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New dispersion model for band gap tracking

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ABSTRACT

The spectroscopic ellipsometry (SE) is known as the best in-situ non-invasive method suitable for thickness and composition measurements of the Si/oxide gates. However, a composition measurement performed by the SE is indirect and it needs a reference. Moreover, thickness and composition cannot be directly related to the relevant device performance parameters. On the other hand, a dielectric function, another optimized parameter of the SE metrology, has a direct relation to the bandgap parameter which is a major factor determining electrical performance of the Si/oxide gates. In this paper we develop and demonstrate a new optical model suitable for band gap tracking. The optical model developed is based on continuous version of the Cody–Lorentz model. This model can intrinsically define a physically meaningful value of the band gap. We show that developed model can be used for device process monitoring.

1. Introduction

The requirement on a good performance of the Si/oxide gate interface is in a very heart of modern microelectronics. In current CMOS technology, device performance is mostly defined by electrical performance of high-K oxide gate. The performance of the gate is characterized in terms of equivalent oxide thickness (EOT), the leakage current, threshold voltage, leakage EOT, and breakdown voltage [1]. The leakage current, in particular, is a key parameter to modern transistor performance affecting the power consumption, and heat generated from the computer chips [2]. During device processing these are the parameters which must be controlled and monitored. These electrical characteristics can be studied by a variety of methods including electrical measurements, transmission electron microscopy, x-ray spectroscopy and scattering, AFM, and photoelectronic spectroscopy [3,4]. However for high production yield, industry needs metrology tools that allow in situ, real-time monitoring during growth without wait for post-deposition electrical characterization or sample transfer to a characterization chamber [5]. The optical metrology, in particular spectroscopic ellipsometry (SE), is known as one of the best in-situ non-invasive characterization method [6,7]. In particular, the SE is suitable for thickness and composition measurements which can be related to technologically important parameters mentioned above. However, a composition measurement performed by the SE is indirect and it needs a reference. Moreover, thickness and composition cannot be directly related to the relevant device performance parameters. On the other hand, a dielectric function, another optimized parameter of the SE metrology, has a direct relation to the bandgap parameter which is a major factor determining electrical performance of the oxide gate. In the SE, a dielectric function is used to be represented by a parameterized optical model. The purpose of this paper is to develop and to demonstrate an optical model which can be used for band-gap tracking being suitable, therefore, for device process monitoring. The optical model developed is a so-called Continuous–Cody–Lorentz model. We demonstrate that the developed model can be applied for band gap monitoring of the high-K dielectric stacks. We finally demonstrate that the band gap found by fitting of experimental data using the developed model correlates to high-K metal gate stacks' electrical performance testing results, in particular, to the leakage current.

There are a few dispersion models which have been used so far in the SE for process monitoring. The most models used for band-gap monitoring are based on direct inversion method [8–10], or on parameterized models [11]. The Bruggeman Effective Model Approximation (BEMA) model [12] is used for composition metrology [8]. Both the BEMA model and the direct inversion method are used to extract dispersion curves which are the real, ε_1, and the imaginary, ε_2, parts of the dielectric function (or refractive index, n, and extinction coefficient, k) from the SE measurements. The BEMA model represents the dielectric function of the layer as an effective composition of assumed dielectric functions of constituents. The optimized effective composition can be related next to the composition of the dielectric layer of interest. The direct inversion method delivers the real and the imaginary parts of the pseudo-dielectric function using a direct inversion of the measured ellipsometric values, α and β or Ψ and Δ, for each measured wavelength. For the band gap monitoring, the calculated dispersion curves are next interpolated in the energy of interest to evaluate the band gap [13,14].

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The main disadvantage of the both BEMA and direct inversion methods in application to process monitoring, is that they do not have a direct connection to monitoring parameters, the band gap and composition in particular, and they need a reference therefore. In addition to this, the inversion method has a number of limitations and constrains. To list some of them: 1. the direct inversion method is an ill-defined mathematical problem. This is because the SE provides two measured values (α and β or Ψ and Δ) for each measured wavelength, but the SE metrology has to deliver three unknowns: ε_1 and ε_2 (or n and k), and the film thickness. Partly this under-defined inverse problem can be resolved by assuming that film thickness is known or that the material is transparent in a part of spectral range, extracting then n and thickness instead of n and k. 2. The real and imaginary parts of optical function derived by the direct inversion method do not satisfy the Kramers–Kronig consistency. As a result optical functions delivered by this method are lack of physical meaning. 3. The direct inversion method is very sensitive to statistical measurement errors. 4. The inversion method is very time consuming which makes it unpractical for in-line applications.

In this paper we demonstrate the state-of-the-art Cody–Lorentz–Continuous (CLC) model. The CLC model is implemented as proprietary model in OLSA (Off-Line Spectral Analysis), a software package for the development and optimization of film dispersion models, available from KLA-Tencor Corporation (Milpitas, CA, U.S.A.). The outline of this paper is the following. In Section 2 we first shortly discuss the conventional Cody–Lorentz (CL) model. We point out the issue with continuity of the derivatives of the CL dispersion functions. In Section 3, we present the developed CLC model. In Section 4, we demonstrate the capability of the developed model in tracking of the technologically important parameters. Section 5 concludes the paper with short remarks.

2. Cody–Lorentz model

The conventional CL model was developed to describe a dielectric function of the amorphous high-K dielectric [15–17]. According to this model, the imaginary part of dielectric function ε_2, is defined as follows.

$$\varepsilon_2^{CL}(E) = \begin{cases} \frac{E_1}{E}\exp\left(\frac{E-E_t}{E_u}\right), & 0<E<E_t \\ G_C(E)L(E), & E\geq E_t \end{cases} \quad (1)$$

In the energy range, $0 < E < E_t$, the CL function (1) describes the Urbach tails where Et is the Urbach transition energy, Eu is the rate of decrease of the Urbach tails, and E_1 is the amplitude of the Urbach function. At $E \geq Et$, the CL function is defined as the Lorentz function, $L(E)$, modulated by the Cody gap function, $G_C(E)$.

It was suggested by Cody that in amorphous dielectrics just above the optical band gap, the optical absorption edge can be described by the function $G_C(E) \propto (E-E_g)^2$ [15]. To satisfy the criteria $G_c(E>>E_g) \rightarrow 1$, the Cody gap function was set to

$$G_c(E) = \frac{(E-E_g)^2}{(E-E_g)^2 + E_p^2} \quad (2)$$

where E_p is the transition energy.

The Lorentz function was invoked into the Cody model to describe the absorption band away from the absorption edge, so that $\varepsilon_2^{CL}(E>>E_g) \rightarrow L(E)$ [12]. The Lorentz function

$$L(E) = \frac{AE_0\Gamma E}{\left(E_0^2-E^2\right)^2 + \Gamma^2E^2} \quad (3)$$

is defined by the amplitude of the Lorentz peak A, the resonant energy E_0, and the width of the peak Γ.

The amplitude of the Urbach function, E_1, is defined by continuity of the dielectric function (1) at $E = E_t$, as follows

$$E_1 = E_tG_c(E_t)L(E_t). \quad (4)$$

The CL model is completely defined by seven fitting parameters in terms of energy including, $E_g, E_p, A, E_0, \Gamma, E_t, E_u$. It must be pointed out that by definition, the CL model sets the correspondence between the main characteristic energies of the model such that [16].

$$E_g \leq E_t < E_0. \quad (5)$$

Inequality (5) implies that the transition energy between Urbach tails and gap region, E_t, cannot be smaller than the band gap energy, E_g, but E_t cannot be larger than the resonant energy, E_0, roughly corresponding to the maximum of the absorption band. Moreover, for the physicality sake, the decay rate of the Urbach tail must be non-negative, $E_u \geq 0$.

The real part of the dielectric function is obtained using the Kramers–Kronig relation:

$$\varepsilon_1^{CL}(E) = \varepsilon_1(\infty) + \frac{2}{\pi}P\int_0^\infty \frac{\xi\varepsilon_2^{CL}(\xi)}{\xi^2-E^2}d\xi. \quad (6)$$

Here $\varepsilon_1(\infty)$ is the high frequency electron part of the dielectric constant and P stands for the principal value of the integral. The dispersion of real and imaginary parts of the conventional CL model is shown by thick dashed curves in Fig. 1(a).

An important limitation of the conventional CL model is that both ε_1 and ε_2 have discontinuous derivatives over E and E_t at $E = E_t$, although condition (4) enforces the continuity of the Cody–Lorentz function itself. Thick dashed curves in Fig. 1(b) show the derivatives $d\varepsilon_1/dE$ and $d\varepsilon_2/dE$, thick dashed curves in Fig. 1(c,d) show the same curves magnifying the region where the discontinuity happens. As a matter of fact derivatives of the dielectric function may be non-continuous to describe some features (defect, excitons, etc.) in absorption coefficient. But the dispersion model would be unphysical if it allows derivatives to be discontinuous with no relation to real features of the material. Moreover, continuity of derivatives is of importance during optimization of the optical model used in the SE metrology. In particular, the discontinuity of derivatives can make the optimization process unstable and derived optical model lack of physical meaning. This is a limitation of the conventional CL model which makes it incapable in tracing the band gap although this model has the band gap as model parameter.

3. Continuous–Cody–Lorentz model

The current state-of-the-art model overcomes the discontinuity of derivatives of the conventional

CL model. The developed CLC model sets up a constraint on continuity of derivatives of the CL function at $E = E_t$. In turn, this constraint redefines the parameter E_u as a function:

$$E_u = \frac{E_1}{\partial E_1/\partial E_t} = \frac{E_t}{2D} \equiv f(E_g, E_p, E_0, \Gamma, E_t), \quad (7)$$

where

$$D = \frac{E_0^4-E_t^4}{\left(E_0^2-E_t^2\right)^2 + \Gamma^2E_t^2} + \frac{E_p^2}{(E_t-E_g)^2 + E_p^2}\cdot\frac{E_t}{(E_t-E_g)}. \quad (8)$$