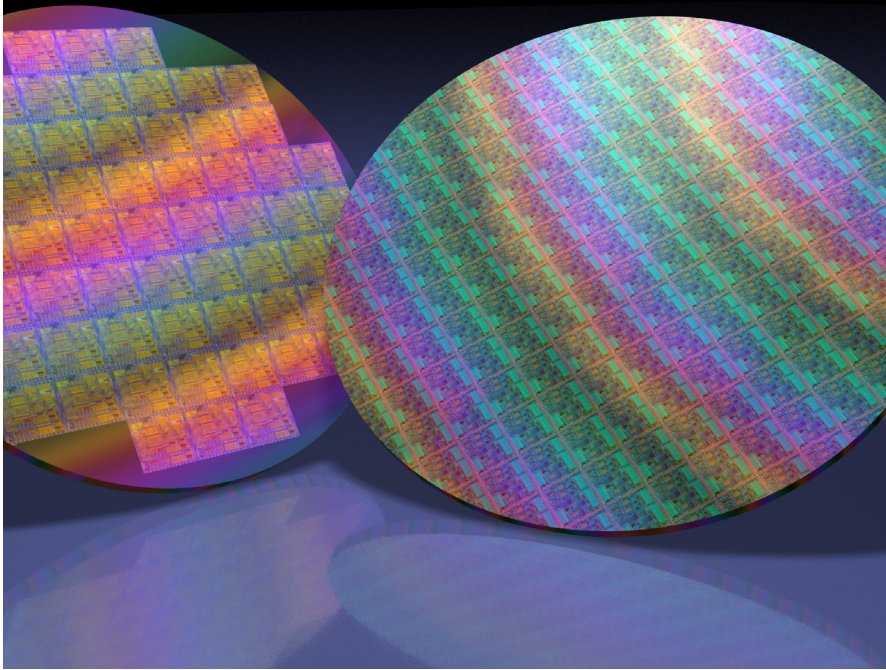Author:

Ian Robertson

PerkinElmer
Seer Green
United Kingdom

Semi-Automated FT-IR Measurements of Elemental Impurities in Silicon Wafers

Introduction

Silicon wafer production is expected to grow in the coming years with increased demand for semiconductors especially in consumer electronics, automotives and the use of silicon devices in the growing solar power industry. A range of different manufacturing methods are used for the production of silicon wafers, the two most common being the Float Zone (FZ) and Czochralski (CZ) processes. The FZ process yields high purity silicon wafers, whereas the CZ process produces wafers with elemental impurities, particularly carbon and oxygen. However, the CZ process has some major advantages over the FZ process such as better thermal stress properties of the wafer, faster and lower cost of manufacturing. In addition, the presence of oxygen impurities can have a positive benefit as it acts as a getter, removing trace metal impurities. Hence, the CZ process is most widely adopted in the industry for silicon wafer manufacturing.

The levels of carbon and oxygen impurities in silicon wafers need to be determined to ensure they are not too high since this can lead to electrically active defects and product failure/rejection. Infrared spectroscopy offers rapid and easy measurement to determine the levels of these impurities according to global standard methods.[1,2,3,4]

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Materials and Methods

The measurement system consists of a PerkinElmer Spectrum 3™ FT-IR spectrometer with MappIR wafer holder and optical system with automation software, as shown in Figure 1.
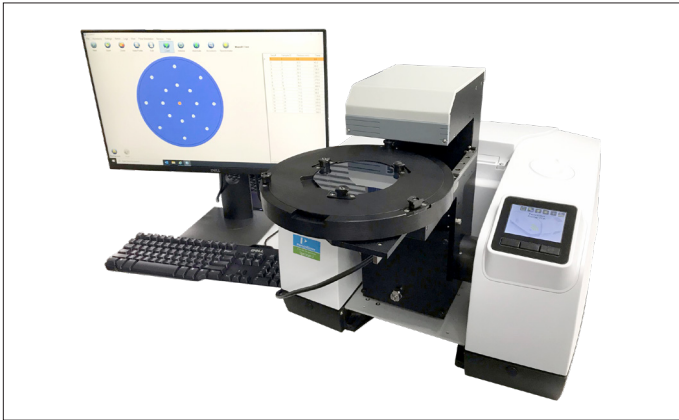

Figure 1. The Spectrum 3 FT-IR and MappIR System.

The system is able to analyze a range of wafer sizes from 2 inches up to 8 inches (MappIR) or 12 inches (Mapp300) in either transmission or reflection mode. The automation software allows automated, unattended mapping of the wafer, collecting spectra across the entire wafer according to pre-set or user-defined mapping arrangements. Data collection is followed by calculations according to the analysis method specified.

Spectra were collected in Transmission mode for a range of 6 inch diameter silicon wafers at a spectral resolution of 4 cm^{-1} using 32 scans for data collection. The Spectrum 3 and MappIR were continuously purged using dry nitrogen to remove atmospheric spectral interferences from the spectra.

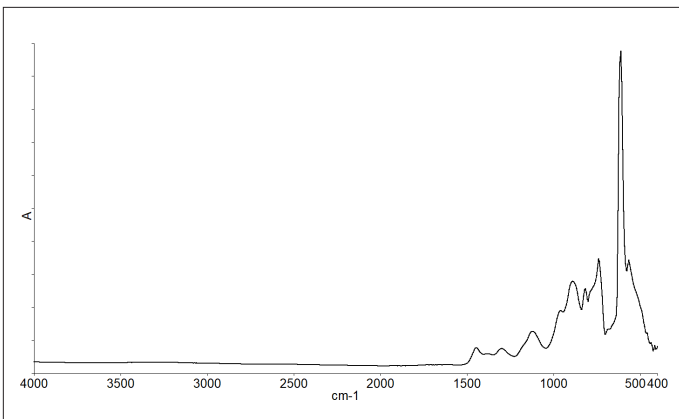A spectrum of a 500 microns thick Float Zone silicon wafer is shown in Figure 2.

Figure 2. The infrared spectrum of a Float Zone silicon wafer.

The infrared spectrum shows that there are several absorption bands below 1500 cm^{-1} due to the silicon lattice vibrations. Figure 3 shows spectra of the same FZ wafer and a CZ wafer overlaid zooming in on the spectral range below 1500 cm^{-1}.
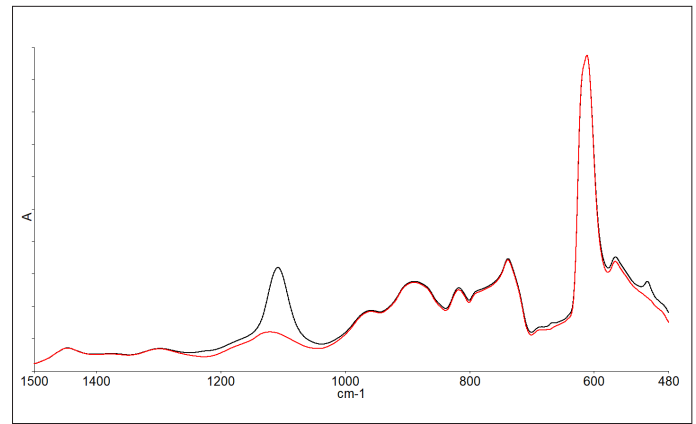

Figure 3. FZ wafer spectrum (red) and CZ wafer spectrum (black) showing spectral differences.

It can be seen from the spectra that there are differences between the 2 wafer spectra especially the additional band around 1100 cm^{-1} in the CZ spectrum. In order to see the spectral differences more clearly and to perform calculations on the spectra the standard methods specify the subtraction of the high purity FZ reference wafer spectrum from the CZ sample being analysed. This generates a spectrum as shown in Figure 4.
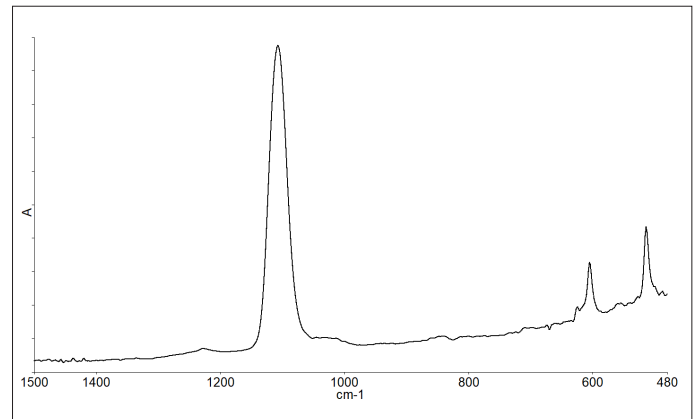

Figure 4. Subtraction spectrum of CZ-FZ wafer spectra showing bands due to impurities in the CZ material.

The bands at 1107 and 513 cm^{-1} are due to the interstitial oxygen present and the band at 605 cm^{-1} is due to the substitutional carbon present. These bands allow for quantitative analysis to be performed on the spectra. Spectra of wafers with a range of different oxygen concentrations are shown in Figure 5.

The calculation methods allow for the use of linear regression of a series of calibration standards or the use of standard calibration factors. Historically, standard reference materials of oxygen in silicon wafers were available from NIST for calibrations. However, these are no longer available so the vast majority of analyses use the standard calibration factors.
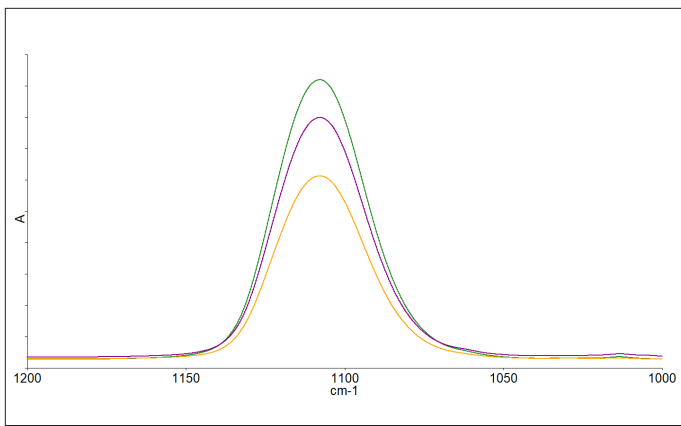
Figure 5. Spectra of high (green), medium (purple) and low (yellow) oxygen concentration wafers after subtraction of a zero oxygen reference FZ wafer spectrum.

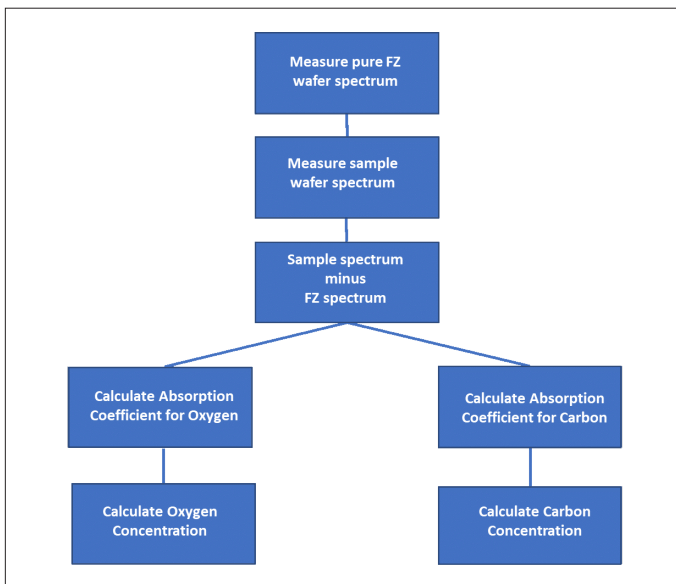The workflow for determining the carbon and oxygen content is as follows, shown in Figure 6:

Figure 6: Carbon and Oxygen Content Determination Workflow.

The absorption coefficients for Oxygen and Carbon can be determined at the peaks 1107 cm^{-1} and 607 cm^{-1} respectively using the following calculation:

Absorption coefficient α = (1/d) Ln (T$_0$ / T)

Where:

T$_0$ is the calculated baseline transmission at the peak position

T is the measured transmission at the peak position

d is the sample thickness (cm)

The concentrations of oxygen and carbon in atoms/cm^3 and parts per million atomic (ppma) are calculated using the following formula:

Oxygen atoms/cm^3 = 3.14*10^{17} **α**

Oxygen ppma = 6.28 **α**

Carbon atoms/cm^3 = 8.2x10^{16} **α**

Carbon ppma = 1.64 **α**

For the sample spectrum shown in Figure 4 the following values were calculated, as shown in Table 1:

Table 1. Calculated values of Figure 4.

	Oxygen	Carbon
Absorption Coefficient, α	2.61	0.384
Atoms/cm^3	8.1954 x 10^{17}	3.1488 x 10^{16}
ppma	16.3908	0.62976

The sample tested was a 6 inch CZ silicon wafer with a thickness of 500 microns, double-side polished (DSP) measured in Transmission.

The AutoPRO7 automation software was used to map the concentrations of carbon and oxygen across the same wafer at the geometries shown in Figure 7.
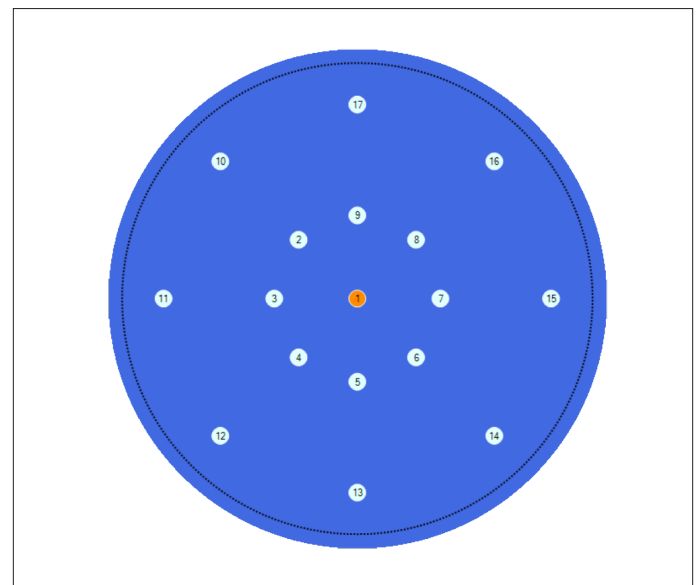

Figure 7: Geometry of the measurement positions in the Auto PRO7 software.

Spectra were collected automatically at the center of the wafer and at 20 and 50mm radii from the center at 45 degree increments giving a total of 17 measurements across the wafer. The spectra are shown in Figure 8.
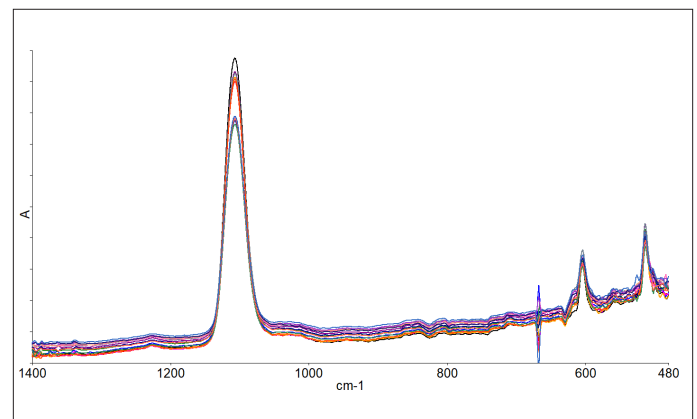

Figure 8. Spectra collected across the wafer.

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It can clearly be seen that there are different intensities in the oxygen peaks in the different measurements. Oxygen and carbon concentrations were calculated for each point and are shown in Table 2.

Table 2. Oxygen and carbon concentrations in the measured silicon wafer.

Sample Name	Oxygen Concentration (atoms/cm³)	Carbon Concentration (atoms/cm³)
1115_B_001	8.21E+17	3.12E+16
1115_B_002	7.56E+17	2.96E+16
1115_B_003	7.59E+17	3.12E+16
1115_B_004	7.62E+17	3.08E+16
1115_B_005	7.64E+17	3.15E+16
1115_B_006	7.67E+17	3.27E+16
1115_B_007	7.60E+17	3.03E+16
1115_B_008	7.49E+17	3.44E+16
1115_B_009	7.60E+17	2.98E+16
1115_B_010	6.24E+17	3.03E+16
1115_B_011	6.19E+17	3.10E+16
1115_B_012	6.26E+17	2.79E+16
1115_B_013	6.18E+17	2.77E+16
1115_B_014	6.22E+17	2.96E+16
1115_B_015	6.26E+17	2.86E+16
1115_B_016	6.33E+17	2.93E+16
1115_B_017	6.18E+17	2.94E+16
Mean Value	6.99E+17	3.03E+16
Std Dev	7.53518E+16	1.67278E+15
RSD%	10.78%	5.52%

The oxygen is shown to vary significantly across the wafer, whereas the carbon measurements are much more consistent. The ideal wafer would have consistent measurements across the entire wafer to avoid inconsistencies when the wafers are cut into smaller individual pieces.

Summary

The PerkinElmer Spectrum 3 with MappIR wafer analysis system is shown to be capable of measuring the levels of impurities present in silicon wafers, a parameter that is very important for the performance of the wafer. The data collection and calculations can be automated with the use of macros in the software and the calculations can be customized according to the regulatory body method required.

Other semiconductor applications can also be performed such as the measurement of coatings and dielectrics as well as Epitaxial films.

The Spectrum 3 can also be used for raw materials identification in the semiconductor industry and can be coupled to a Spotlight FT-IR microscope for defect analysis.

References

1. SEMI MF1188-1105 Test Method for Interstitial Oxygen Content of Silicon by Infrared Absorption with Short Baseline.

2. SEMI MF1391-93 (Reapproved 2000) Test Method for Substitutional Atomic carbon Content of Silicon by Infrared Absorption.

3. National Standards of the People's Republic of China GB 1557-89, GB/T 1558.

4. JEITA EM-3503 Standard Test Method for Substitutional Atomic Carbon Content of Silicon by Infrared Absorption.

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