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Spectroscopic Phase-Modulated Ellipsometry
---Application to thin film metrology---

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Feature Article
特集論文

Spectroscopic Phase-Modulated Ellipsometry
--- Application to thin film metrology ---

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Abstract

Recent advances in thin film technology, especially in semiconductor one, are providing new opportunities and challenges for the development and application of spectroscopic ellipsometry in thin film metrology. Nowadays precise determination of film thicknesses, optical properties and surface morphology are extremely important to produce high quality devices .

The article shows why spectroscopic phase-modulated ellipsometry is extensively used for the characterization of materials (insulators, semiconductors and metals). Main application fields, particularly in semiconductor technology, of this popular optical technique are discussed. Through typical examples accuracy and sensivity aspects are illustrated.

1. Introduction

Thin film materials pervade our everyday life. We are familiar with transparent conductors in LCD watches and computer displays, antireflection coatings, glass coatings for both color and energy efficiency, a large variety of microelectronic and optoelectronic devices, hard coating... Without thin film technology our way of life would not be the same.

Only about 25 years ago the variety of deposition and etching techniques for preparing thin films based devices was relatively limited. Now a certain level of process sophistication and system integration has been achieved and, consequently, more and more precise characterization of the thin films used is required in order to produce quality devices.

The sensitivity of ellipsometry to thin films and surfaces has been well known for over a century. However, it is only in the last two decades that this non-destructive technique has become an automated, fast, sensitive and highly reliable tool for thin film structures characterization.

2. Spectroscopic ellipsometry : Theory and data analysis

Spectroscopic ellipsometry measures the change in the polarization state of probing light, introduced by its interaction (through reflection or, more rarely, transmission) with the sample under study, and as a function of wavelength. This change is usually described by two angles (Ψ) and (Δ), which express the ratio of the complex reflection coefficients Rp and Rs of the sample (the indices 《 p 》and《 s 》, stand for light polarized parallel (p) and perpendicular (s) to the plane of incidence - see **Fig. 1**):

分光位相変調エリプソメトリ --- 薄膜評価への応用 ---

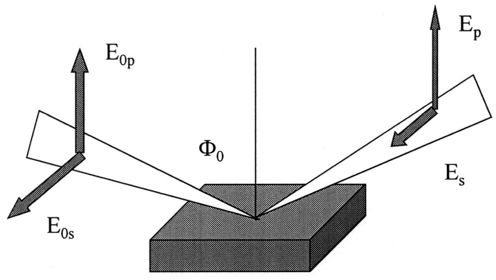
１．はじめに

薄膜材料は，時計やパソコンの各種電子デバイス材料として日常生活に深く浸透しており，今や薄膜なしでは生活が成立たない。薄膜莁成技術は急速に進展しているが，良質の薄膜を作るためには評価方法の向上が不可欠だ。エリプソメトリは薄膜の特性評価として優れた手段で，ここ20年間に自動化･高感度･高信頼化が急速に進んでいる。

２．分光エリプソメトリ：理論とデータ解析

分光エリプソメトリは，物質に光を照射し，主に反射光の偏光状態の変化を波長の関数として測定・解析し，薄膜の光学的性質を知る手法である。（**図１**）

薄膜の反射率は，基板と薄膜の組成，厚さ，表面アラサにより決り，偏光のパラメータ(Ψ)および(Δ)によって記述される。ΨとΔの計算値と実測値との平均二乗誤差(χ^2)が最小化なるような条件を見出すことにより，薄膜の光学特性を解析する。（**式１**）



$$E_p = r_p E_{0p} \qquad E_s = r_s E_{0s}$$

Fig.1 Polarization of reflected light

$$\rho = Rp/Rs = \tan \Psi \exp(i\,\Delta)$$

The reflection coefficients are determined by the optical properties and composition of the substrate and the overlying layers, by their thicknesses and morphology, and by surface roughness. In order to deduce the unknown parameters of the sample under investigation, a model which optically describes the sample structure is built. This model contains initial estimates of the parameters sought. The parameters are then varied to generate a set of calculated Ψ^{calc} and Δ^{calc} that fits best the measured data.

Data fitting consists in minimizing the mean-square deviation χ^2 between calculated and measured ellipsometric parameters (Ψ and Δ):

$$\chi^2 = \Sigma_{t=1..N}\ \Sigma_{\Phi=1..M}[\Psi^{calc}(\lambda_{i,}\Phi_j) - \Psi^{exp}(\lambda_{i,}\Phi_j)]^2 + [\Delta^{calc}(\lambda_{i,}\Phi_j) - \Delta^{exp}(\lambda_{i,}\Phi_j)]^2 \ / \ (2N-P-1) \ ......\ (1)$$

where the sum is taken over all measured wavelengths λ_i and angles of incidence Φ_j; P is the number of unknown material parameters and N, the number of experimental data points . The values of the varied parameters obtained after a χ^2 minimum has been achieved are then taken to be the best statistical estimates of the material parameters descibing the sample properties.

3. Spectroscopic Phase-Modulated Ellipsometry(SPME): Principle of operation and instrumentation

The optical set-up of SPME in the UV-visible range is displayed in **Fig.2**. The excitation head consists of a light source, a polarizer and a photoelastic modulator. After reflection on the sample the emerging light beam goes through an analyzer and a monochromator before being detected by the detector. The last three optical elements form the detection head.

The photoelastic modulator consists of a fused silica block glued to a piezoelectric crystal quartz bar oscillating at the frequency of 50 kHz. This generates a periodic phase shift $\delta(t) = A \sin(\omega t)$ between two orthogonal amplitude components of the transmitted beam.

The detected intensity takes the general form :

$$I(t) = Io + Is \sin(\omega t) + Ic \cos(2\omega t)$$

Where Is and Ic are function of (Ψ , Δ).

In the UVISEL system , the Fourier analysis of the signal is carried out by a Digital Signal Processor. This fast microprocessor system (cycle time < 100 ns) is especially dedicated to fast fourier transform computation. Finally the DC and the first two harmonics of the signal are continuously transmitted to a PC. The intensity ratios then directly yield the ellipsometric parameters Ψ and Δ characterizing the sample under study.

３．分光位相変調エリプソメトリ(SPME)：動作原理と測定装置

SPMEの光学系は，光源，偏光子および光弾性変調器，検光子，分光器，および検出器とにより構成されている。(**図２**)

石英製の光弾性変調器により，反射光の直交する振幅成分に位相のズレ$\delta(t)=A \sin(\omega t)$を生じさせ，光強度を測定する。UVISELでは，専用のDPSを使って高速フーリエ変換し，偏光解析パラメータΨとΔを解析する。(**式２**)

４. 用途

4.1 フラット・パネル・デイスプレイ(FPD)

分光エリプソメトリは，面積が広く多層構造のFPDの評価に適している。

(1)SiO2/ガラス

ガラス基板上に石英薄膜を蒸着するが，膜厚の均一性が特に重要である。SPMEにより広い面積にわたり，厚さのマッピングが高い精度で測定できる。(**図３，４**)

(2)アモルファスシリコンおよび多結晶シリコン／ガラス

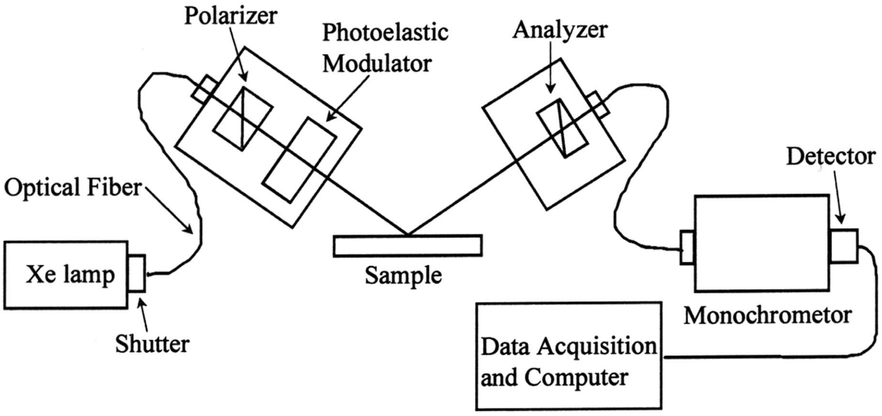


Fig.2 Schematic diagram of the Spectroscopic phase modulated ellipsometer

4. Applications

4.1 Flat panel display (FPD)

The application of spectroscopic ellipsometry in the field of the flat panel display often involves thin film thickness uniformity and optical properties measurements of a large-area multilayer structures.

(1)SiO$_2$ / Glass

Silica films are currently deposited as initial layers on glass substrates before further film deposits. Therefore, the thicknes uniformity of the silica layer is of crucial importance for the quality of the whole multilayer structure. Phase-modulated ellipsometry is particularly well adapted to the characterization of transparent materials (e.g. silica) since it gives a precise absolute measurement of the ellipsometric phase Δ. Thus, a typical thickness mapping of a large-area silica-deposited glass substrate by SPME is characterized by an Å-scale precision (see **Fig. 3, 4**).

(2) a-Si and poly-Si / Glass

Amorphous and polycrystalline silicon (**Fig. 5**) are the building materials of the actual thin film transistor (TFT) technology. The former is easy to deposit and process while the latter exhibits superior electrical properties (higher carrier mobility). The degree of crystallinity, thickness

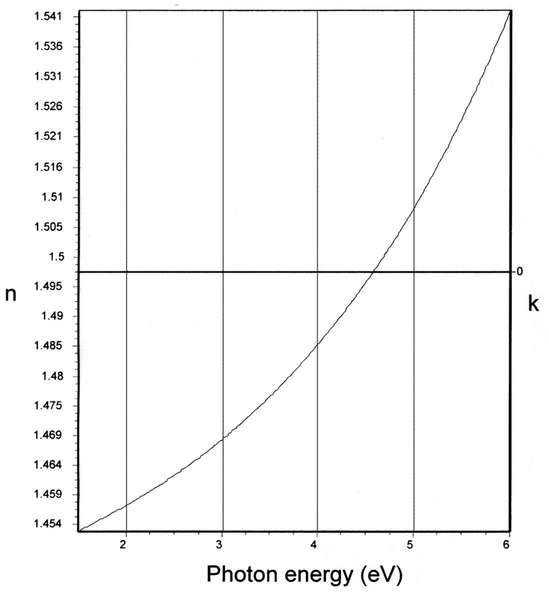


Fig.3 n,k of SiO$_2$/Glass

アモルファスシリコンと多結晶シリコンは，薄膜トランジスタ(TFT)によく使われているが，結晶性，厚さの均一性，表面粗さ，酸化度が重要である。SPMEで膜特性を解析することにより，蒸着工程の制御が容易になり最適化がはかれる。**図5**にガラス上のポリシリコン膜の屈折率を示す。

(3) 透明の導電性酸化物膜(ITO, SnO$_2$)

ITO, SnO$_2$膜は透明電極として広く使われているが，蒸着条件によっては光学定数が急激に変化する。(**図6**) SPMEにより，光学定数の傾斜状態，表面の厚さと粗さなど，さらには，電気的な特性も評価することができる。

(4)多層膜

FPDの製造工程では多層膜の蒸着がキー・プロセスである。SPMEを使ってFPD各点における光学パラメータを即測定解析し，さらにパネル全面にわたり完全自動マッピングが可能である。

4.2 リソグラフィー

リソグラフ用光源の多様化に伴い，各種のホトレジスト，反射防止膜，半導体・絶縁体・金属用のエリプソメタータが求められている。SPMEは，遠紫外から近赤外まで広い波長範囲にわたって測定できる。これら物質の光学定数を正確に求めることは，ホトリソグラフィープロセスばかりでなく，マイクロデバイスの作製全般の最適化にとって大変重要である。

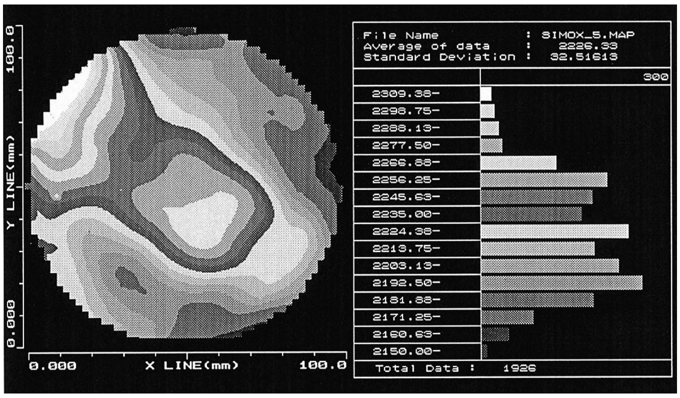


Fig.4 Mapping SIMOX (Si)

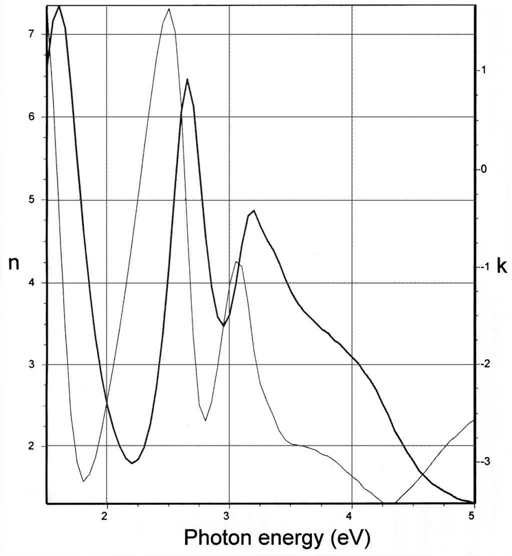


Fig.5 Pseudo <n,k> POLY-Si/Glass

uniformity, surface rougness and oxidation are the clue parameters to be monitored for a high quality TFT fabrication.

Owing to its high sensitivity and the use of advanced optical constant models SPME is capable of determination of the optical and morphological properties of both a-Si and poly-Si layers . With its help the deposition processes can be better understood and controlled and, consequetly, optimized .

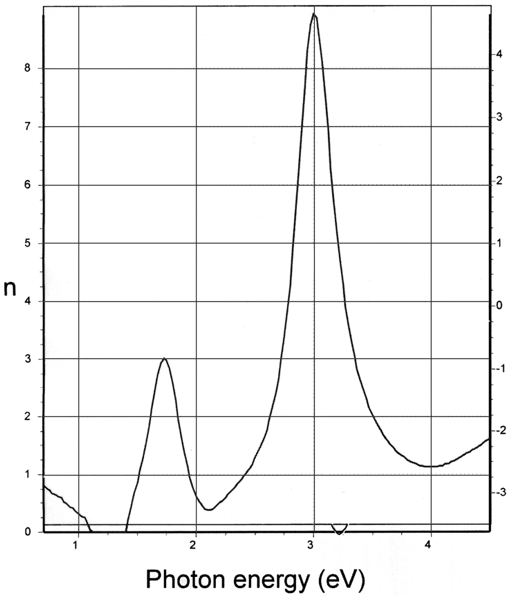


Fig.6 Pseudo <n> of SnO$_2$/Glass

(3)Transparent Conducting Oxides (ITO and SnO$_2$)

Transparent conducting oxides (especially indium tin oxide, ITO) are widely used as transparent electrodes since they combine high electrical conductivity with good optical transmissivity. Because of the particular deposition conditions these films are known to exhibit an optical constants gradient and non-negligible surface roughness thus making their optical characterization delicate(**Fig.6**). SPME inherently possesses the required sensitivity in order to successfully characterize such films. Thus, the use of a graded model of the optical constants of the layers enables the determination of essential material parameters such as index profile, surface thickness and roughness . Moreover, through modeling the of the free-carrier absorption in the films SPME provides valuable information on their electrical resistivity.

5．結論

本稿では，SPMEの応用例は分光位相変調エリプソメトリの持つ潜在能力ほんの一部を紹介したに過ぎない。SPMEの高い感度と精度，充実したソフトウエアは，薄膜のキャラクタライゼーション用として幅広い用途が期待されている。

（抄訳：半導体システム企画開発部　永井良典）

(4)Multilayers

An essential step in the FTP fabrication process is the deposition of multilayered thin film coatings. The determination of the thickness and the optical porperties of each individual layer represents a classical problem in ellipsometry and is successfully solved by SPME. Multilayer structures comprising a great number of layers, gradients, periodicity and substrate backside reflection are currently used in modeling SPME measurement results. Once the parameters of the structure having been determined at a given (x, y) point of the FPD, a fully automated mapping procedure can be performed over the entire surface of the panel.

4.2 Lithography

Photolithography is one of the basic processes in the production of microelectronic devices. The actual integrated circuits (particularly high-density memories) require smaller and smaller patterns thus pushing the wavelegth of the lithography light to the deep UV (DUV). Therefore, the probing light of the characterization optical technique (e.g. ellipsometry) must follow this trend and, as a consequence, large spectral range DUV (down to 190 nm) SPME has become available. The list of materials studied in this《extreme》, spectral region includes various photoresists, antireflective coatings, semiconductors (poly-Si), insulators , and metals. SPME is capable of their optical characterization down from DUV up to near IR. The precise determination of the optical constants of these materials using SPME is of great importance for the optimization of the photolithographic process and the microdevice fabrication in general .

5. Conclusion

Spectroscopic phase-modulated ellipsometry, being a non-desctuctive, fast, precise and easy-to-use optical technique is on the way of becoming an invaluable tool for the thin film materials characterization. The application fields cited above are only a part of a whole list of various actual and potential applications of SPME to microelectronics or elsewhere. With the increasing complexity and lowering the size of the samples SPME has an ensured future owing to its high instrumentational sensitivity and accuracy, and advanced modeling software capabilities.

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