Application Note

220-AT-0222

Evaluation of Si Wafer Surface Condition Using 65-degree incident ATR PRO650G

1. Introduction

Measuring/analyzing the semiconductor surface of an Si substrate or the like is mandatory for knowing the condition or the contamination condition of thermally oxidized film that functions as insulating film. For the surface analysis, such measures as XPS (X-ray photoelectron spectroscopy, ESCA) and SIMS (secondary ion mass spectrometry) are popularly employed, and such measures give elemental information on the sample surfaces. On the other hand, infrared spectroscopy (IR) easily obtains information on the molecular bonding condition, which cannot be analyzed by XPS or SIMS in a nondestructive manner. For the surface analysis in IR, the ATR method is popularly employed. For the 45-degree incident ATR, which is used in general, measurement of samples of Si wafers or the like with a high refractive index was difficult, since it does not satisfy the total reflection conditions required for ATR measurement. With the single reflection 65-degree incident ATR we developed recently (Fig. 1), Ge with a high refractive index (n = 4.0) is used for the prism, and the incident angle of light to the sample is set at 65 degrees, thereby obtaining information on the topmost surface and measuring samples with a high refractive index, such as Si (refractive index=approx. 3.4) and rubber containing carbon whose refractive index is 2.8 or higher. (See Table 1: JASCO FT/IR application data 280-AT-0003)

Fig. 1: Single Reflection 65-degree Incident ATR (ATR PRO650G)

Table 1: Comparison of 65-degree Incident ATR and 45-degree Incident (Existing Type) ATR

Incident Angle	Prism	Lower Measurement Limit at Low Wavenumber Side	n_1	n_2	Penetration Depth (For 1000 cm^{-1}, n_2=1.5)
65º	Ge	- 700 cm^{-1}	4.0	3.6	0.48 µm
45º	Ge	- 700 cm^{-1}	4.0	2.8	0.66 µm

n_1 : Refractive index of prism
n_2 : Upper limit of measurable refractive index of sample (Upper limit that satisfies the total reflection conditions)

2. Features of Single Reflection 65-degree Incident ATR (ATR PRO650G)

The ATR PRO650G (Fig. 1) features a slip clutch to prevent damage to the sample or prism as standard equipment for a design that does not allow application of pressures exceeding a certain level during the process of bonding the sample and the prism. Furthermore, a wide space is secured around the top panel, thereby enabling measurement of the center part of the sample even for a six-inch Si wafer. In addition, since a polarizer and an analyzer can be introduced to the light path as an option, analysis of the molecular orientation condition of the sample surface can also be executed.

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3. Measurement Conditions

System: FT/IR-4100 Measurement Method: ATR method (Reflection: Single)
Resolution: 4 cm^{-1} Detector: DLATGS
Aperture: 3.5 mm Integration: 128 times
Accessory: ATR PRO650G (Prism: Ge)

4. Results and Discussion

As a sample, measurement was made of the Si wafer surface on which a natural oxide film was generated. For comparison purposes, the measurement was made using a 45-degree incident ATR and the transmission method. Fig. 2 shows the spectra obtained by overwriting the measurement results of the 45-degree incident ATR on it, and Fig. 3 shows the spectra obtained by standardizing and overwriting the measurement results of the transmission method. From Fig. 2, it can be seen that the spectrum of the 45-degree incident ATR does not satisfy the total reflection condition required for the ATR measurement, and the spectrum presents significant distortion making it difficult to evaluate the surface condition. On the other hand, with the 65-degree incident ATR, since the spectrum satisfies the total reflection condition, the spectrum does not present any distortion and the base line remains flat. From Fig. 3, the absorption peak in the vicinity of 1235 cm^{-1}, which can be attributed to the natural oxide film, is noted, and a slight amount of organic substances adhere to the surface starting from the peak at 3000 to 2800 cm^{-1}, which can be attributed to C-H adsorption. On the other hand, the results measured by the transmission method reveal adsorption in the vicinity of 1100 cm^{-1}, which can be attributed to the Si-O in the Si wafer substrate, but the adsorption peak at around 1235 cm^{-1}, or the peak that can be attributed to C-H adsorption, cannot be determined. More specifically, this reveals that using the 65-degree incident ATR enabled acquisition of information on the top surface of samples that could not be determined by the transmission method.

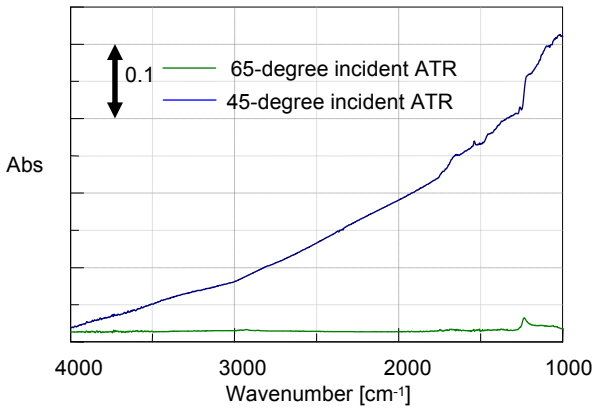

Fig. 2: Oxide Film Spectrum on Si Wafer
(Offset Indication)

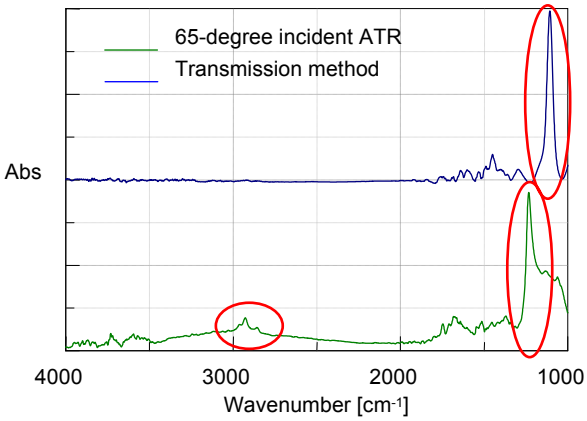

Fig. 3: Oxide Film Spectra on Si Wafer
(Standardized; Offset Indication)

As stated above, using the single refraction 65-degree incident ATR enables evaluation of the surface condition of substrates such as Si wafers with a high refractive index in a nondestructive manner. As further development, applications for the qualitative/quantitative evaluation of the adhesion condition of organic substances on the Si wafer surface and the quantitative evaluation of oxide films by evaluating the peak height and area at around 1235 cm^{-1}, estimation of SiO and SiO_2 percentages in the oxide film utilizing the fact that the adsorption peak position is different between SiO (around 1100 cm^{-1}) and SiO_2 (around 1235 cm^{-1}) can be expected.

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