Overview of VASE: Basic Theory and Applications

• Reference: J.A Woolam[1]

Introduction

- Mathematical theory is based on Fresnel reflection/transmission equations
 - These come from solutions to Maxwell's equations
 - p polarised: ${\pmb E}$ field parallel to plane of incidence
 - s polarised: E field perpendicular to plane of incidence (parallel to surface)
- Ellipsometric measurement:

$$\tan(\Psi)e^{i\Delta}=\rho=\frac{r_p}{r_s}$$

- Spectroscopic Ellipsometry (SE): Measure ρ as a function of λ
- Variable Angle SE (VASE): Measure ρ as a function of λ and angle of incidence.
- Measure *ratio* of 2 values \implies accurate and reproducable
- Measure Δ (phase quantity), sensitive to presence of thin films
- VASE gathers many data points off a single sample, and is well suited to modelling and fitting

What can be Determined by VASE?

- Layer thickness
- Surface/interfacial roughness
- Optical constants \implies any parameter that depends on these
- Gradients in properties vs depth in film
- Optical anisotropy

$$\begin{aligned} \langle \epsilon \rangle &= \langle \epsilon_1 \rangle + i \langle \epsilon_2 \rangle \\ &= \langle \tilde{n} \rangle^2 = \left(\langle n \rangle + i \langle k \rangle \right)^2 \\ &= \sin(\phi)^2 \left[1 + \tan(\phi)^2 \left(\frac{1 - \rho}{1 + \rho} \right) \right] \end{aligned}$$

Data Analysis

- Ellipsometry doesn't directly measure film parameters; measures Ψ and Δ
- Necessary to perform a model dependent analysis of Ψ and Δ data
- VASE increases data points recorded \implies good for fitting model to data
- Procedure:
 - 1. Aquire Data
 - 2. Use assumed model to predict expected data
 - 3. Compare generated to experimental data, and adjust model parameters to fit
- Fitting algorithm Marquardt-Levenberg
- Objective minimise (root) Mean Squared Error (MSE)

$$\text{MSE} = \sqrt{\frac{1}{2N - M} \sum_{i=1}^{N} \left[\left(\frac{\Psi_i^{\text{Mod}} - \Psi_i^{\text{Exp}}}{\sigma_{\Psi_i}^{\text{Exp}}} \right)^2 + \left(\frac{\Delta_i^{\text{Mod}} - \Delta_i^{\text{Exp}}}{\sigma_{\Delta_i}^{\text{Exp}}} \right)^2 \right]}$$

- Iterative process; start with simple model and refine
- "...the danger in making the model more complex is that paramters become correlated, in which case multiple sets of paramters will give the same good MSE fit."

Considerations for VASE Analysis

- Initial guesses must be close to the actual value
- Or the regression algorithm could finish on a secondary minimum, as shown in 1



Figure 1: From [1]

References

[1] John A. Woolam et al. Overview of variable angle spectroscopic ellipsometry (vase), part i: Basic theory and typical applications. *Optical Metrology*, 2000.