# Application Note

220-AT-0222

## Evaluation of a Si Wafer Surface Using a 65-degree Incident Angle ATR

### 1. Introduction

Measuring the surface of a Si semiconductor substrate or other materials is required knowledge of the surface or contamination condition of thermally oxidized films that function as an insulating film for the semiconductor. For the surface analysis, such techniques as XPS (X-ray photoelectron spectroscopy, ESCA) and SIMS (secondary ion mass spectrometry) are popularly employed, and such methods provide 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 non-destructive manner. For the surface analysis using mid-IR, the ATR method is popularly employed. For the 45-degree incident ATR, the most common configuration, measurement of samples of Si wafers with a high refractive index is difficult, since this configuration does not satisfy the total reflection conditions required for ATR measurements. With the single-reflection 65-degree incident ATR recently developed (Figure 1), a Ge crystal 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 providing measurements of samples with a high refractive index, such as Si (refractive index=approx. 3.4) and carbon black filled rubbers whose refractive index can be 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 and 45-degree (Standard) ATR Accessories

| 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)

We recently executed measurements of a natural oxide film on Si wafer surfaces using a single reflection 65-degree incident ATR as an application example of the new ATR accessory.

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

The ATR PRO650G (Figure 1) features a slip clutch pressure clamp to prevent damage to the sample or prism during application of pressure to ensure proper contact of the sample with the ATR crystal. Furthermore, a large sampling surface is available on the top panel, enabling measurements of the center portion of a sample, even as large as a six-inch Si wafer. In addition, since an optional polarizer and analyzer can be added to the light path, analysis of the molecular orientation of the sample surface can also be obtained.

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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 Accumulations: 128 times
Accessory: ATR PRO650G (Prism: Ge)

### 4. Results and Discussion

Measurement was performed of a Si wafer surface on which a natural oxide film was present. For comparison purposes, the measurement was made using a 45-degree incident ATR and the transmission method. Figure 2 displays the overlaid spectra obtained of the measurement results using the 45-degree and 65-degree incident ATR accessories, and Figure 3 shows the spectra obtained by normalizing the measurement results of the transmission method and comparing to the spectrum of the 65-degree ATR. From Figure 2, it can be seen that the spectrum of the 45-degree incident ATR does not satisfy the total refraction 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 refraction condition, the spectrum does not present any distortion and the base line remains flat. From Figure 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 contamination of the surface is present based on the peaks from 3000 to 2800 $cm^{-1}$, which can be attributed to C-H adsorptions. Also, the results obtained by the transmission method reveal absorptions in the vicinity of 1100 $cm^{-1}$, which can be attributed to the Si-O in the Si wafer substrate, but the absorption peak at around 1235 $cm^{-1}$ cannot be positively determined. These results demonstrate that using the 65-degree incident ATR enabled acquisition of information on the very surface of samples that could not be determined by using the transmission method.

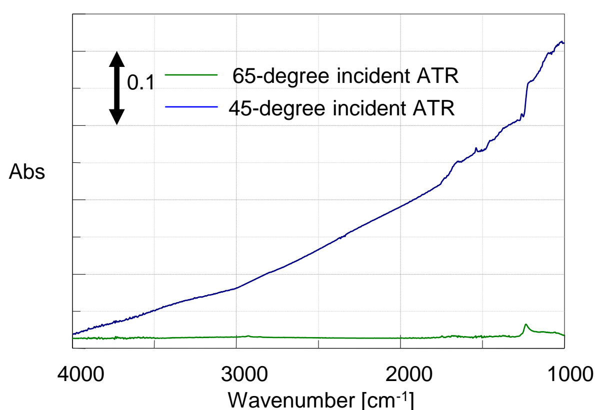


Fig. 2: Oxide Film Spectrum on Si Wafer
(Offset Indication)

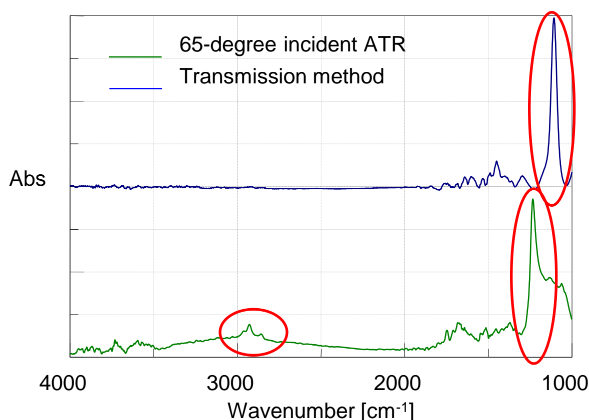


Fig. 3: Oxide Film Spectra on Si Wafer
(Standardized; Offset Indication)

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. In the future, applications for the qualitative and quantitative evaluation of the adhesion condition of organic substances on the Si wafer surface will be evaluated. The quantitative evaluation of oxide films based on the peak height and area at around 1235 $cm^{-1}$ and the estimation of SiO and $SiO_2$ percentages in the oxide film will be examined.

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