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On determining the optical properties and layer structure from spectroscopic ellipsometric data using automated artifact minimization method

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ABSTRACT

An ellipsometric analysis method is presented and applied to simulated and measured ellipsometric data. It is shown that the Kramers–Kronig consistency of numerically inverted dielectric curves is lost, if interference related structures are present in the inverted dielectric function. Based on this observation, the root mean square of the self consistency curve is found to be appropriate to find the Kramers–Kronig consistent dielectric function, which belongs to a physically correct layer structure. Furthermore, it is shown that the effect of restricted photon energy range, typical to real life ellipsometric measurements, can be handled by adding an integration constant and one or two Sellmeier oscillators, whose parameters are fitted, to the Kramers–Kronig integrated dielectric function. The limitations of the method are also discussed, both on simulated and measured data.

1. Introduction

Optical characterization methods play an important role in high-tech semiconductor processing and glass manufacturing industries as they are non-destructive and require no sample preparation. Among these techniques spectroscopic ellipsometry stands out due to its high sensitivity and versatility. Ellipsometry has, however, a major drawback. It is an indirect technique, which means that a model based analysis must be performed, since in the majority of cases the optical properties of a sample cannot be derived directly from the measured data. Moreover, ellipsometric modeling does require not only the description of the layer structure of the investigated sample, but also the mathematical description of the dispersion of optical properties of the materials under study. The latter requires a priori knowledge regarding the shape of the dielectric function or considerable experience when recently developed materials are analyzed. Both can be avoided, however, by using the so called exact numerical inversion method. In case of this method, after constructing the model of the layer structure and assigning guess values for the real and imaginary parts of the unknown complex dielectric function (ε_1, ε_2) for the first wavelength point, Ψ, Δ pairs (or alternatively Re(ρ), Im(ρ) pairs) are calculated and compared to the experimental ones. Then a fitting algorithm is used to tune the ε_1 and ε_2 values until the calculated and experimental Ψ, Δ pairs agree within a preset limit. This process is repeated for each spectral point in turn, wavelength by wavelength, using the optimum ε_1, ε_2 value pair of the actual spectral point as initial guess values for the consecutive spectral point [1].

Incorrect layer structure and/or thicknesses generate artifacts in the complex dielectric function. However, this inherent property of the method – as it was pointed out by Aspnes et al. in 1984 [2] and Arwin et al. [3] – can assist in finding the correct layer structure and the proper complex dielectric function of the unknown layer in the numerical inversion method. In these artifact minimization processes the thickness of each layer is varied from an initial value and after each modification a numerical inversion is performed. This process is repeated until i) the interference related structures in the low absorption spectral region of the ε_2 curve [2] or ii) the effects of the substrate are eliminated [3]. It must be noted, that the method selects the best artifact free ε_1, ε_2 curves via the supervision of the dielectric curves by an expert, and thus is rather subjective.

In this paper we describe an improved interference related artifact minimization method, which selects the best ε_1, ε_2 curve pairs in an unsupervised manner and concomitantly guarantees a physically correct, Kramers–Kronig consistent solution of the complex dielectric function.

2. Experimental details

For the purpose of presenting and testing the method ellipsometric data of a SiO_2 substrate/amorphous silicon layer/surface roughness system with different layer thicknesses was simulated and analyzed. The optical data of the glass substrate and amorphous silicon were taken from Ref. [4] and from SOPRA database, respectively. To extrapolate

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the data of a-Si at photon energies above 5.1 eV, the tabulated data were fitted with a Tauc–Lorentz (TL) oscillator (position: 3.58 eV, amplitude: 173.7 eV, broadening: 2.22 eV and band gap: 1.40 eV) [5,6]. The optical properties of the roughness layer were described by an effective medium approximation, assuming a 50–50% mixture of the ambient and film. Simulations were performed at 55°, 60° and 65° angle of incidence and at photon energies between 1 and 20 eV with 0.01 eV steps, if not stated otherwise. For simulating measurement errors Gaussian noise with standard deviation of 0.0005 was added to the ellipsometric data. All simulations, numerical inversions and artifact minimization procedure were performed using a purpose written Mathcad code, whose proper operation was thoroughly tested. After each numerical inversion the Kramers–Kronig integral of the dielectric curves was numerically estimated [7] by the trapezoidal rule. The real part of the dielectric function at the ith photon energy was calculated according to the following expression:

$$\varepsilon_1^i = 1+\frac{1}{\pi}\left(\begin{array}{l}\sum_{j=1,j\neq i-1,j\neq i}^{N-1}\left(\frac{E^j\cdot\varepsilon_2^j}{E^{j2}-E^{i2}}+\frac{E^{j+1}\cdot\varepsilon_2^{j+1}}{E^{j+1\,2}-E^{i2}}\right)\left(E^{j+1}-E^j\right)+\\ +\left(\frac{E^{i-1}\cdot\varepsilon_2^{i-1}}{E^{i-1\,2}-E^{i2}}+\frac{\left(E^i-\delta\right)\cdot\varepsilon_2\left(E^i-\delta\right)}{\left(E^i-\delta\right)^2-E^{i2}}\right)\left(E^i-\delta-E^{i-1}\right)+\\ +\left(\frac{\left(E^i+\delta\right)\cdot\varepsilon_2\left(E^i+\delta\right)}{\left(E^i+\delta\right)^2-E^{i2}}+\frac{E^{i+1}\cdot\varepsilon_2^{i+1}}{E^{i+1\,2}-E^{i2}}\right)\left(E^{i+1}-\left(E^i+\delta\right)\right)\end{array}\right), \tag{1}$$

where N is the number of photon energies in the measurement range ($E_h - E_H$), δ – denoting the radius at the vicinity of the pole at E^i – was chosen to be 0.001 eV and $\varepsilon_2(E^i \pm \delta)$ is calculated by linearly interpolating the ε_2 data. Eq. (1) was evaluated only at photon energies between $E_h + 0.5$ eV and $E_H - 0.5$ eV to exclude any distortion in ε_1 that may be caused by any absorption peaks right outside the integration limits.

The application of the minimization method is presented on two different real samples. Ellipsometric data of a pulsed laser deposited $TiO_{2-x}N_x$ thin film (substrate temperature 400 °C, nitrogen concentration of the background gas mixture 90%) reported earlier [8] were reanalyzed. The second sample was a HfO_2 thin film purchased from UAB Altechna, whose ellipsometric spectra were measured with a Semilab rotating compensator ellipsometer at 70° angle of incidence, in the 1.25–4.2 eV photon energy range. In both cases the substrate was fused silica whose optical properties were also determined by ellipsometry. Conventional ellipsometric data analysis of the HfO_2 film was done using the SEA software [9].

3. Results and discussion

Kramers–Kronig consistency is an inherent property of materials, describing the interdependence of the real and imaginary parts of the complex dielectric function. The connection between ε_1 and ε_2 is given by the Kramers–Kronig relations [10]:

$$\varepsilon_1(E) = 1+\frac{2}{\pi}P\int_0^\infty \frac{E'\varepsilon_2(E')}{E'^2-E^2}dE', \tag{2}$$

$$\varepsilon_2(E) = -\frac{2E}{\pi}P\int_0^\infty \frac{\varepsilon_1(E')-1}{E'^2-E^2}dE', \tag{3}$$

where E and E' denote photon energies and P denotes the principal value of the integral. Physically correct dielectric functions must satisfy these Kramers–Kronig relations. However, the numerical inversion procedure does not inherently guarantee Kramers–Kronig consistent dielectric functions. Thus the Kramers–Kronig consistency of the ε_1, ε_2 curve pairs originating from numerical inversion should be checked. Although this Kramers–Kronig consistency check is usually considered as a constraint, in the following it will be used to assist in deriving the correct layer structure and the proper (i.e. artifact free) complex dielectric function. In order to determine these unknown structural and optical parameters, the ε_1, ε_2 curve pair that fulfills the Kramers–Kronig relations to the most has to be selected from a systematically generated, large set of ε_1, ε_2 curve pairs. This selection can be done by comparing the real part of the numerically inverted dielectric function with its Kramers–Kronig integrated imaginary part and choosing the ε_1, ε_2 curve pair, where the difference is minimal, i.e. by choosing the ε_1, ε_2 curve pair, which is most self consistent.

In the followings we will describe how to find such an optimum (i.e. most Kramers–Kronig consistent) ε_1, ε_2 curve pair in an automated way. In addition to this, the applicability and limitations of the method will also be discussed by analyzing both simulated and experimentally measured ellipsometric data.

3.1. Exemplification of the method

Fig. 1 a), b) and c) show the real part of the simulated complex reflectance ratio for a four phase (glass substrate/amorphous silicon/surface roughness/air) system at 3 different a-Si thicknesses, namely 20, 50 and 100 nm, respectively. In all three cases, the thickness of the surface roughness layer was 5 nm. The generated ellipsometric data were analyzed using the numerical inversion method. The real part of the numerically inverted dielectric functions (solid curve) is plotted in Fig. 1 d), e) and f) when the a-Si layer was set to be 96% of the exact thickness values, i.e. 19.2, 48.0 and 96.0 nm, respectively. These dielectric curves are accompanied by the corresponding Kramers–Kronig

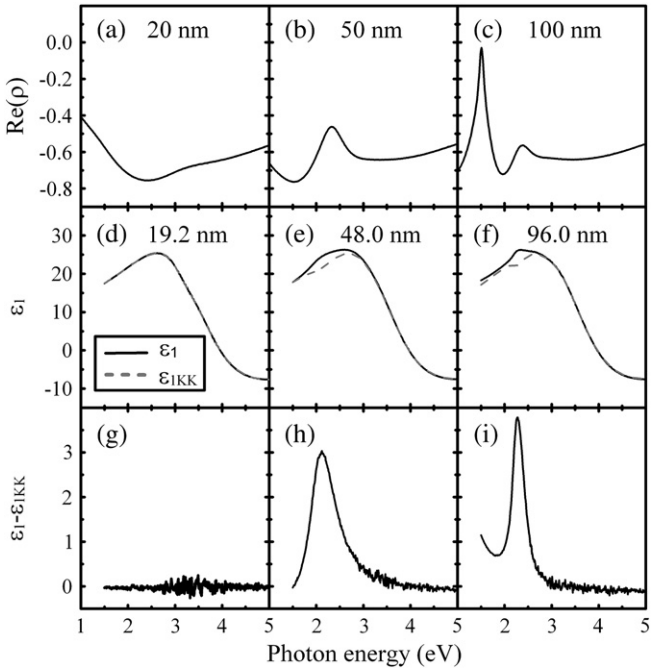

Fig. 1. a), b) and c) the real part of the complex reflectance ratio for a simulated glass substrate/a-Si (20, 50 and 100 nm, respectively)/roughness (5 nm) sample at 55° angle of incidence; d), e) and f) numerically inverted (solid black) and Kramers–Kronig integrated (dashed gray) dielectric functions when the thickness of the a-Si layer was supposed to be 19.2, 48.0 and 96.0 nm thick, respectively; g), h) and i) non-normalized self consistency curves. Although simulations, numerical inversion and Kramers–Kronig integration were performed in the 1–20 eV photon energy range, the curves are presented only up to 5 eV for better visualization of the appearing interference structures.