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### Resolving lateral and vertical structures by ellipsometry using wavelength range scan

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#### ABSTRACT

For most thin film structures, by changing the wavelength range to fit ellipsometric spectra, the values of the fitted parameters also change to a certain extent. The reason is that compared with the ellipsometric sensitivity many thin films are vertically non-uniform. In absorbing films with significant dispersion in the used wavelength range, the penetration depth of probing light can show large variations depending on the wavelength. Consequently, the value of a fitted parameter for a certain wavelength range is a weighted sum of structural information over different depth ranges corresponding to the different wavelengths. By changing the wavelength range, the range of penetration depths can be adjusted, and the fitted values can be plotted as a function of the probed depth range calculated directly from the determined or tabulated extinction coefficients. We demonstrate the results on deposited polycrystalline thin films. The advantage of this approach over the parameterization of structural properties as a function of depth is that the wavelength scan approach requires no parameterized depth distribution model for the vertical dependence of a layer property. The difference of the wavelength scan method and the vertical parameterization method is similar to the difference between the point-by-point and the parameterized dielectric function methods over the used wavelength range. The lateral structures strongly influence the ellipsometric response, as well. One of the most remarkable effects is when the lateral feature sizes approach the wavelength of the probing light. In this case the effective medium method is not valid any more, since scattering and depolarization occurs. By scanning the wavelength range, the limit wavelength of the onset of scattering can be found, and used for the determination of the corresponding critical lateral period length.

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#### 1. Introduction

Thin films created by most frequently used techniques like deposition (sputtering, evaporation, ablation, etc.), etching (e.g. porous silicon) or ion implantation are usually non-uniform both laterally and vertically on the scale of ellipsometric sensitivity [1-4] (sensitivity of a fit parameter is related here to the uncertainty, i.e., the 90% confidence limits of the fitted parameters). The vertical inhomogeneity is usually measured by dividing the surface region into numerous layers and fitting a characteristic parameter in each layer separately or as a defined function of depth [5,6,2]. In the first case, we have numerous fit parameters [7] (if a good depth resolution is aimed), whereas in the second case, we have to assume a depth distribution function [6]. However, utilizing the fact that the penetration depth of light is a strong function of wavelength in

http://dx.doi.org/10.1016/j.tsf.2014.02.008 0040-6090/ © 2014 Published by Elsevier B.V. semiconductors in the photon energy range around the critical points, a model independent "direct" depth scan can be performed.

The wavelength dependence can also be utilized for resolving lateral surface features, if their period is comparable with the wavelength of illumination. The dielectric function of composite media can be calculated using the effective medium approximation (EMA), if the size of the distinct phases is significantly smaller than the wavelength of illuminating light. It has been shown by Egan and Aspnes that the EMA is considerably influenced when component sizes approach the illumination wavelength [8]. Recently, we have shown that this effect can be used for the estimation of silicon nanosphere sizes comparable to the wavelength [4].

The aim of this article is to point out the potential of wavelength range scan for the resolution of both vertical and lateral features. The capabilities of vertical scan were demonstrated on a series of polycrystalline silicon layers with different thicknesses. In case of lateral features, we show that the limit wavelength of EMA correlates with a characteristic lateral feature size in a resist pattern prepared by electron beam lithography.

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**Fig. 1.** Micrograph of the sample with a hole size of nominally 120 nm and a period of 280 nm measured by scanning electron microscopy. The circular areas are exposed with e-beam and removed from the resist layer.

#### 2. Experimental details

Polycrystalline silicon [9] layers have been created using low pressure chemical vapor deposition on single-crystal Si wafers with ~100 nm thermal oxide at a deposition temperature of 640 °C, pressure of 27 Pa, and flow rate of 100 sccm. Polycrystalline silicon layers with the same deposition parameters but varied deposition times were created in the thickness range from 50 to 500 nm.

For the studies of the lateral structure, crystalline silicon wafers were spin coated with 300 nm photoresist. Then circular areas in a hexagonal order were removed from the resist using electron beam lithography (Fig. 1). The diameter of the circular part as well as the period have been varied in the range of 90–170 nm and 200–330 nm, respectively. Patterned areas as large as 0.3 mm by 0.6 mm were created so that the patterned area is suitable for the ellipsometric measurement with microspot.

We used a Woollam M-2000DI rotating compensator spectroscopic ellipsometer with a microspot of 0.3 mm beam diameter to measure the patterned areas. The ellipsometer is equipped with an X–Y mapping stage that can be positioned with a precision of a few microns. Using ellipsometry [10] we measure the complex reflectance ratio  $\rho = r_p/r_s =$ tan  $\Psi e^{i\Delta}$ , where  $r_p$  and  $r_s$  are the complex reflection coefficients of the light polarized parallel and perpendicular to the plane of incidence, respectively;  $\Psi$  and  $\Delta$  are the ellipsometric angles. Because the M-2000DI is a multichannel ellipsometer [11] that is capable of measuring  $\Psi - \Delta$ spectra in the wavelength range of 193–1690 nm (Fig. 2) within one



**Fig. 2.** Measured ellipsometric angles on the sample created by e-beam lithography with a nominal hole size of 100 nm. The angle of incidence was 60°. Note the irregular, distorted line shapes in the UV range.



Fig. 3. Measured and fitted  $\Psi - \Delta$  spectra for the ~500-nm thick polycrystalline silicon sample. The angle of incidence is 75°. The inset shows the optical model. "Poly" denotes the polycrystalline silicon layer modeled by the effective medium composition of c-Si, nc-Si and void. The roughness layer is modeled by the effective medium composition of 50% void and 50% "Poly". In this study, the wavelength range from 240 to 840 nm was used, because the nc-Si reference is only available for these wavelengths.

second with a precision of 0.05° for both, a high resolution (50 micron) mapping over an area of approximately 1 mm by 1 mm could be performed in as little as 10 min to locate the exact position of the patterned area. To increase the sensitivity we measured at angles of incidence as small as possible to avoid that the measurement spot gets elongated too much and reaches the non-patterned area. The typical angle of incidence for the electron beam-patterned samples was 60°.

#### 3. Resolving vertical features

The layer structure of the polycrystalline silicon wafers was modeled using a single-crystalline Si (c-Si) substrate, a SiO<sub>2</sub> layer created by thermal oxidation, a polycrystalline silicon layer with an effective medium composition of fine-grained polycrystalline silicon (nc-Si, [12]), c-Si and void (for density correction), as well as a surface roughness layer with 50% void and 50% layer material. Fig. 3 shows the optical model and a typical fit on the thickest layer (tm25). The fitted model parameters for the different samples are compiled in Table 1. In this study we focus on  $f_{\nu}$ , the volume fraction of void, which is a density correction of the polycrystalline silicon layer in the model. Note that it changes with the layer thickness significantly.

The variation of  $f_v$  in depth can also be estimated based on the fact that the penetration depth of illuminating light depends on the used wavelength range. The extinction coefficient (k) of the polycrystalline silicon layer (which is related to the absorption) has a characteristic feature around the E<sub>1</sub> (360 nm) and E<sub>2</sub> (300 nm) critical points, as shown in Fig. 4. The optical penetration depth (OPD) in Fig. 4 was calculated

#### Table 1

Fitted parameters of polycrystalline silicon layers. Only the deposition time was varied in order to obtain changing layer thicknesses. The uncertainty of parameter fit for the volume fractions and layer thicknesses is below 1% and 1 nm, respectively.  $d_b$  and  $d_r$  denote the thicknesses of the polycrystalline silicon layer and its surface roughness, respectively.  $f_{c-Sin}$   $f_{nc-Sin}$   $f_{v,d1}$  and  $f_{v,d2}^{(c)}$  denote the volume fractions of c-Si, nc-Si, void, and the corrected value of void, respectively. The fitted thickness of the buried oxide layer (not included in the table) is ~120 nm.  $d_{b,c}$  is the depth which is equivalent to the penetration depth scale of Table 2 – see the method of calculation and the description in the text.

Sample	$\frac{d_r}{(nm)}$	$\frac{d_b}{(nm)}$	$\frac{d_{b,c}}{(nm)}$	$\frac{f_{\text{c-Si}}}{\%}$	$\frac{f_{\text{nc-Si}}}{\%}$	$\frac{f_{\nu,d}}{\%}$	$\frac{f_{v,d}^{(c)}}{\%}$
tm22	3.0	57	436	49.7	48.2	2.1	2.1
tm23 tm24	3.2 4.0	113 276	380 217	51.0 38.8	47.3 56.9	1.7 6.0	1.7 4.2
tm25	4.3	493	0	32.2	60.9	12.0	7.7

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