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Characterization of complex inter-layer dielectric stack by spectroscopic ellipsometry: A simple method to reduce parameters correlations

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ABSTRACT

The accurate and stable measurements of inter-layer dielectric (ILD) film thicknesses and optical properties in a multi-layer stack have been always a key factor in semiconductor development and manufacturing. Spectroscopic ellipsometry is one of the most adapted optical metrology techniques to perform such measurements but it requires the use of one of the multi-parameter non-linear optimization methods due to its indirect nature. It creates a big challenge for analysis of multi-layer structures since the number of simultaneously determined model parameters is restricted due to parameter cross-correlations. This paper describes a simple way to reduce the correlations for single-angle ellipsometric measurements when applied to monitor the thicknesses of the dielectric films (silicon oxide, ultra low-k dielectric and low-k dielectric barrier/etch stop films) in a multi-layer stack. The method is based on inclusion of a thin Ta metal layer (~160 Å thick) into the multi-layer structure in order to suppress the inter-layer correlations, thereby allowing an accurate determination of the thicknesses of individual films in the thin-film stack. The optical characterization of all layers in the spectral range of 200–800 nm (6.20–1.55 eV) has been performed using an “additive” thin-film stack approach. The method was employed for analyzing the multi-layer ILD test stack with up to five-layer film structures in which four of the films are dielectric. The final model uniqueness and accuracy of the obtained ellipsometric solution were also verified.

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1. Introduction

Measurements of inter-layer dielectric films thicknesses and optical properties in the back-end-of-line (BEOL) [1] process always have been an important task for interconnect metrology in semiconductor development and manufacturing [2–4] since those properties directly influence device performance. One of the most convenient and well-established optical metrology techniques to perform such measurements is ellipsometry. Ellipsometry measures the changes in the polarization state of light upon reflection from a sample surface at non-normal (oblique) incidence (although transmission ellipsometry at normal incidence can be used for optically anisotropic samples) and those changes typically expressed either in terms of two values (ellipsometric angles) called Psi (Ψ) and Delta (Δ) or a complex number ρ (complex reflectance ratio) (all additional details can be found in standard references [5–9]). Those measured values can be used to determine the fundamental optical properties (complex dielectric function, $\varepsilon = \varepsilon_1 + i\varepsilon_2$, or complex refractive index, $N = n + ik$) of various materials and thicknesses of thin films (from monoatomic layers up to a few microns, in some cases). The complex dielectric function depends only on the intrinsic characteristics of the material (namely, it can be interpreted in terms of material electronic structure) and, therefore, it gives an opportunity to characterize other important material properties such as composition, phase structure, doping, stress, uniformity and electrical properties. Typically, *no special sample preparation is required* which makes ellipsometry a very fast measurement technique. In general, the sample is unaltered as the measurement itself does not cause any damage since ellipsometry uses relatively weak light sources. However, we should bear in mind that ellipsometry is an *indirect* characterization method which requires appropriate modeling analysis depending on the nature of the monitored or controlled processes to achieve accurate and reliable results. Ellipsometric analysis compares the measured data with a suitable optical model in which some parameters (layers thickness(es) and/or optical properties) are allowed to vary to minimize so-called the *merit function* (or *error function*), i.e., the function which determines the quality of fit [10].

Multi-layer stacks of dielectric films present a significant challenge for routine in-line process monitoring and control required to accomplish maximum production yield. These stacks cannot be characterized by single-wavelength ellipsometry which uses a monochromatic light source and, therefore, results in only single pair of ellipsometric parameters (Ψ, Δ). The latter makes it impossible to determine thicknesses of three or more films [11] since the number of unknowns (thicknesses) exceeds the number of measured parameters (Ψ and Δ) and the nonlinear ellipsometric equation cannot be directly inverted (the system is mathematically undetermined). Even the method of multiple angles of incidence might be not sufficient due to possibility of strong cross-

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correlations between the model parameters [12], which are a root cause of great uncertainties of the parameters, and also this method generally is not commercially available for production environments.

Spectroscopic ellipsometry (SE) involves measurements of Ψ and Δ as functions of wavelength λ (multi-wavelength approach). Therefore, it provides more information and allows the measurements of the individual-layer thicknesses in complex multi-layer structures. Additionally, SE can be used to determine the complex index of refraction as a function of wavelength λ (material dispersion; $N = f(\lambda)$) for chosen individual film layer. It has been shown that spectroscopic approach can be applied to various multi-layer cases: for instance, absorbing semiconducting alloys [13–15], oxide–nitride–oxide (ONO) and oxide–poly-Si–oxide (OPO) stacks [16], near-surface ion-implantation-induced damaged layers in semiconductors [17–20], metallic multi-layer structures [21], buried barrier oxide layer [22], etc. Variable-angle spectroscopic ellipsometry (VASE), a variant of SE, is an even more powerful technique for multi-layer optical measurements since the ellipsometric angles Ψ and Δ are measured as functions of both wavelength and angle of incidence (AOI) which results in higher sensitivity and accuracy due to additional optical paths for various AOI's [23–25]. As an example of VASE application to complex multi-layer structure we can refer to characterization of a silicon nitride (Si_3N_4)/silicon oxynitride (SiO_xN_y)/silicon dioxide (SiO_2) dielectric stack [26]. However, in some cases VASE still might not provide sufficient information for unambiguous multi-layer optical analysis and is also very rarely used for high-throughput industrial applications due to longer measurement time. Thus, in-line monitoring and control is usually performed on production metrology equipment at a single AOI, which is typically fixed and, therefore, cannot be optimized for particular applications in a production environment. Unfortunately, if the thin films in a multi-layer stack have comparable optical properties for a selected spectral range and, therefore, there is a quite bad contrast between the layers, a strong correlation between, at least, some layers thicknesses generally occurs and differentiation of the film thicknesses can be a problem. In other words, the thickness alterations of various layers can compensate each other and optical analysis may become unstable resulting in multiple local minima instead of the unique global one. As a well-known example of this issue we can mention thin ONO stack measurements which are very much affected by severe correlation between top and bottom oxide layers [27–29]. Those measurements are also complicated by existence of interface layers (sometimes not so very well-defined) between nitride and oxide layers [30,31]. To overcome this particular issue and decorrelate layers thicknesses, the following approaches were suggested: (i) the complementary use of deep ultraviolet (DUV) [32] ellipsometric and reflectometric spectra collected from the same location on a sample and their simultaneous analysis [27]; (ii) the combination of angle-resolved single-wavelength reflectometry (beam profile reflectometry), angle-averaged single-wavelength ellipsometry (beam profile ellipsometry), and DUV spectroreflectometry [33]. Those multi-technology techniques allow significant reduction of ONO layer cross-correlations and, therefore, the thickness uncertainties but are not available in most production metrology tools and also suffer from being significantly time consuming and impractical for real-time in-line monitoring.

In the present work, we report the characterization of a multi-layer ILD test stack with up to five-layer film structure in which four of the films are dielectric measured by an ex situ single-angle spectroscopic ellipsometer. For this purpose, the optical properties of the individual films in the structure of interest (silicon oxide (TEOS, tetraethylorthosilicate)/ultra low-k (ULK) dielectric/low-k dielectric barrier/etch stop film (BLOK™)/metal film/silicon oxide (TEOS)/silicon oxide-Si interface/Si substrate) have been investigated using an "additive" thin-film stack approach. The parameters of interest in the present study are the thicknesses of each layer. In practice, the thicknesses of the layers above the bottom TEOS film appear to be correlated with its thickness which significantly reduces accuracy and stability of the ellipsometric measurements. In order to suppress such correlations, an additional thin absorbing metal layer was introduced within a typical ILD test structure. Such inclusion will not affect device performance or ability to function since it can be applied only to appropriate structures in the test areas or on the test wafers. As demonstrated, a distinctive "screening" effect from the presence of the metal layer is a key factor to reduce thicknesses correlations between the dielectric films and it provides a unique solution for the thicknesses. The final model uniqueness and accuracy of the obtained ellipsometric solution were also verified. No other results on such ellipsometric characterization approach have been reported so far.

2. Experiment

2.1. Sample preparation

Two sets of five unpatterned test wafers, each with typical ILD structure on standard 300 mm silicon (100) wafers, were prepared using an Applied Materials Producer™ SE tool for dielectric chemical vapor deposition and an Applied Materials Endura™ tool for metal physical vapor deposition. The details of all used deposition processes (power, working pressure, deposition rates, etc.) are beyond the scope of this paper. One set of four-layer test wafers had the following structure: LDR (low deposition rate) TEOS/UV-cured ULK/BLOK/TEOS/Si substrate, another set of five-layer test wafers had an additional thin Ta metal layer between the BLOK and TEOS films (Fig. 1).

2.2. Measurements and analysis

Ex situ spectroscopic ellipsometry measurements were made at room temperature using rotating-compensator spectroscopic (190–800 nm) ellipsometer (RCSE) [34], one of the measurement modules in a KLA-Tencor Opti-Probe® OP9000 metrology tool. The RCSE performs measurements at AOI of ~65° using up to 512 different wavelengths. The time-dependent signal $I(t)$ at each wavelength is described by the general formula [9]

$$I(t) = I_0[1 + \alpha_2 \cos(2\omega t) + \beta_2 \sin(2\omega t) + \alpha_4 \cos(4\omega t) + \beta_4 \sin(4\omega t)], \quad (1)$$

where ω is the compensator rotation frequency and α_2, α_4, β_2 and β_4 are the normalized Fourier coefficients from which the ellipsometric parameters Ψ and Δ can be determined. The Fourier coefficient α_2 is usually set to zero by choice of coordinate system. Thus, the Opti-Probe RCSE has the non-modulated DC (total reflectivity) signal which always normalized to the Si reference and the modulated signal with three Fourier coefficients related to the rotating compensator and normalized to the DC signal.

All fits to the measured data were performed by using a commercial GO™ (Global Optimizer, Version 1.2a) software for optical characterization of thin films. Its non-linear optimization procedure adjusts the optical model parameters to minimize an error between experimental and

Fig. 1. Sketch of the multi-layer ILD structures with (right) and without (left) additional thin Ta metal layer used in present study.

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