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Optical Modeling of Fluorocarbon Polymer Thin Films on Silicon Substrates

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Introduction

Spectroscopic ellipsometry (SE) is an excellent nondestructive characterization technique for determining thin film layer thickness and/or optical constants. Furthermore, a combination of variable incidence angle and variable wavelength (spectroscopic) capabilities provides the highest possible sensitivity and accuracy in measurements of multilayer structures. In this article, we report on the optical properties, characterized by variable-angle spectroscopic ellipsometry (VASE), of fluorocarbon (FC) polymer thin films grown on silicon substrates by vapor phase (VP) deposition and spin-on process. Lorentz and Cauchy models were used to simulate the measured SE spectra of the FC polymer thin films. The surface roughness effect of FC thin films was included in the model by assuming a roughened surface FC layer under the Bruggeman effective medium approximation (EMA) to obtain accurate FC optical constants.

The linear FC polytetrafluoroethylene (PTFE) is better known under several trademarks such as Teflon®, Fluon®, or Hostaflon®. Because it has many remarkable properties, including a low dielectric constant of 2.1, low coefficient of friction between 0.05 and 0.08, low permeability constant, and biocompatibility, this motivates the desire to produce thin film coatings. The known biocompatibity of bulk Teflon™ suggests these coatings could be used in a variety of biomedical applications including lead wires for pacemakers, catheter inserts, neural probes, and implantable tubing.

Experimental

Silicon wafers were cut into 13 mm × 15 mm and were precleaned in a solution mixture of H_2SO_4 and H_2O_2 (4:1) followed by HF treatment before the deposition. Finally, the samples were rinsed with deionized (DI) water and dried with N_2. FC722 (solute, 98% C_6F_{14} with 2 % proprietary fluoropolymer) and FC40 (solvent, $C_{12}F_{20}$) were provided by 3M Co. as source liquids for the deposition of FC films. FC chemicals were vapor phase (VP) deposited on the surface of silicon wafer. For the VP deposition, 1000 μl of 1:5 mixture of FC chemicals was placed in a vacuum oven. In the case of spin-on process, FC mixture were spun coated at 1000 rpm for 30 sec and baked at 100 °C for 15 min in air condition.

Ellipsometric measurements were performed with a computer-controlled variable angle spectroscopic ellipsometer of the rotating analyzer type (J. A. Woollam Co.). The dynamic measurements were carried out at an angle of incidence of 70°. The angle of incidence of 70° was chosen to maximize the sensitivity near the Brewster angle of the films. Data were fitted to a multilayer model (in which each layer was characterized by its thickness and refractive index) using Lorentz and Cauchy models. Optical modeling and data analysis were done using a Woollam Company WVASE32™ software package. The quality of the SE fit was determined by the mean-square error (MSE):

$$MSE = \frac{1}{2N-M}\sum_{i=1}^{N}\left[\left(\frac{\Psi^{mod}-\Psi^{exp}}{\sigma^{exp}_{\Psi,i}}\right)^2+\left(\frac{\Delta^{mod}-\Delta^{exp}}{\sigma^{exp}_{\Delta,i}}\right)^2\right],$$

where N is the number of (Ψ, Δ) pairs, M is the number of variable parameters in the model, and σ is the standard deviations of the experimental data points.

Results

To accurately simulate the obtained ellipsometric spectra, we performed a regression analysis in two steps assuming a three-phase model (ambient/FC/Si) and a four-phase model (ambient/roughened FC/FC/Si). First, the regression analysis was performed using the three-phase model and a best-fit MSE value was obtained. Then, the four-phase model was used to improve the best-fit result. The surface roughness layer was assumed to be a mixture of FC films and voids under the Bruggeman EMA. We found that the best-fit MSE was reduced when surface roughness was included. The Lorentz model allows us to simulate the optical constants of the FC films with a minimum number of parameters while maintaining Kramers-Kronig consistency between the real and imaginary parts of the optical constants. FC films are nearly transparent over the visible spectrum, so it is possible to assume k = 0 over part of the visible spectrum in the Cauchy model. Since the optical properties of the FC films were unknown, the Lorentz model and the Cauchy model were used to fit the measured spectra in the above analysis.