FEATURE ARTICLE

Full Automatic Spectroscopic Ellipsometer UT-300

Part 3 : Examples of the Multilayer Analysis

Seiichi Hirakawa*, Nataliya Nabatova-Gabain*,
Yoko Wasai*, Hiroshi Iida*

*HORIBA JOBIN YVON Co., Ltd.

Abstract

The UT-300 spectroscopic ellipsometer is a fully-automated measurement system developed specifically for use on semiconductor production lines. The spectroscopic ellipsometer serves as the main component of the system for recipe verification. Although the UT-300 is intended for analysis of the most advanced types of films using state-of-the-art techniques, the authors focus on the basics in this article, describing the spectrum analysis steps required to perform multilayer analysis and providing guidelines on the effective use of the instrument.

1 Principles of Spectroscopic Ellipsometer

A spectroscopic ellipsometer (SE) measures the change in polarization between incident light and reflected light, and calculates the film thickness (d) and complex refractive index (n, k) from the measured change.[1,2] The change in polarization, defined as amplitude Ψ and phase shift Δ , depends on parameters such as wavelength (λ), incidence angle (ϕ), film thickness, and complex refractive index. The relationship between these parameters is expressed by

$$(d, n, k) = f\ (\Psi, \Delta, \lambda, \phi)$$

However, if the incidence angle is fixed and a single-wavelength ellipsometer is used for measurement, this relationship can be expressed as

$$(d, n, k) = f(\Psi, \Delta)$$

Although there are three unknown quantities in the above equation, only two independent variables can be measured with a single-wavelength ellipsometer. Therefore, one of the three unknown quantities (d, n, k) must be fixed as a known quantity.

More variables can be measured using a single wavelength if the incidence angle is varied. However, since there is clear correlation between ($\Psi_{\phi 1}$, $\Delta_{\phi 1}$) and ($\Psi_{\phi 2}$, $\Delta_{\phi 2}$), corresponding to different incidence angles, it is difficult to determine d, n, and k precisely.

By contrast, with a multi-wavelength spectroscopic ellipsometer, the parameters are expressed as follows:

$$(d, n\ (\lambda), k\ (\lambda)) = f\ (\Psi, (\lambda), \Delta, (\lambda))$$

Three unknown quantities can be determined at the same time because the film thickness is constant, independent of the wavelength.

In addition, as the number of layers of multilayer films increases, the number of unknown quantities also increases; (d_1, n_1, k_1), (d_2, n_2, k_2), ... Therefore, only a multi-wavelength spectroscopic ellipsometer is capable of measuring d, n, and k of a multilayer film.

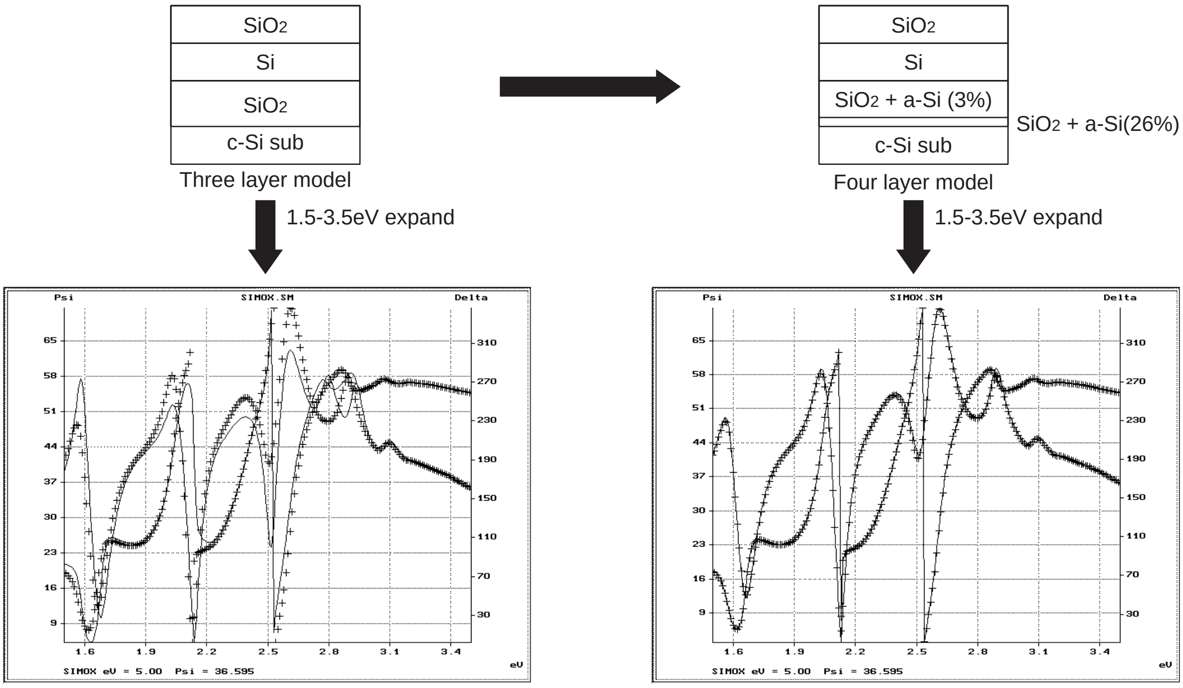
2 Examples of Multilayer Film Analysis

An example of analysis of a substrate formed using separation by implanted oxygen (SIMOX) is shown in Fig.1.

The measurement results are displayed in terms of Ψ and Δ (+++) for each wavelength, and the simulation spectra are displayed by solid lines. In general, the wavelength of spectra are represented by energy (eV: electron volt) to make it easier to determine the change in polarization. (1 eV = 1.2398μm from $E = hn$.)

The measured Ψ and Δ take the substrate and all layers into account, and are expressed as follows, where they are specifically indicated by Ψ_E and Δ_E.

$$(\Psi_E, \Delta_E) = f\ (d_1, d_2, ...d_n, n_0, n_1, ...n_n, k_0, k_1, ...k_n)$$



Model	Film thickness(Å)				X2*
	Inter layer	SiO2	Si	SiO2	
Three layer model		3909.4	2258.2	1121.6	96.33
Four layer model	483.6	3274.1	2266.7	1123.2	4.88

Fig.1 Example of Multilayer Film Analysis (SIMOX)

Consequently, the specific analysis procedure is comprised of the following steps: (1) Assume the initial values for each layer such as (n_0, k_0) for the substrate and (d_1, n_1, k_1) for the first layer, and calculate the totals (Ψ_M, Δ_M) for modeling simulation, and (2) fit the measured spectra (Ψ_E, Δ_E) and simulated spectra (Ψ_M, Δ_M) when the values of the two data sets are sufficiently close. For actual production lines, some fitted recipes should be prepared.

In the SIMOX analysis example, the measured data agree practically with the data obtained from the four-layer model, in which an interface layer is placed on the Si substrate. The error between the measured data and the data obtained from the model is represented by χ^2, that is, the least square error. As in the table in Fig.1, χ^2 of the four-layer model is obviously smaller than that of the three-layer model.

Generally, short wavelength (high energy) light is affected by surface roughness, whereas long wavelength (low energy) light passes the rough surface easily, thus providing more information about the interface. In this example, the Si layer is placed as the second layer from the top, preventing ultra-violet rays of 3 eV or greater (400 nm or shorter) from passing through the layer. Therefore, the interface conditions are not reflected in the spectra, and no changes are seen in the three an four layer models above 3 eV.

As described above, the spectroscopic ellipsometer is based generally on mathematical processes. Therefore, some results may be difficult to understand, and thus a physical approach is indispensable for proper analysis.

3 Optical Constants

The optical constants of bulk SiO_2 (oxide film) and Si_3N_4 (nitride film) are well known, and numerical data for the refractive index of each wavelength can be found in various texts.3) By contrast, there is almost no numerical data for ferroelectric substances, novel materials such as low-k film, polycrystalline silicon (p-Si), SiOx, or SiON.

For the above materials, one of two analytical methods are applied; (1) effective medium approximation (EMA), in which two materials of known refractive index are combined, and (2) dispersion, in which the refractive index is dealt with as a function of wavelength.

3.1 Effective Medium Approximation (EMA)

A typical example is polycrystalline silicon (p-Si). The refractive index of p-Si can be determined by mixing crystalline silicon (c-Si) and amorphous silicon (a-Si). The index of crystallization can also be derived from the ratio of the mixed crystal.

Another typical example is mixing the surface layer and air and then analyzing the roughness.

SiGe, which is a material used in cellular phones, is given below (Fig.2) as a specific application. As shown in the figure, several SiGe spectra having different Ge concentrations are seen between the crystalline silicon (c-Si) spectrum and the crystalline germanium (c-Ge) spectrum. Note that the dielectric constant spectra of the imaginary part are also displayed here (dielectric constant is square of refractive index). Several SiGe materials with differing refractive indexes, dependent on the Ge concentration, are publicly available, allowing the Ge concentration to be found by mixing such SiGe. Currently, even SiGe with low Ge concentration can be analyzed using advanced analysis technology.

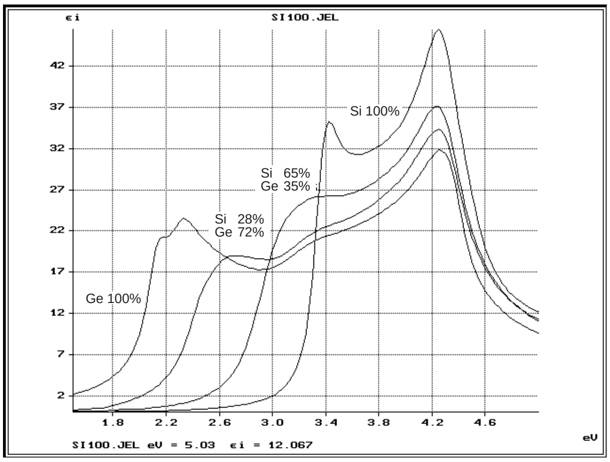


Fig.2 Dielectric Constant Spectra of a Thin SiGe Film (imaginary part)

3.2 Dispersion

(1) Equation of nth Degree

In the range where refractive index changes simply with wavelength, an equation of the *n*th degree of wavelength can be used. A typical equation is the Cauchy's dispersion formula. However, currently it is rarely used because fitting is divergent, complicated refractive indexes with peaks cannot be expressed, and physical analysis is impossible.

(2) Oscillator Model (Classical Mechanics)

The dielectric constant can also be expressed using an oscillator model. This method is intuitive and easy to understand. For example, if the formula does not have an imaginary part, the material is transparent, and if the formula has a free electron term, the material is conductive.

Although this method features convergent fitting, this feature requires only a small number of initial parameters to be selected carefully beforehand. For a novel material, the initial parameters of a similar material should be selected because the tendency of wavelength dispersion in terms of the dielectric constant is first classified into general categories such as insulators (oxide film etc.), metals, and semiconductors, and is then classified into specific categories such as transference electrodes (ITO etc.).

(3) Oscillator Model (Quantum Mechanics)

The dispersion formula can be applied to a wide range of materials using an oscillator model based on quantum mechanics with the appropriate superposition of oscillators. Although this model has the advantage of using a formula with intrinsic optical bandgaps, it also has a drawback in its divergent fitting. The initial parameters should be selected in the same way as in the case of classical mechanics.

(4) Miscellaneous

In addition to the above approaches, appropriate dispersion formulas can be prepared for each material. A compound semiconductor is a typical example.

Here, polysilicon (formed at a low temperature), as used for high-resolution liquid crystal displays, is described as an example (Fig.3, 4, and Table 1).[4)]The dispersion formula for the dielectric constant includes parameters E_1 (eV) and Γ_1 (eV) (omitted for brevity). As Γ_1, the spectrum width of the peak at E_1 energy, becomes narrower, the electron mobility becomes higher. As shown in the figure, high electron mobility means large grain size. If the grain size is infinitely large, it is crystalline silicon (c-Si).

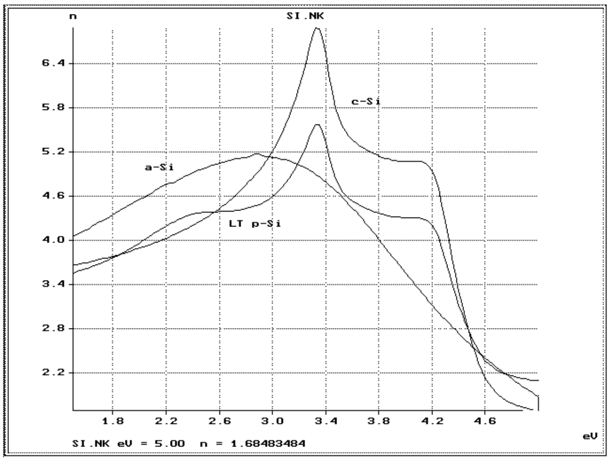


Fig.3 Refractive Index Spectra of Thin Polycrystalline Silicon Film Formed at Low Temperature (*n*)

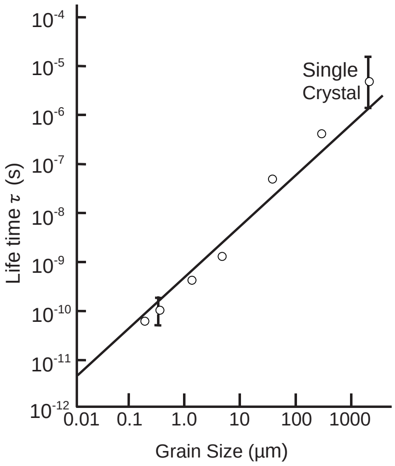


Fig.4 Relationship between Γ_1, Mobility, Life Time, and Grain Size

	E_1(eV)	Γ_1(eV)
Crystalline silicon (c-Si)	3.37	0.069
Polycrystalline silicon (p-Si:doped)	3.36	0.098
Polycrystalline silicon (p-Si:undoped)	3.49	0.319
Low temperature polycrystalline silicon (LT p-Si)	3.37	0.069

Table 1 E_1 and Γ_1 of Various Silicon Films

4 Difficulty in Thin Film Analysis

The change in light polarization is proportional to the product of the refractive index and the mass of the transmitted light (film thickness × beam diameter). Therefore, if the beam diameter is constant, the relationship can be expressed as:

Change in light polarization $\propto$ film thickness (d) × refractive index (n, k)

The change in light polarization for an ultra thin film is so small and the correlation between the film thickness and the refractive index is so large that it is difficult to analyze the film thickness and the refractive index separately.

Here, an oxide film (SiO_2) on silicon (Si) is discussed. If the film is thicker than 1000Å, the film quality is considered to be the same as that of the bulk, and thus the refractive index of the bulk can be used for the film. To measure such a thick film, an optical interferometer is generally used.

However, film thinner than 1000Å is difficult to measure with a standard interferometer due to the limitations of optical wavelength. Although the structure of a 100 to 1000Å-thick SiO_2 film differs from the structure of the bulk, with a corresponding variation in refractive index, an ellipsometer can be used because the variation in the refractive index occurs only in the high energy range beyond the detectable wavelength range of the ellipsometer. A single-wavelength ellipsometer is generally used for measuring 100 to 1000Å-thick film.

If the film is thinner than 100Å, specifically if the film is an ultra thin oxide film 10 to 20Å thick - equal to the thickness of several molecules - some consider it meaningless to discuss the refractive index, which is a physical constant of a bulk.

In a quality control processes, the deviation from the target film thickness is controlled. If the values must be controlled to within an error of ±1%, for example, this corresponds to 100Å for a 1µm film and 10Å for a 1000Å film. Thus, it is extremely difficult to deal with 10Å-thick film.

The refractive index of an oxide film (SiO_2) is shown in Fig.5.

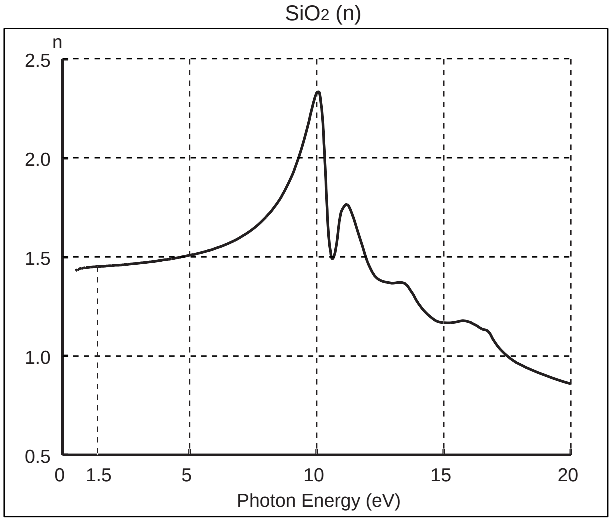


Fig.5 Refractive Index Spectra of Thin Silicon Dioxide Film (*n*)

An ellipsometer generally uses the wavelength of 5.0 to 1.5 eV (or 6.5 to 1.5 eV) for measurement; however, the refractive index of insulators show only a small change within this range, thus making measurement and analysis difficult.

As each layer is thick enough and has its own distinct refractive index in SIMOX, the difference between the measured data and the data obtained from the model can be identified on a display. As an exception, χ^2 is used as the index in analyzing the ultra thin film described above.

However, by combining highly precise measurements and state-of-the-art analysis methods, even ultra thin films can be evaluated, which has previously been considered practically impossible.

Only two examples are given here; a four-layer oxide film (Fig.6), and an ONO film (Fig.7). In an ultra-thin oxide film, the difference in the structure of the oxide film, due to differences in the gases used (NO gas or N_2O gas), can also be detected.

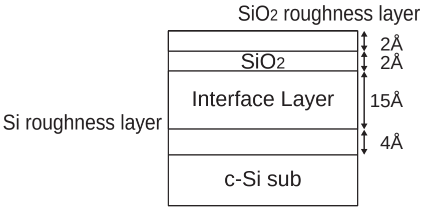


Fig.6 Example of Multilayer Structure: SiO_2 (four layers)

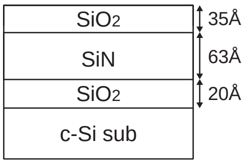


Fig.7 Example of Multilayer Structure: ONO

5 Conclusion

Spectroscopic ellipsometers serve as highly precise film thickness measurement systems, and provides various other information because it can measure many parameters. However, a full understanding of sample characteristics and the appropriate analysis techniques is required in order to realize effective analysis. In addition, the optimum recipe should be prepared in collaboration with the user in order to maximize the throughput.

References

[1] E. Wolf and M. Born
PRINCIPLE OF OPTICS
(TOKAI UNIVERSITY PUBLISHER)

[2] R. M. A. AZZAM and N. M. BASHARA
ELLIPSOMETRY AND POLARIZED LIGHT

[3] Edward D. Palic
Handbook of Optical Constants of Solids I & II

[4] A. K. Ghosh, C. Fishman and T. Feng
JOURNAL OF APPLIED PHYSICS
Vol. 51, p.446-454 (January, 1980)

Seiichi Hirakawa

Manager
Semiconductor Sales Department

HORIBA JOBIN YVON Co., Ltd.

Nataliya Nabatova-Gabain

Job leader
Semiconductor Sales Marketing Department

HORIBA JOBIN YVON Co., Ltd.

Yoko Wasai

Application engineer
Semiconductor Sales Department

HORIBA JOBIN YVON Co., Ltd.

Hiroshi Iida

Application engineer
Semiconductor Sales Department

HORIBA JOBIN YVON Co., Ltd.