

## Application News

# No.A445

### Spectrophotometric Analysis

## Determination of Interstitial Atomic Oxygen and Substitutional Atomic Carbon in Silicon Wafers and Hydrogen in Silicon Nitride Films on Silicon Wafers by FTIR

Worldwide silicon wafer production is steadily increasing due to increasing demand not only for semiconductors that has continued for decades, but for solar cells as well, where demand has been expanding since 2000. In both applications, however, control of the various types of impurities that can occur is required for ensuring the quality of silicon wafers. Quantitative analysis of interstitial oxygen and substitutional carbon in silicon wafers is known to be relatively easy using infrared spectroscopy. Furthermore, infrared spectroscopy can also be used for the determination of hydrogen in silicon nitride films that are deposited on the surface of silicon wafers as anti-reflective and insulating coatings. Here, we introduce examples of this type of measurement on such samples using the IRsolution Macro Program.

### ■ Determination of Interstitial Atomic Oxygen and Substitutional Atomic Carbon in Silicon Wafers

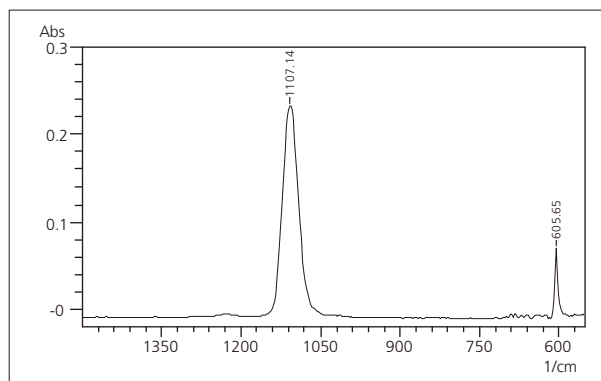
Infrared spectroscopy has been established as a method for determining the concentrations of interstitial atomic oxygen and substitutional carbon in monocrystalline Si wafers. These are commonly determined using the ASTM<sup>1), 2)</sup> methods, on which the Chinese National Standards<sup>3)</sup> are based. In Japan, the standard method for measurement of substitutional atomic carbon using infrared absorption is specified in JEITA EM-3503<sup>4)</sup>. With these quantitation methods, the absorption coefficients are obtained from the characteristic peaks of oxygen (1107 cm<sup>-1</sup>) and carbon (607 cm<sup>-1</sup>) shown in Fig. 1 using Expression (1) below, and calculation is conducted by multiplying the predetermined coefficient by these values.

$$\text{Absorption coefficient } \alpha = (1/d) \ln (T_0 / T) \dots\dots\dots (1)$$

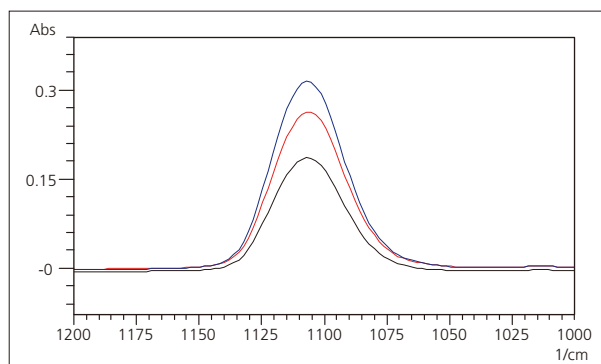
T<sub>0</sub>: Baseline transmission at peak position

T: Transmission at peak position d: Sample thickness (cm)

This measurement requires the use of a standard wafer that contains no carbon or oxygen in order to offset the absorption of silicon itself that exists at the position overlapped by each of those absorptions. Fig. 2 shows the transmission spectra obtained from measurement of 3 types of silicon wafers (2 mm thick) with different concentrations of interstitial atomic oxygen. Quantitation values as those shown in Fig. 3 can be obtained in addition to the infrared spectra by using the special Macro Program.



**Fig. 1 Infrared Spectrum of Interstitial Atomic Oxygen and Substitutional Atomic Carbon in a Silicon Wafer**



**Fig. 2 Infrared Spectra of Silicon Wafers with Differing Concentrations of Interstitial Oxygen**

<Result of Oxygen Content>	
Date&Time: 2011/12/08 13:37:35	
Sample No.: H-6 20111208-2	
Reference No.: R-6	
Peak Wavenumber: 1105.2 cm <sup>-1</sup>	
Baseline Wavenumber: 1160.0 - 1040.0 cm <sup>-1</sup>	
Sample Thickness: 2mm	
Reference Thickness: 2mm	
Constant1: 3.14*E17	
Constant2: 6.28	
Instrument: IRAffinity-1	
Temperature: 24	
Half Width: 33.4cm <sup>-1</sup>	
Absorption Factor: 3.532	
Atoms/cm3: 1.109E+18	} Quantitation Values
ppma: 22.181	

**Fig. 3 Results Calculated by Macro Program**

## ■ Quantitation of Hydrogen in Silicon Nitride Films on Silicon Wafers

SiN film used as anti-reflective coating on crystalline silicon solar cells is known to undergo passivation due to hydrogen exposure during its formation. Hydrogen passivation refers to the inactivation of dangling bond defects in silicon by forming Si-H bonds. Also, quantitation of Si-H and N-H bonds in SiN film using infrared spectroscopy has been proposed by Lanford et al<sup>5)</sup>.

Fig. 4 shows a transmission spectrum of SiN film, in which the Si-H peak is seen in the vicinity of 2180 cm<sup>-1</sup>, and the N-H peak near 3300 cm<sup>-1</sup>. Fig. 5 shows an example of the measurement screen displayed using the Macro Program, and Fig. 6 shows an example of the output quantitative results.

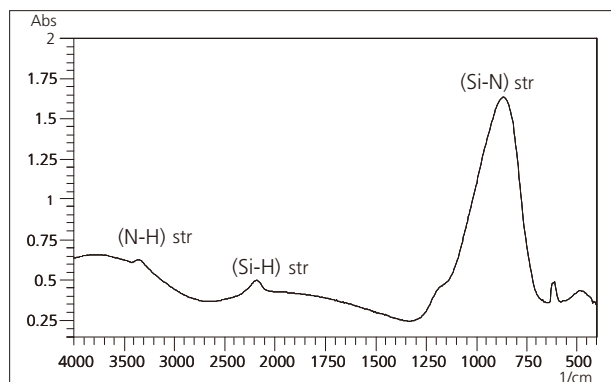


Fig. 4 Transmission Spectrum of SiN Film

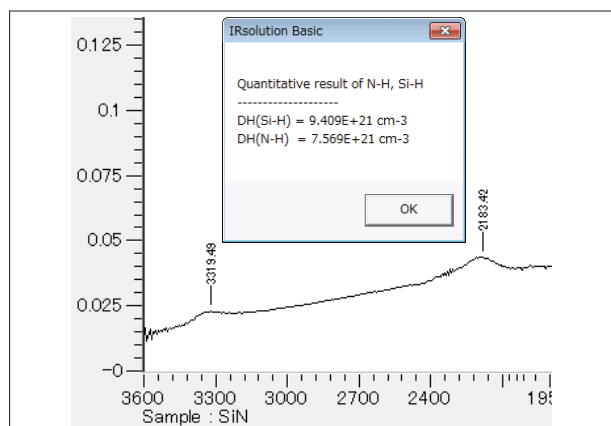


Fig. 5 Image of Macro Program Used for Quantitative Result

<Result of Oxygen Content>	
Date&Time: 2012/04/27 15:09:26	
Sample No.: No. 300 test	
Reference No.: CZ	
Si-H Peak Wavenumber: 2183.4 cm <sup>-1</sup>	
Si-H Baseline Wavenumber: 2400.0 - 2000.0 cm <sup>-1</sup>	
N-H Peak Wavenumber: 3319.5 cm <sup>-1</sup>	
N-H Baseline Wavenumber: 3500.0 - 3150.0 cm <sup>-1</sup>	
Sample Thickness: 0.16μm	
Constant1: 1.36*1E17	
Constant2: 1.90*1E17	
Instrument: IRAffinity-1	
Temperature: 24	
DH(Si-H): 9.409E+21 cm <sup>-3</sup>	} Quantitation Values
DH(N-H): 7.569E+21 cm <sup>-3</sup>	

Fig. 6 Results Calculated by Macro Program

## ■ Quantitation of Hydrogen in Silicon Nitride Films Formed at Different Temperatures

Here, the quantitation results are shown for a sample in which SiN anti-reflective film (80 nm thick) was formed on both sides of monocrystalline Si wafers. The films were formed on the 200 μm thick monocrystalline Si wafers at 3 different temperatures (350 °C, 400 °C, 450 °C), and transmission measurement was conducted using the conditions shown in Table 1. The obtained infrared spectra are shown overlaid in Fig. 7. Differences in the Si-H peak intensities due to the different forming temperatures are clearly observed. Table 2 shows the quantitative values of hydrogen determined from these peaks. The results showed that, whereas the quantity of hydrogen associated with N-H is nearly constant regardless of the film forming temperature used, the quantity of Si-H hydrogen is at its maximum at 350 °C.

Table 1 Analytical Conditions

Instrument	: IRAffinity-1
Resolution	: 4 [1/cm]
Accumulation	: 40
Apodization	: Happ-Genzel
Detector	: DLATGS

Table 2 Hydrogen Bond Density in Each Sample

Sample	N-H (cm <sup>-3</sup> )	Si-H (cm <sup>-3</sup> )
Processing temperature 350 °C	5.03E+22	8.76E+22
Processing temperature 400 °C	4.78E+22	7.33E+22
Processing temperature 450 °C	5.09E+22	5.90E+22

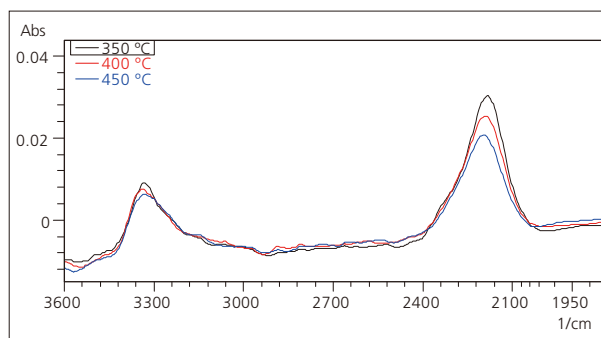


Fig. 7 Infrared Spectra of Silicon Nitride Films Formed at Different Temperatures

### [References]

- 1) ASTM F1188-02 Standard Test Method for Interstitial Atomic Oxygen Content of Silicon by Infrared Absorption with Short Baseline (Withdrawn 2003)
- 2) ASTM F1391-93 (2000) Standard Test Method for Substitutional Atomic Carbon Content of Silicon by Infrared Absorption (Withdrawn 2003)
- 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
- 5) W. A. Lanford, etc: J.Appl.Phys. 49, 2473 (1978)

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