	18	1.4
7N:5N edge	49	13	1.2
Typical SIMS detection limits	0.5	1.0	0.02
SEMI PV Si wafer specification	100	80	no spec

Note that each of the C and O numbers for the corner, center, and edge samples are averages of two separate measurements on two separate wafers.

Feedstock Analysis

Table 1 shows that the 7N Si feedstock has no detectable C or O above the 5E15/cm^3 and 1E16/cm^3 detection limits, respectively. This is as expected for a Siemens-based polysilicon process. The 7N Si feedstock does have detectable N which is about an order of magnitude higher than what is typically found in electronic-grade Si substrates used for semiconductor devices. The 5N UMG-Si feedstock was found to have much higher levels of C, O and N than the 7N Si feedstock and the SIMS data indicates that the nitrogen is present in precipitate form, presumably silicon nitride. Previous analyses of UMG-Si samples cooled in non-silicon nitride lined molds showed no detectable N so this N may come from a Si nitride furnace liner. The carbon level in the 5N Si feedstock is below the SEMI PV Si wafer specification for mc-Si wafers, but the oxygen level is not.

Block Analysis

The direct solidification of 7N into blocks for Si wafers adds C, O and N far above the original 7N feedstock, but the C and O are still less than the SEMI PV Si solar wafer specifications. This data indicates that use of the higher purity and cost 7N Si feedstock for forming solar-grade Si is not justified, as the subsequent processing adds much higher levels of C, O and N.

While one would expect somewhat higher impurity levels in a block formed with the 80:20 7N/5N mix, compared to the pure 7N block, this was not the result. The carbon level is actually lower in the 80:20 samples than in the 7N block samples, while the O levels are somewhat higher. The levels of N contamination are fairly similar between the two blocks. The block grown from 7N feedstock and the block grown from the mix of 7N and 5N feedstock were grown in different direct solidification furnaces. The unexpected C reduction from mixing pure 7N with “dirty” 5N feedstock may be due to differences in the C contamination from the different furnaces.