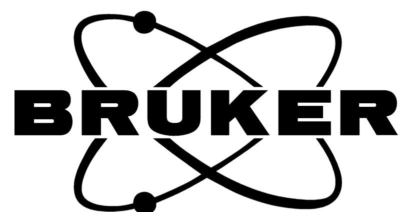
# OPUS
Spectroscopy Software

Version 6

## User Manual

# SEMI



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This manual is the original documentation for the OPUS spectroscopic software.

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# 1 Introduction

The software package OPUS/SEMI is intended for analyses in the field of semiconductor quality control.

On the basis of an absorbance spectrum of a wafer, this OUS function calculates the impurity concentration of interstitial oxygen (Oi) and substitutional carbon (Cs) in silicon wafers.

OPUS/SEMI provides evaluation methods based on the following ASTM and DIN standards:

- ASTM F 1188-93a Oxygen
- ASTM F 1391-92 Carbon
- DIN 50438-1 A (93) Oxygen
- DIN 50438-1 B (93) Oxygen
- DIN 50438-2 (82) Carbon

Besides the evaluation methods based on the above listed ASTM and DIN standards, the following methods are available:

- The pseudo ASTM method which requires that the wafer thickness is already known.
- The ratio method which automatically computes the wafer thickness from the silicon matrix peaks.
- A special ratio method which is designed to deal with strongly curved baselines which can occur when analyzing samples with a rough surface and/or free charge carriers.

**Note:** For the calculation algorithms of the available evaluation methods refer to chapter 3.

The *CARBon-OXygen Analysis* function of OPUS/SEMI is suited for two types of wafers having different surface treatments:

- Double-side polished or polish-etched wafers
- Single-side polished wafers with etched back surfaces

# 2 Carbon - Oxygen Analysis

Before starting a *Carbon - Oxygen Analysis*, acquire an absorbance spectrum of a pure silicon wafer produced by float-zoning (reference wafer) and an absorbance spectrum of a silicon wafer containing Oi- and Cs-impurities (test wafer that is to be analyzed).

**Note:** When setting up the general measurement parameters, define a resolution of 4.0 and a zerofilling factor of 2.

After the measurement, load the files containing the absorbance spectra (reference and sample spectra) into OPUS. (See figure 1.)

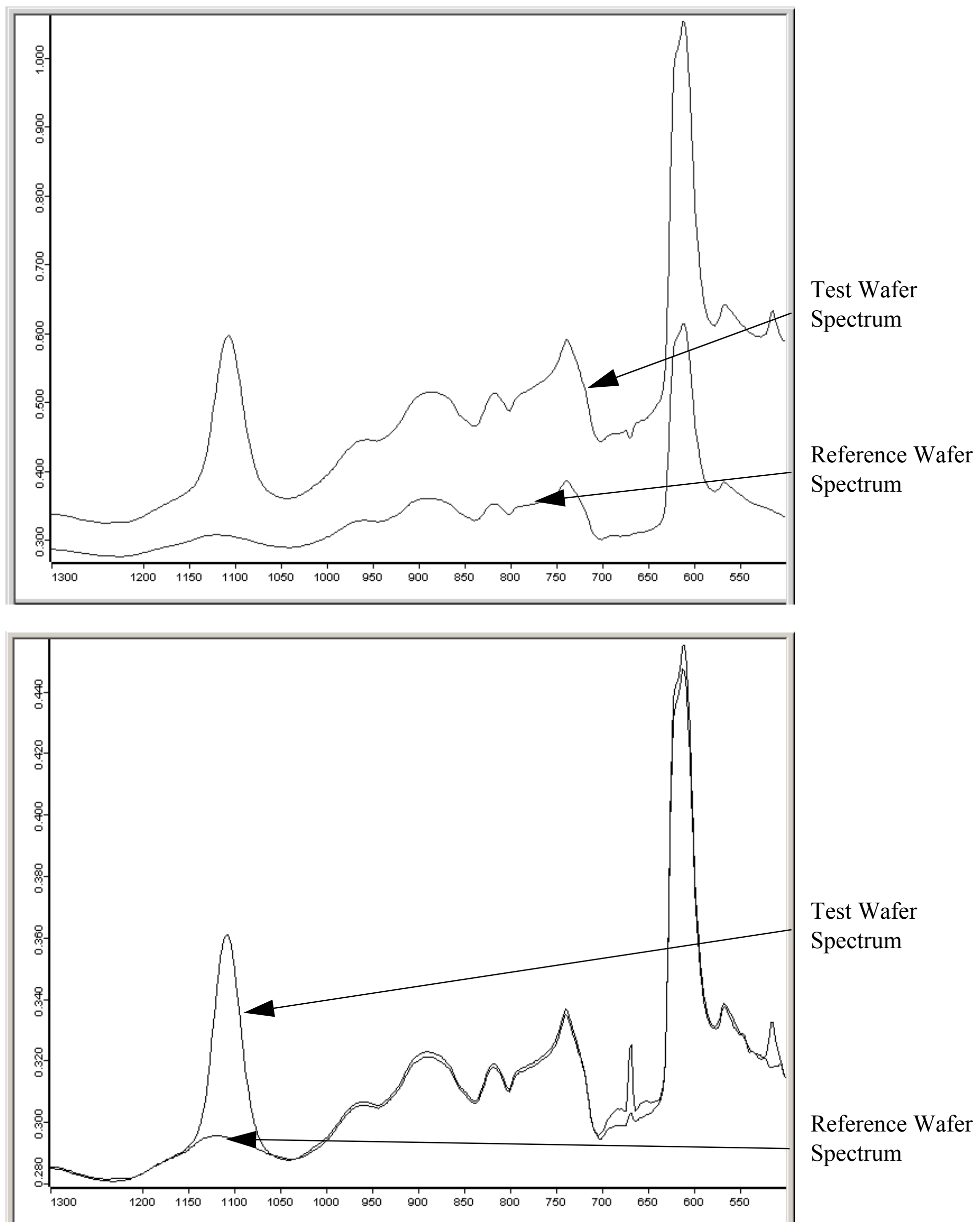


Figure 1: Absorbance Spectra for the Carbon - Oxygen Analysis

## 2.1 Select Files

To determine the impurity concentrations of interstitial oxygen (Oi) and substitutional carbon (Cs) in a silicon wafer, select in the OPUS *Evaluate* menu the *CARBon-OXygen Analysis* function. The following dialog window appears:

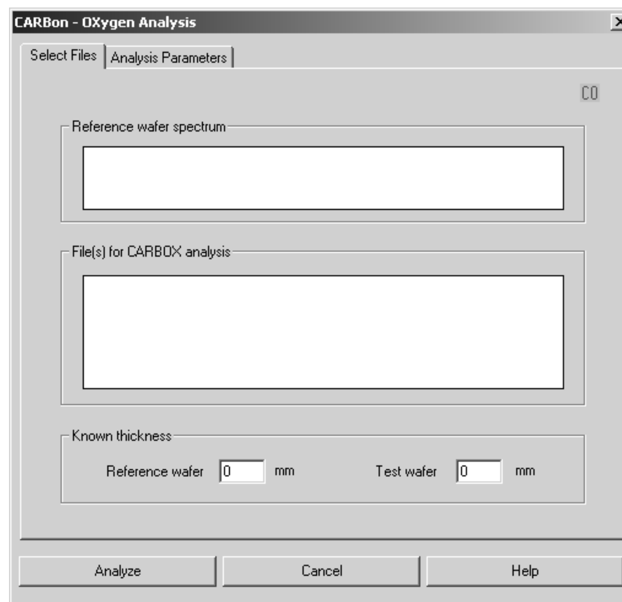


Figure 2: Carbon-Oxygen Analysis Dialog Window - Select Files

Drag and drop the absorbance data block of the reference wafer in the upper field *Reference wafer spectrum* and the absorbance data block(s) of the test wafer(s) in the lower field *File(s) for CARBOX analysis*.

**Note:** The OPUS function *CARBon - OXygen Analysis* accepts only absorbance data blocks.

**Note:** This OPUS function allows also the evaluation of a 3D data block (of the test wafer). In this case, the concentrations $O_i$ and $C_s$ are displayed as traces.

Enter the thickness values (in mm) of the reference and the test wafer in the corresponding fields, provided that these values are known. For all evaluation methods - except for *RATIO Method 1* and *RATIO Method 2* - the thickness values of the reference and the test wafer need to be entered. If the thickness is unknown, enter the value *0*. In this case, the thickness is calculated using the silicon phonon peak at 610cm$^{-1}$. (The algorithm for the wafer thickness calculation is described in detail in chapter 3).

# 2.2 Analysis Parameters

Click on the *Analysis Parameter* tab. The following dialog window appears:

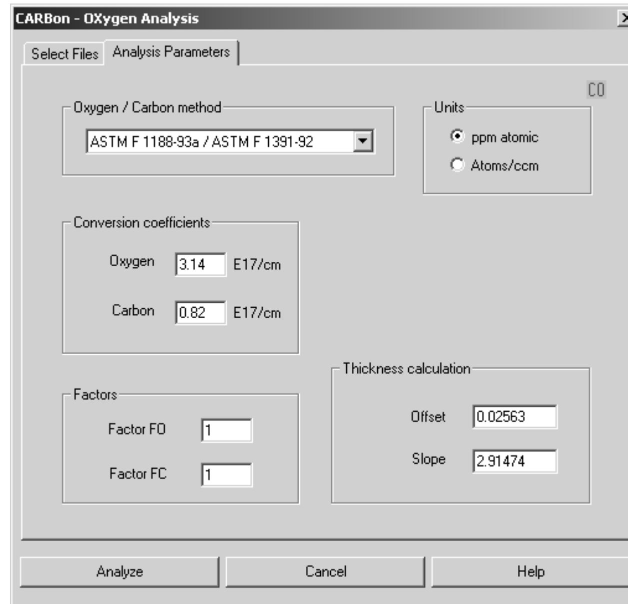


Figure 3: Carbon-Oxygen Analysis Dialog Window - Analysis Parameters

## 2.2.1 Oxygen / Carbon Methods

In this dialog window, you specify the parameters for the carbon-oxygen analysis. The following evaluation methods are available:

- ASTM F 1188-93a / ASTM F 1391-92
- DIN 50438-1 A (93) / ASTM F 1391-92
- DIN 50438-1 B (93) / ASTM F 1391-92
- RATIO-Method 1
- RATIO-Method 2
- Pseudo ASTM
- No Oxygen Analysis / DIN 50438-2 (82)

The methods for calculating the interstitial oxygen concentration are:

- ASTM F 1188-93a
- DIN 50438-1 A (93)
- DIN 50438-1 B (93)
- RATIO-Method 1
- RATIO-Method 2
- Pseudo ASTM

The methods for calculating the substitutional carbon concentration are:

- ASTM F 1391-92
- RATIO-Method
- Pseudo ASTM
- DIN 50438-2 (82)

The **RATIO - Methods 1** and **2** are suited for double-side polished wafers and for wafers with a rough backside. Using these methods, the height of the oxygen peak (at $1107cm^{-1}$) and the height of the carbon peak (at $605cm^{-1}$) are calculated for both spectra (i.e. the reference wafer spectrum and the test wafer spectrum). For this purpose, proper baselines are fitted. Then, a so-called ratio factor is calculated using the silicon peak at $738cm^{-1}$. The oxygen and carbon peak heights of reference wafer spectrum are multiplied with this ratio factor and subtracted from the peak height of the test wafer spectrum. Using the corrected peak heights, the software calculates the oxygen and carbon concentrations by dividing these peak heights by the height of the baseline corrected silicon peak at $617cm^{-1}$ of the test wafer spectrum and multiplying it by appropriate proportional factors.

In case of RATIO-Method 1, linear baselines are fitted, whereas in case of RATIO-Method 2 a quadratic polynomial is used for the oxygen baseline. This method can be used for spectra with a strong curved baseline.

The **Pseudo ASTM Method** can only be used for silicon slices polished on both sides.

Taking the multiple reflections on both wafer surfaces into account, the formula for calculating the transmittance spectrum ($T=10^{-Absorbance}$) is:

$$T = \frac{(1-R)^2 e^{-\alpha d}}{1 - R^2 e^{-2\alpha d}}$$

with $d$ being the wafer thickness and $R$ being the reflectivity (0.3). Using the this formula, the absorption coefficient $\alpha$ is calculated.

The $\alpha$-values for the peak and the baseline point are evaluated and then the baseline value is subtracted from the peak value. This is done for both the reference wafer spectrum and the test wafer spectrum. Then, the $\alpha$-values from the reference measurement are subtracted from those of the test wafer spectrum. These corrected $\alpha$-values are proportional to the impurity concentrations.

**Note:** The complete calculation algorithms for all evaluation methods are described in chapter 3.

If you are not sure which oxygen / carbon method you should use, select ASTM F 1188-93a (oxygen) and ASTM F 1391-92 (carbon).

## 2.2.2 Other Analysis Parameters

In the group field *Units*, specify the unit (*ppm atomic* or *atoms/ccm*) in which the concentration values in the Quant report are to be displayed by clicking on the corresponding option button.

In the group field *Conversion Coefficients*, specify the conversion coefficients for oxygen and carbon. These conversion coefficients are multiplied by the absorption coefficients for the oxygen peak and the carbon peak to get the concentration values. For the evaluation methods based on ASTM standards, the default values of the conversion coefficients are: oxygen: 3.14 E17/cm and carbon: 0.82 E17/cm.

The multiplication factors **Factor FO** (oxygen) and **Factor FC** (carbon) have the default value 1. If you measure calibration wafers with known oxygen and carbon concentrations you can use these factors for your calibration.

In the group field *Thickness Calculation* you specify the *Offset* and the *Slope*. The default parameters are only valid for double-side polished wafers and a certain thickness range (approx. from 0.3 to 2.5mm). If your wafer does not fulfill the above mentioned conditions concering surface treatment and thickness, you need to change these default values.

**Note:** It is better to work with known thickness values than to calculate them on the basis of the FT-IR spectrum as described in chapter 3, section 3.1.

In case of the method DIN 50438-1 A (93), the concentration of the free charge carriers needs to be entered as well. See figure 4.

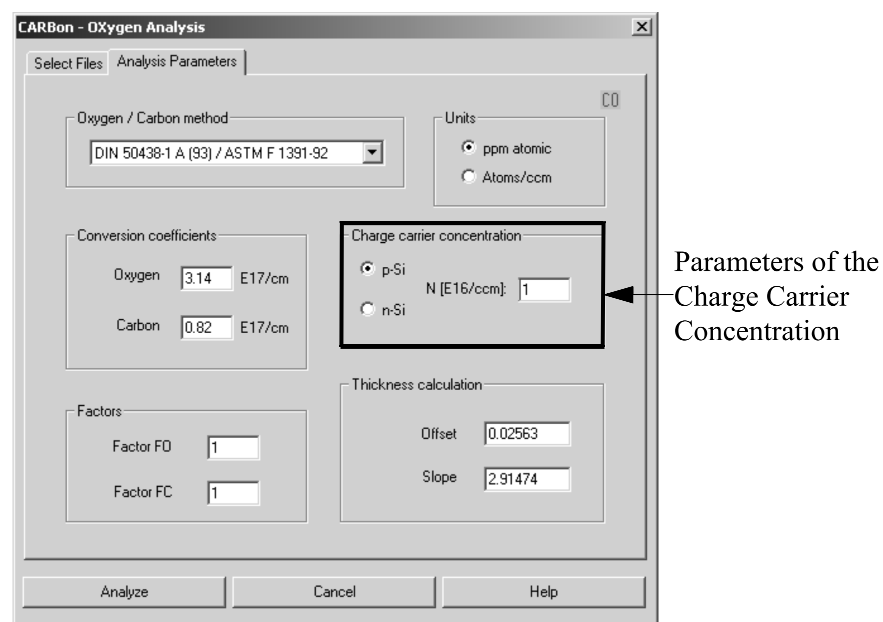


Figure 4: Analysis Parameters of the Charge Carrier Concentration

## 2.3 Analysis Results

After having entered all analysis parameters, click on the *Analyze* button. (See figure 4.) The results of a carbon-oxygen analysis are stored in a Quant data block (figure 5) which is attached to the test wafer spectrum file. To display the analysis results, double-click on the Quant data block. As a result, the OPUS report window opens.

Depending on the number of analyses (e.g. using different methods) you have performed, there are several carbon oxygen analysis reports displayed in form of a directory tree. Clicking on one of them displays the corresponding analysis result.

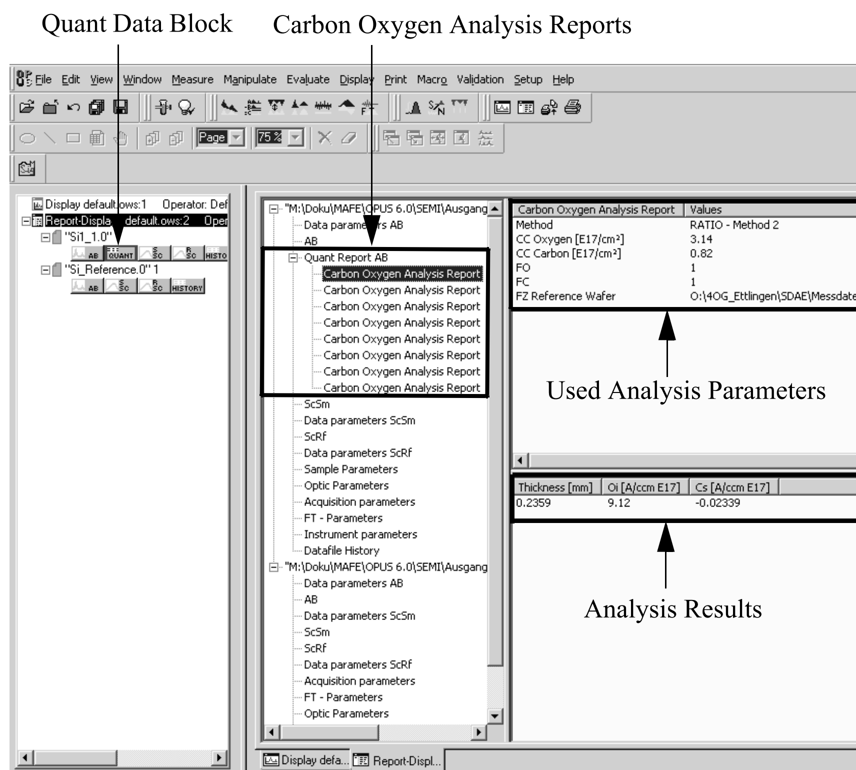


Figure 5: OPUS Report Window

# 3 Calculation Algorithms

This chapter describes the calculation algorithms of the different methods for determining the oxygen and the carbon impurity concentrations.

## 3.1 Calculation of the Wafer Thickness

For the calculation of the wafer thickness, the silicon phonon peak at $610cm^{-1}$ in the absorbance spectrum is used.

1) The absorption values of the three data points at the wavenumbers 617.18, 619.1 and $615.26cm^{-1}$ are averaged. (The data point nearest to the specified wavenumber is chosen.)

**Note:** These data points are not exactly in the center of the peak, but slightly off-center.

2) The baseline is a straight line calculated by fitting the six data points (the data point at $651.9cm^{-1}$ and the two neighboring data points as well as the data point at $576.68cm^{-1}$ and the two neighboring data points) using the least-squares method.

3) The y-value of the baseline at $617.18cm^{-1}$ is determined.

4) This value is subtracted from the absorption value calculated in step 1. The result is called $A_D$.

5) The wafer thickness is calculated using the following empirical formula:

$$d[mm] = 0.02563 + 2.91474 \bullet A_D$$

with 0.02563 being the default *Offset* value and 2.91474 being the default *Slope* value.

**Note:** This formula can only be used for double-side polished wafers having a certain thickness range (approx. from 0.3 to 2.5mm).

For a more flexible thickness calculation, the parameters *Offset* (a) and *Slope* (b) in the above formula are free parameters:

$$d[mm] = a + b \bullet A_D$$

## 3.2 Ratio 1 Method - Oxygen

1) The data point at 1107.08cm$^{-1}$ and two data points on the right and two data points on the left (totally 5 data points) are used for a least squares fit to a parabola.

2) The y-value of this parabola ($A_P$) at the wavenumber 1107.08cm$^{-1}$ is determined.

3) A linear baseline is calculated by fitting six data points (the data point at 1299.9cm$^{-1}$ and two neighboring data points as well as the data point at 940cm$^{-1}$ and two neighboring data points) using the least squares method.

4) The y-value of the baseline ($A_B$) at 1107.08cm$^{-1}$ is determined.

5) The difference $A_P - A_B$ for both the test wafer spectrum and the reference wafer spectrum are calculated. The results are $A_T$ (absorption value of the test wafer spectrum) and $A_R$ (absorption value of the reference wafer spectrum).

6) For the calculation of the so-called ratio factor (R), the silicon peak at 738cm$^{-1}$ is used. The y-values of the data points at 740.6, 738.0 and 736.0cm$^{-1}$ are averaged. The calculated average value $ASI_P$ is taken as intensity of the peak maximum.

7) For the calculation of the baseline, five data points are used. The absorption value of the left baseline point (BL) is the mean value of the y-values at 1043.4, 1041.5 and 1039.6cm$^{-1}$. The absorption value of the right baseline point (BR) is the mean value of the y-values at 700 and 698cm$^{-1}$. The value of the baseline ($ASI_B$) at 738 cm$^{-1}$ is calculated using the following formula:

$$ASI_B = \frac{(BL \bullet 40 + BR \bullet 300)}{340}$$

8) The difference $ASI_P - ASI_B$ for both the test wafer and the reference wafer spectrum are calculated. The results are $ASI_T$ and $ASI_R$.

9) The ratio factor $R$ is calculated as follows:

$$R = \frac{ASI_T}{ASI_R}$$

10) The absorption value of oxygen ($A_o$) is calculated using the following equation:

$$A_O = A_T - R \bullet A_R$$

11) The oxygen concentration $c_o$ is calculated using the following formula:

$$c_O = 6.4\ cm^{-1} \bullet \frac{A_O}{A_D} \bullet 3.14 \bullet 10^{17} cm^{-2}$$

with $A_D$ being the absorption value (at 610cm$^{-1}$,silicon peak) which has been calculated in the course of the thickness calculation for the test wafer spectrum (See section 3.1.) The factor *3.14* is the conversion coefficient (oxygen) which can be changed by the user in the *CARBon-OXygen Analysis* dialog window.

12) Then, the calculated oxygen concentration value is multiplied by the factor FO (Factor Oxygen), which can be specified by the user:

$$C_O = c_O \bullet FO$$

**Note:** The thickness value is not used for the oxygen concentration calculation. Only the baseline corrected absorption value $A_D$ of the silicon peak at 610cm$^{-1}$ has an influence on the oxygen concentration calculation.

## 3.3 Ratio 2 Method - Oxygen

The difference between *Ratio 1 Method* and *Ratio 2 Method* concerns only step 3. For determining the absorption value of the baseline ($A_B$), a parabola is fitted.

A parabolic baseline is calculated by fitting the following 12 data points:

- data point at 1299.9cm$^{-1}$ and the two neighboring data points
- data point at 1180cm$^{-1}$ and the two neighboring data points
- data point at 1040cm$^{-1}$ and the two neighboring data points
- data point at 940cm$^{-1}$ and the two neighboring data points

## 3.4 Ratio Method - Carbon

1) The data point at 605.6cm$^{-1}$ and two data points on the right and two data points on the left (totally 5 data points) are used for a least squares fit to a parabola.

2) The y-value of the parabola ($A_P$) at the wavenumber 605.6cm$^{-1}$ is determined.

3) A linear baseline is calculated by fitting six data points (the data point at 622.97cm$^{-1}$ and the two neighboring data points as well as the data point at 567.04cm$^{-1}$ and the two neighboring data points) using the least square method.

4) The y-value of the baseline ($A_B$) at 605.6cm$^{-1}$ is determined.

5) The difference $A_P - A_B$ for both the test wafer spectrum and the reference wafer spectrum are calculated. The results are $A_T$ (absorption value of the test wafer spectrum) and $A_R$ (absorption value of the reference wafer spectrum).

6) For the calculation of the so-called ratio factor (R), the silicon peak at 738cm$^{-1}$ is used. The y-values of the data points at 740.6, 738.0 and 736.0cm$^{-1}$ are averaged. This average value $ASI_P$ is taken as intensity of the peak maximum.

7) For the calculation of the baseline, five data points are used. The absorption value of the left baseline point (BL) is the average value of the y-values at the wavenumbers 1043.4, 1041.5 and 1039.6cm$^{-1}$. The absorption value of the right baseline point (BR) is the average value of the y-values at the wavenumbers 700 and 698cm$^{-1}$. The value the baseline ($ASI_B$) at 738cm$^{-1}$ is calculated using the following formula:

$$ASI_B = \frac{(BL \bullet 40 + BR \bullet 300)}{340}$$

8) The difference $ASI_P - ASI_B$ for both the test wafer spectrum and the reference wafer spectrum are calculated. The results are $ASI_T$ and $ASI_R$.

9) The ratio factor *R* is calculated as follows:

$$R = \frac{ASI_T}{ASI_R}$$

10) The absorption value of carbon ($A_C$) is calculated using the following equation:

$$A_C = A_T - R \bullet A_R$$

11) The carbon concentration $c_C$ is calculated using the formula:

$$c_C = 10.14\ cm^{-1} \bullet \frac{A_C}{A_D} \bullet 8.2 \bullet 10^{16} cm^{-2}$$

with $A_D$ being the absorption value (at 610cm$^{-1}$, silicon peak) which has been calculated in the course of the thickness calculation for the test wafer spectrum. (See section 3.1.) The factor *8.2* is the conversion coefficient (carbon) which can be changed by the user in the *CARBon-OXygen Analysis* dialog window. The carbon concentration value is multiplied by the factor FC, which can be specified by the user:

$$C_C = c_C \bullet FC$$

**Note:** The thickness value is not used for the oxygen concentration calculation. Only the baseline corrected absorbance value $A_D$ of the silicon peak at 610cm$^{-1}$ has an influence on the oxygen concentration calculation.

## 3.5 Pseudo ASTM Method - Oxygen

1) The thickness of reference wafer and test wafer are determined by either measuring the thickness using a caliper gauge or calculating the thickness using the silicon phonon peak at 610cm$^{-1}$ in the absorbance spectra. (See section 3.1.)

**Note:** First the oxygen absorption coefficients are calculated separately for test wafer spectrum and reference wafer spectrum.

2) The data point at 1107.08cm$^{-1}$ and two data points on the right and two data points on the left (totally 5 data points) are used for a least squares fit to a parabola.

3) The y-value of this parabola ($A_P$) at the wavenumber 1107.08cm$^{-1}$ is determined.

4) A linear baseline is calculated by fitting six data points (the data point at 1299.9cm$^{-1}$ and the two neighboring data points as well as the data point at 940cm$^{-1}$ and the two neighboring data points) using the least squares method.

5) The y-value of the baseline ($A_B$) at 1107.08cm$^{-1}$ is determined.

6) The absorption coefficients $\alpha$ for $A_P$ and $A_B$ are calculated using the following formula:

$$\alpha = -\frac{1}{d} \ln \frac{-(1-R)^2 + \sqrt{(1-R)^4 + 4T^2R^2}}{2TR^2}$$

with $d$ being the wafer thickness, R (ratio factor) having the value 0.3 and T = $10^{-A}$.

7) The absorption coefficient calculated for the baseline point is subtracted from the absorption coefficient calculated for the peak at 1107cm$^{-1}$ ($\alpha_P$ - $\alpha_B$). The results are net absorption coefficients for the test wafer and the reference wafer ($\alpha_T$ and $\alpha_R$).

8) To calculate the absorption coefficient for oxygen $\alpha_O$ the net absorption coefficient of the test wafer is subtracted from the net absorption coefficient of the reference wafer:

$$\alpha_O = \alpha_T - \alpha_R$$

9) The oxygen concentration $c_O$ is calculated by multiplying the absorption coefficient $\alpha_O$ by a calibration factor:

$$c_O = 3.14 \bullet 10^{17}\ cm^{-2}\ \alpha_O$$

This calibration factor is also called conversion coefficient. The default value is 3.14 x $10^{17}cm^{-2}$. This value can be changed by the user in the *CARBon-OXygen Analysis* dialog window.

10) The oxygen concentration value $c_O$ (calculated in step 9) is multiplied by the factor FO (default value FO=1), which can be specified by the user in the *CARBon-OXygen Analysis* dialog window:

$$C_O = c_O \bullet FO$$

## 3.6 Pseudo ASTM Method - Carbon

1) The thickness of reference wafer and test wafer are determined by either measuring the thickness using a caliper gauge or by calculating the thickness using the silicon phonon peak at 610$cm^{-1}$ in the absorbance spectra. (See section 3.1.)

**Note:** First the carbon absorption coefficients are calculated separately for test wafer spectrum and reference wafer spectrum.

2) The data point at 605.6$cm^{-1}$ and two data points on the right and two data points on the left (totally 5 data points) are used for a least squares fit to a parabola.

3) The y-value of the parabola ($A_P$) at the wavenumber 605.6$cm^{-1}$ is determined.

4) A linear baseline is calculated by fitting six data points (the data point at 622.97$cm^{-1}$ and the two neighboring data points as well as the data point at 567.04$cm^{-1}$ and the two neighboring data points) using the least squares method.

5) The y-value of the baseline ($A_B$) at 605.6$cm^{-1}$ is determined.

6) The absorption coefficients $\alpha$ for $A_P$ and $A_B$ are calculated using the following formula:

$$\alpha = -\frac{1}{d} \ln \frac{-(1-R)^2 + \sqrt{(1-R)^4 + 4T^2R^2}}{2TR^2}$$

with $d$ being the wafer thickness, $R$ (ratio factor) having the value 0.3 and T = $10^{-A}$.

7) The absorption coefficient calculated for the baseline point is subtracted from the absorption coefficient calculated for the peak (at 605cm$^{-1}$) $\alpha_P$ - $\alpha_B$. The results are net absorption coefficients for the test wafer and the reference wafer ($\alpha_T$ and $\alpha_R$).

8) To calculate the absorption coefficient for carbon ($\alpha_C$), the net absorption coefficient of the test wafer is subtracted from the net absorption coefficient of the reference wafer:

$$\alpha_C = \alpha_T - \alpha_R$$

9) The carbon concentration $c_C$ is calculated by multiplying the absorption coefficient $\alpha_C$ by a calibration factor:

$$c_C = 8.2 \bullet 10^{16}\ cm^{-2}\ \alpha_C$$

This calibration factor is also called conversion coefficient. The default value is 8.2 x 10$^{16}$cm$^{-2}$. This value can be changed by the user in the *CARBon-OXygen Analysis* dialog window.

10) The carbon concentration value $c_C$ (calculated in step 9) is multiplied by the factor FC (default value FC=1), which can be specified in the *CARBon-OXygen Analysis* dialog window:

$$C_C = c_C \bullet FC$$

# 3.7 ASTM F 1188-93a Method - Oxygen

1) The thickness of reference wafer and test wafer are determined by either measuring the thickness using a caliper gauge or by calculating the thickness using the silicon phonon peak at 610cm$^{-1}$ in the absorbance spectra. (See section 3.1.)

2) The absorbance spectrum of the reference wafer is multiplied by the factor $d_m / d_r$ (with $d_m$ being the thickness of the test wafer and $d_r$ being the thickness of the reference wafer).

3) The normalized absorbance spectrum of the reference wafer is subtracted from the absorbance spectrum of the test wafer.

4) The maximum absorbance value of the oxygen peak at 1107cm$^{-1}$ is determined.

5) This data point plus two data points on the right and two data points on the left (totally 5 data points) are used for a least squares fit to a parabola.

6) The wavenumber of the parabola vertex $v_{max}$ and the corresponding absorption value $A_P$ are determined.

7) On the basis of the spectrum calculated in step 3, a linear baseline is calculated by fitting data points in the regions from 900 to 1000cm$^{-1}$ and from 1200 to 1300cm$^{-1}$ using the least squares method.

8) The absorption value of the baseline $A_B$ at the wavenumber $v_{max}$ is determined.

9) The transmittance values, which correspond to the absorbance values $A_P$ and $A_B$, are calculated:

$$T_P = 10^{-A_P} \qquad T_B = 10^{-A_B}$$

10) The absorption coefficients $\alpha_P$ and $\alpha_B$ for the peak maximum and the baseline point are calculated using the following formula:

$$\alpha = -\frac{1}{d} \ln \frac{(0.09 - e^{1.7d}) + \sqrt{(0.09 - e^{1.7d})^2 + 0.36\, T^2 e^{1.7d}}}{0.18\, T}$$

with $d$ being the thickness of the test wafer.

11) The absorption coefficient for oxygen $\alpha_O$ is calculated:

$$\alpha_O = \alpha_P - \alpha_B$$

12) The oxygen concentration $c_O$ is calculated by multiplying the absorption coefficient $\alpha_O$ by a calibration factor (IOC-88):

$$c_O = 3.14 \bullet 10^{17}\ cm^{-2}\ \alpha_O$$

This calibration factor is also called conversion coefficient. The default value is 3.14 x 10$^{17}$cm$^{-1}$. This value can be changed by the user in the *CARBon-OXygen Analysis* dialog window.

13) The oxygen concentration value $c_O$ is multiplied by the factor FO (default value FO=1), which can be specified by the user in the *CARBon-OXygen Analysis* dialog window.

$$C_O = c_O \bullet FO$$

# 3.8 ASTM F 1391-92 Method - Carbon

1) The thickness of reference wafer and test wafer are determined by either measuring the thickness using a caliper gauge or by calculating the thickness using the silicon phonon peak at 610cm$^{-1}$ in the absorbance spectra. (See section 3.1.)

2) The absorbance spectrum of the reference wafer is multiplied by the factor $d_m / d_r$ (with $d_m$ being the thickness of the test wafer and $d_r$ being the thickness of the reference wafer).

3) The normalized absorbance spectrum of the reference wafer is subtracted from the absorbance spectrum of the test wafer.

4) The maximum absorbance value of the carbon peak at 605cm$^{-1}$ is determined.

5) This data point plus two data points on the right and two data points on the left (totally 5 data points) are used for a least squares fit to a parabola.

6) The wavenumber of the parabola vertex $v_{max}$ and the corresponding absorption value $A_P$ are determined.

7) On the basis of the spectrum calculated in step 3, a linear baseline is calculated by fitting data points in the regions from 550 to 570cm$^{-1}$ and from 630 to 650cm$^{-1}$ using the least squares method.

8) The absorption value of the baseline $A_B$ at the wavenumber $v_{max}$ is determined.

9) The absorption coefficient for carbon $\alpha_C$ is calculated using the following formula:

$$\alpha_C = \frac{23.03}{d}(A_P - A_B)$$

with $d$ being the thickness of the test wafer.

10) The carbon concentration $c_C$ is calculated by multiplying the absorption coefficient $\alpha_C$ by a calibration factor:

$$c_C = 8.2 \bullet 10^{16}\ cm^{-2}\ \alpha_C$$

This calibration factor is also called conversion coefficient. The default value is 8.2 x 10$^{16}$cm$^{-2}$. This value can be changed by the user in the *CARBon-OXygen Analysis* dialog window.

**Note:** The conversion coefficient (0.82 x $10^{17}$cm$^{-2}$) is valid for spectra acquired at room temperature. But this method can also be used for spectra acquired at cryogenic temperatures (below 80 K). In this case, the absorption band peak is at 607.5cm$^{-1}$ and the recommended conversion coefficient is 0.37 x $10^{17}$cm$^{-2}$.

11) The carbon concentration value $c_C$ is multiplied by the factor FC (default value FC=1) which can be specified by the user in the *CARBon-OXygen Analysis* dialog window.

$$C_C = c_C \bullet FC$$

## 3.9 DIN 50438-1 A (93) Method - Oxygen

1) The thickness of reference wafer and test wafer are determined by either measuring the thickness using a caliper gauge or by calculating the thickness using the silicon phonon peak at 610cm$^{-1}$ in the absorbance spectra. (See section 3.1.)

2) The absorbance spectrum of the reference wafer is multiplied by the factor $d_m / d_r$ (with $d_m$ being the thickness of the test wafer and $d_r$ being the thickness of the reference wafer).

3) The absorbance spectra are converted into transmittance spectra (Tr = $10^{-Abs}$).

4) A so-called comparison spectrum is calculated by dividing the test wafer spectrum by the reference wafer spectrum.

5) The minimum transmittance value of the oxygen peak at 1107cm$^{-1}$ is determined.

6) This data point plus two data points on the right and two data points on the left (totally 5 data points) are used for a least squares fit to a parabola.

7) The wavenumber of the parabola vertex $v_{min}$ and the corresponding transmittance value $T_M$ are determined.

8) On the basis of the spectrum calculated in step 4, a linear baseline is calculated by fitting data points in the regions from 1025 to 1040cm$^{-1}$ and from 1180 to 1195cm$^{-1}$ using the least squares method.

9) The transmittance value of the baseline $T_B$ at the wavenumber $v_{min}$ is determined.

10) The absorption coefficient for oxygen $a_O$ is calculated using the following formula:

$$\alpha_O = \frac{-\ln(A + \sqrt{A^2 + B^2})}{d}$$

with:

$$A = \frac{T_B}{2T_M}(1 - B^2)$$

$$B = \frac{1}{R}\exp(\alpha d)$$

$$\alpha = \alpha_A = \alpha_{phon} + \alpha_N$$

$$\alpha_{phon} = 0.85\ cm^{-1}$$

$$p\text{-}Si:\ \alpha_N = 1.43 \bullet 10^{-16}\ cm^2\ N(p)$$

$$n\text{-}Si:\ \alpha_N = 0.32 \bullet 10^{-16}\ cm^2\ N(n)$$

with N(n) and N(p) being the free charge carrier concentrations for p- and n-type silicon.

11) The oxygen concentration $c_O$ is calculated by multiplying the absorption coefficient $\alpha_O$ by a calibration factor:

$$c_O = 3.14 \bullet 10^{17}\ cm^{-2}\ \alpha_O$$

This calibration factor is also called conversion coefficient. The default value is 3.14 x $10^{17}cm^{-2}$. This value can be changed by the user in the *CARBon-OXygen Analysis* dialog window.

12) The concentration value $c_O$ is multiplied by the factor FO, which can be specified by the user in the *CARBon-OXygen Analysis* dialog window:

$$C_O = c_O \bullet FO$$

# 3.10 DIN 50438-1 B (93) Method - Oxygen

1) The thickness of reference wafer and test wafer are determined by either measuring the thickness using a caliper gauge or by calculating the thickness using the silicon phonon peak at $610cm^{-1}$ in the absorbance spectra. (See section 3.1.)

2) The absorbance spectrum of the reference wafer is multiplied by the factor $d_m / d_r$ (with $d_m$ being the thickness of the test wafer and $d_r$ being the thickness of the reference wafer).

3) The absorbance spectra are converted into transmittance spectra ($Tr = 10^{-Abs}$).

After that, the leveled transmittance spectrum of the test wafer is calculated as follows:

4) $\Theta_a$ is the transmittance value at $1107cm^{-1}$ of curve a in figure 6.

5) This spectrum (curve a in figure 6) is leveled linearly in such a way that the transmittances values at the wavenumbers $1200cm^{-1}$ and $1025cm^{-1}$ are identical. (See curve b in figure 6).

6) $\Theta_b$ is the transmittance value at $1107cm^{-1}$ of the linearly leveled spectrum. (See curve b in figure 6).

7) The linearly leveled spectrum (curve b in figure 6) is multiplied by $\Theta_a / \Theta_b$. The result is the leveled spectrum. (See curve c in figure 6).

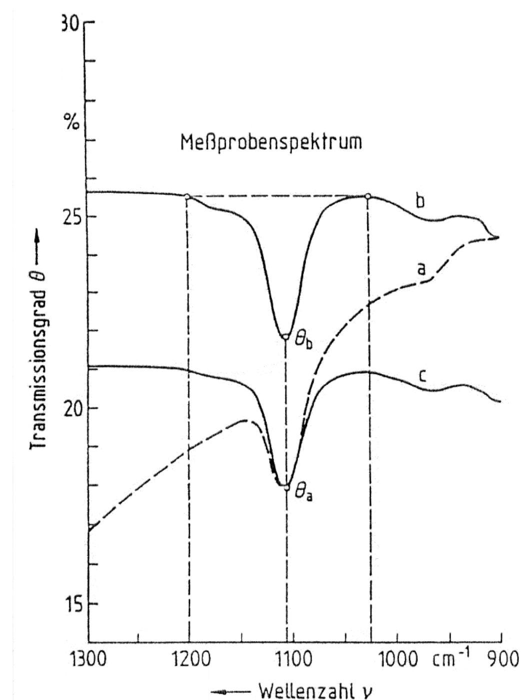


Figure 6: Leveling the Spectrum of a single-side polished Test Wafer

(Source: DIN 50438-1: Prüfung von Materialien für die Halbleitertechnologie - Bestimmung des Verunreinigungsgehaltes in Silicium mittels Infrarot-Absorption - Teil 1, Berlin: Beuth Verlag GmbH (1995-07).

8) $\Theta_t$ is the transmittance value at 1188cm$^{-1}$ of the leveled spectrum. (See curve c in figure 6).

After that, the adjusted transmittance spectrum of the reference wafer is calculated as follows:

9) The transmittance value $\Theta_r$ at 1188cm$^{-1}$ in the reference spectrum is determined. This value has been corrected for thickness (step 2 and 3).

10) This spectrum is multiplied by the factor $\Theta_t / \Theta_r$. The result is an adjusted transmittance spectrum.

11) $\Theta_R$ is the transmittance value at 1107cm$^{-1}$. This value is required for the calculation of absorption coefficient $\alpha_B$. (See step 13.)

12) The leveled test wafer spectrum (curve c in figure 6) is divided by the adjusted reference wafer spectrum to obtain the comparison spectrum $T$.

13) The absorption coefficient $\alpha_B$ is calculated using the following formula:

$$\alpha_B = \frac{-\ln\left( D + \sqrt{D^2 + 11.111}\right)}{d}$$

with $d$ being the thickness of the test wafer. The parameter $D$ is calculated as follows:

$$D = \frac{-2.722}{\Theta_R}$$

Using the comparison spectrum $T$, the values $T_M$ and $T_B$ are calculated as follows:

14) The minimum transmittance value of the oxygen peak at 1107cm$^{-1}$ is determined.

15) This data point plus two data points on the right and two data points on the left (totally 5 data points) are used for a least squares fit to a parabola.

16) The wavenumber of the parabola vertex $\nu_{min}$ and the corresponding intensity value $T_M$ are determined.

17) A linear baseline is calculated by fitting data points in the regions from 1025 to 1040cm$^{-1}$ and from 1180 to 1195cm$^{-1}$ using the least squares method.

18) The transmittance value of the baseline $T_B$ at the wavenumber $\nu_{min}$ is determined.

19) The absorption coefficient for oxygen $\alpha_O$ is calculated using the following formula:

$$\alpha_O = \frac{-\ln(A + \sqrt{A^2 + B^2})}{d}$$

with:

$$A = \frac{T_B}{2T_M}(1 - B^2)$$

$$B = \frac{1}{R}\exp(\alpha_B d)$$

with $\alpha_B$ being the absorption coefficient which has been calculated in step 13 and *d* being the thickness of the test wafer.

20) The oxygen concentration is calculated by multiplying the absorption coefficient $c_O$ by the calibration factor:

$$c_O = 3.14 \bullet 10^{17}\, cm^{-2}\, \alpha_O$$

This calibration factor is also called conversion coefficient. The default value is $3.14 \times 10^{17} cm^{-2}$. This value can be changed by the user in the *CARBon-OXygen Analysis* dialog window.

21) The oxygen concentration value is multiplied by the factor FO which can be specified by the user in the *CARBon-OXygen Analysis* dialog window:

$$C_O = c_O \bullet FO$$

# 3.11 DIN 50438-2 (82) Method - Carbon

1) The thickness of reference wafer and test wafer are determined by either measuring the thickness using a caliper gauge or by calculating the thickness using the silicon phonon peak at 610cm$^{-1}$ in the absorbance spectra. (See section 3.1.)

2) The absorbance spectrum of the reference wafer is multiplied by the factor $d_m / d_r$ (with $d_m$ being the thickness of the test wafer and $d_r$ being the thickness of the reference wafer).

3) The absorbance spectra are converted into transmittance spectra ($Tr = 10^{-Abs}$).

4) A so-called comparison spectrum is calculated by dividing the test wafer spectrum by the reference wafer spectrum.

5) The minimum transmittance value of the carbon peak at 605cm$^{-1}$ is determined (provided that the spectrum has been acquired at room temperature).

**Note:** In case the spectrum has been acquired at cryogenic temperatures, the minimum transmittance value of the carbon peak at 607.5cm$^{-1}$ is determined.

6) This data point plus two data points on the right and two data points on the left (totally 5 data points) are used for a least squares fit to a parabola.

7) The wavenumber of the parabola vertex $v_{min}$ and the corresponding transmittance value $T_M$ are determined.

8) The baseline is constructed as a tangent to the comparison spectrum in such a way that the spectrum contacts it at least at one point on each side of the absorption band, but it is not cut at any point.

9) The transmittance value of the baseline $T_B$ at the wavenumber $v_{min}$ is determined.

10) The absorption coefficient for carbon $\alpha_C$ is calculated using the following formula:

$$\alpha_c = \frac{\ln(T_B / T_M)}{d}$$

11) The carbon concentration $c_c$ is calculated by multiplying the absorption coefficient $\alpha_C$ by a calibration factor:

$$c_c = 1.0 \bullet 10^{17}\ cm^{-2}\ \alpha_c$$

This calibration factor is also called conversion coefficient. The default value is 1.0 x $10^{17}cm^{-2}$. This value can be changed by the user in the *CARBon-OXygen Analysis* dialog window.

**Note:** The conversion coefficient (1.0 x $10^{17}cm^{-2}$) is valid for spectra acquired at room temperature. But this method can also be used for spectra acquired at cryogenic temperatures (below 80 K). In this case, the absorption band peak is at $607.5cm^{-1}$ and the recommended conversion coefficient is 0.45 x $10^{17}cm^{-2}$.

12) The concentration value $c_c$ is multiplied by the factor FC, which can be specified by the user in the *CARBon-OXygen Analysis* dialog window:

$$C_c = c_c \bullet FC$$

# Appendix

## ASTM and DIN Standards

As already mentioned in chapter 1, the OPUS/SEMI software supports the following ASTM and DIN standards:

- ASTM F 1188-93a Oxygen
- ASTM F 1391-92 Carbon
- DIN 50438-1 A (93) Oxygen
- DIN 50438-1 B (93) Carbon
- DIN 50438-2 (82) Carbon

It is highly recommended to purchase these standards. You can order them, for example, at the Beuth Verlag GmbH (www.beuth.de) or at ASTM International (www.astm.org). This appendix quotes the scope or range of application and purpose of the following standards:

- ASTM F 1188-93a
- ASTM F 1391-92
- DIN 50438-1
- DIN 50438-2 (82)

## ASTM F 1188-93a[1]

**Standard Test Method for Interstitial Atomic Oxygen Content of Silicon by Infrared Absorption**

### 1. Scope

1.1 This test method covers the determination of the interstitial oxygen content of single crystal silicon by infrared spectroscopy. This test method requires the use of an oxygen-free reference specimen. (...)

1.2 The useful range of oxygen concentration measurable by this test method is from 1 x $10^{16}$ atoms/$cm^3$ to the maximum amount of interstitial oxygen soluble in silicon.

1.3 The oxygen concentration obtained using this test method assumes a linear relationship between the interstitial oxygen concentration and the absorption coefficient of the 1107$cm^{-1}$ band associated with interstitial oxygen in silicon.

1.4 (...)

1. ASTM F 1188-93a (Published 1993): Standard Test Method for Interstitial Atomic Oxygen Content of Silicon by Infrared Absorption. ASTM International, West Conshohocken, Pennsylvania, U.S.

# ASTM F 1391-92[1]

**Standard Test Method for Substitutional Atomic Carbon Content of Silicon by Infrared Absorption**

## 1. Scope

1.1 This referee test method covers the determination of substitutional carbon concentration in single crystal silicon. Because carbon may also reside in interstitial lattice positions, when in concentrations near the solid solubility limit, the result of this test method may not be a measure of the total carbon concentration.

1.2 The useful range of carbon concentration measurable by this test method is from the maximum amount of substitutional carbon soluble in silicon down to about 0.1 parts per million atomic (ppma), that is, $5 \times 10^{15} cm^{-3}$ for measurements at room temperature, and down to about 0.01 ppma, that is, $0.5 \times 10^{15} cm^{-3}$ at cryogenic temperatures (below 80 K).

1.3 This test method utilizes the relationship between carbon concentration and the absorption coefficient of the infrared absorption band associated with substitutional carbon in silicon. At room temperatures (about 300 K), the absorption band peak is at $605 cm^{-1}$ or 16.53µm. At cryogenic temperatures (below 80 K), the absorption band peak is at $607.5 cm^{-1}$ or 16.46µm.

1.4 This test method is applicable to slices of silicon with a resistivity higher than 3Ω-cm for p-type and higher than 1Ω-cm for n-type. Slices an be any crystallographic orientation and should be polished on both surfaces.

1.5 This method is intended to be used infrared spectrophotometers that operate in the region from 2000 to $500 cm^{-1}$ (5 - 20µm).

1.6 This test method provides procedure and calculation sections for the cases where the thickness values of test and reference specimens are both closely matched and not closely matched.

1.7 (...)

1.ASTM F 1391-92 (Published 1992): Standard Test Method for Substitutional Atomic Carbon Content of Silicon by Infrared Absorption. ASTM International, West Conshohocken, Pennsylvania, U.S.

# DIN 50438, Part 1[1]

**Testing of Materials for Semiconductor Technology: Determination of Impurity Content in Semiconductors by Infrared Absorption - Part 1: Oxygen**

## 1. Range of Application and Purpose

The Methods A and B of this standard serve to determine with high precision the oxygen content of silicon by non-destructive optical infrared means. Only the interstitial oxygen content of the silicon is detected by these methods. The total oxygen content may be greater than the interstitial oxygen content. (...)

The range of application of the methods is limited to plane-parallel mono- or polycrystalline silicon wafers with thicknesses d > 0.03 cm and charged carrier concentrations $N \leq 2x10^{16}$ $cm^{-3}$, and is independent of crystal orientation. The methods are applicable to both of the currently used types of specimens having different surface treatments and thicknesses:

- Double-side polished or polish-etched wafers with a thickness $d \geq 0, 006$ cm (Method A)
- One-side-polished wafers with etched back surfaces and thicknesses $d \geq 0, 003$ cm (Method B)

Specimens having only sawed or only lapped surfaces do not fulfill the requirements of this standard.

The measurement range for oxygen concentration lies between $c_o = 2.5 \times 10^{15} cm^{-3}$ and the solubility of oxygen of about $2.5 \times 10^{18} cm^{-3}$ at the melting point of silicon. (...)

1.DIN 50438, Part 1 (1993): Testing of Materials for Semiconductor Technology Determination of Impurity Content in Semiconductors by Infrared Absorption Oxygen in Silicon. Berlin: Beuth Verlag GmbH.

# DIN 50438, Part 2[1]

**Testing Materials for Semiconductor Technology: Determination of Impurity Content in Silicon Using Infrared Absorption - Part 2: Carbon**

## 1. Range of Application and Purpose

The process, according to this standard, is used to determine the carbon content of silicon. The absorption coefficient of substitutional carbon at a wave number of 605 $cm^{-1}$ (16.5µm - absorption band) is used to measure carbon content.

Therefore, this procedure does not apply to carbon that may be present in another form in the silicon lattice or chemically linked or is precipitated at gain boundaries or other places. With this limitation, the application range of the procedure covers plane-parallel, two-sided polished test pieces of single-crystal or polycrystalline silicon with charge carrier concentrations under $5 \times 10^{16} cm^{-3}$, regardless of conductivity type and crystal orientation. The measurement range for the carbon concentration lies between $5 \times 10^{15} cm^{-3}$ and about $3 \times 10^{18} cm^{-3}$.

Due to the strong silicon lattice absorption (absorption coefficient $K_G \approx 8 cm^{-1}$ for wave number 605 $cm^{-1}$ (2)), that is superimposed on the (605$cm^{-1}$) band generated by the carbon, the carbon content can only be determined using a differential process.

1.DIN 50438, Part 2 (1982): Testing of Materials for Semiconductor Technology: Determination of Impurity Content in Silicon Using Infrared Absorption - Carbon. Berlin: Beuth Verlag GmbH.

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