Parameters and conventions used in TFCompanion

TFCompanion follows common naming convention using subscripts $_s$ and $_p$ (e.g. R_s, R_p) indicating p-polarization (in the plane of incidence) and s-polarization (perpendicular to plane of incidence). TFCompanion support several different representations of Ellipsometry parameters that are described in this document. Both reflectance and transmittance Ellipsometry parameters are supported; _T is added to the name of the parameter to indicate that it is related to Transmission Ellipsometry. Two different sign conventions (Azzam and Beaglehole) of Ellipsometry parameters are supported as well as Delta convention and can be selected in configuration defaults setup.

I. Reflectance, Transmittance and Absorption parameters.

Measured parameters (intensity) indicated by capital characters, amplitudes indicated by small characters.

a). Reflectance parameters

R_p- reflectance of the p-polarized light; $R_p=|\boldsymbol{r_p}|^2$

R_s- reflectance of the s-polarized light; $R_s=|\boldsymbol{r_s}|^2$

Reflectance – unpolarized reflectance; Reflectance= $\frac{\boldsymbol{R_p}+\boldsymbol{R_s}}{2}$

Normal Reflectance – reflectance at 0 angle of incidence (from the normal to the surface). The presence of Normal Reflectance as a separate parameter allows to calculate it simultaneously with other angle dependent parameters.

b). Transmittance parameters

Note. Transmittance is calculated from ambient to substrate (substrate is infinite). Substrate should be set as void.mat (and any finite thickness material as a first layer).

T_p- transmittance of the p-polarized light; $T_p=|\boldsymbol{t_p}|^2$

T_s- transmittance of the p-polarized light; $T_s=|\boldsymbol{t_s}|^2$

Transmittance – unpolarized transmittance $\frac{\boldsymbol{T_p}+\boldsymbol{T_s}}{2}$

Normal Transmittance – transmittance at 0 angle of incidence (from the normal to the surface).

c). Absorption parameters

Note. Absorption is calculated indirectly as a complimentary parameter using equation R+T+A=1 (R-reflectance, T – transmittance, A- absorption) for each type of the absorption units.

A_p- absorption of the p-polarized light; $A_p=1-\boldsymbol{T_p}-\boldsymbol{R_p}$

A_s- absorption of the p-polarized light; $A_s=1-\boldsymbol{T_s}-\boldsymbol{R_s}$

Absorption – unpolarized absorption $\frac{\boldsymbol{A_p}+\boldsymbol{A_s}}{2}$

Normal Absorption – absorption at 0 angle of incidence (from the normal to the surface).

II. Ellipsometry parameters

TFCompanion supports conventional system independent Ellipsometry parameters and system dependent Ellipsometry parameters (as of build 06282005). All parameters are supported for reflectance and transmittance Ellipsometry.

a). System independent Ellipsometry parameters

Conventional ellipsometry parameters (Δ,Ψ) for isotropic system are defined using following equation:

$$\rho = \frac{\boldsymbol{r}_p}{\boldsymbol{r}_s} = \mathrm{Re}(\rho) + \boldsymbol{i}\,\mathrm{Im}(\rho) = \tan\Psi\, \boldsymbol{e}^{i\Delta} \text{ for reflectance ellipsometry}$$

$$\text{where } \tan\Psi = \frac{|\boldsymbol{r}_p|^2}{|\boldsymbol{r}_s|^2} = \frac{\boldsymbol{R}_p}{\boldsymbol{R}_s};$$

$$\Delta = \text{Phase\_Rp} - \text{Phase\_Rs}$$

$$\text{alternative representation: } X = \frac{2\mathrm{Re}(\rho)}{(1+\tan\Psi^2)};\ Y = \frac{2\mathrm{Im}(\rho)}{(1+\tan\Psi^2)}$$

and

$$\tau = \frac{\boldsymbol{t}_p}{\boldsymbol{t}_s} = \mathrm{Re}(\tau) + \boldsymbol{i}\,\mathrm{Im}(\tau) = \tan\Psi\, \boldsymbol{e}^{i\Delta} \text{ for transmittance ellipsometry}$$

$$\text{where } \tan\Psi = \frac{|\boldsymbol{t}_p|^2}{|\boldsymbol{t}_s|^2} = \frac{\boldsymbol{T}_p}{\boldsymbol{T}_s};$$

$$\Delta = \text{Phase\_Tp} - \text{Phase\_Ts}$$

$$\text{alternative representation: } \boldsymbol{X\_T} = \frac{2\mathrm{Re}(\tau)}{(1+\tan\Psi^2)};\ \boldsymbol{Y\_T} = \frac{2\mathrm{Im}(\tau)}{(1+\tan\Psi^2)}$$

Delta – ellipsometry **Δ** parameter.
Psi - ellipsometry **Ψ** parameter.
CosDelta – ellipsometry **cosΔ** parameter
TanPsi – ellipsometry tan**Ψ** parameter
Phase_Rp –absolute phase (θ_p) of R_p
Phase_Rs –absolute phase (θ_s) of R_s
Delta_T – ellipsometry **Δ** parameter for transmission.
Psi_T - ellipsometry **Ψ** parameter for transmission.
CosDelta_T – ellipsometry **cosΔ** parameter for transmission
TanPsi_T – ellipsometry tan**Ψ** parameter for transmission
Phase_Tp –absolute phase (θ_p_T) of T_p
Phase_Ts –absolute phase (θ_s_T) of T_s
X, Y parameters provide alternative of **Δ, Ψ** representation
X_T, Y_T parameters provide alternative of **Δ_T, Ψ_T** representation.

The interesting property of X, Y parameters is that they are also directly measured quantity in PME (Photoelastic modulator ellipsometry). Assuming A=P=45deg (Analyzer/Polarizer azimuth angle).

The following expression shows the connection:

$$\boldsymbol{X} = \frac{\boldsymbol{I}_{2f}}{\boldsymbol{I}_{dc}} = \frac{4\boldsymbol{J}_2(\delta_0)\mathrm{Re}(\rho)}{1+\tan\Psi^2+2\boldsymbol{J}_0(\delta_0)\mathrm{Re}(\rho)} = \frac{2\cos\Delta}{1+\tan\Psi^2}$$

$$\boldsymbol{Y} = \frac{\boldsymbol{I}_{f}}{\boldsymbol{I}_{dc}} = -\frac{4\boldsymbol{J}_1(\delta_0)\mathrm{Im}(\rho)}{1+\tan\Psi^2+2\boldsymbol{J}_0(\delta_0)\mathrm{Im}(\rho)} = \frac{2\sin\Delta}{1+\tan\Psi^2}$$

where $\boldsymbol{I}_f$ is the signal at PM oscillation frequency;

$\boldsymbol{I}_{2f}$ is the signal at double PM frequency;

$\boldsymbol{I}_{dc}$ is the DC component of the signal;

J_n is a Bessel function on n[th] order

b). System dependent ellipsometry parameters

Measurement system does not, normally, measure conventional ellipsometry parameters directly, instead the system specific parameters are measured and conventional ellipsometry parameters are calculated by taking into account system configuration.

1. Rotating analyzer ellipsometer (RAE) or Rotating polarizer ellipsometer (RPE).

RAE or RPE are some of the most simple and widely used ellipsometry measurement systems.
The time –dependent signal collected from the detector can be expressed in the following form:

$\boldsymbol{I}(\boldsymbol{t}) = \boldsymbol{I}_0\{1+\boldsymbol{\alpha}\cos(2\boldsymbol{ft})+\boldsymbol{\beta}\sin(2\boldsymbol{ft})\}$,

where $\boldsymbol{f}$ is the frequency of rotating element.

α,β parameters are directly measured values in RAE or RPE system and, in the case of isotropic system, they can be related to the tanΨ and cosΔ values using following equations:

$$\tan\Psi = \tan\boldsymbol{P}\left(\frac{1+\alpha}{1-\alpha}\right)^{1/2};$$

$$\cos\Delta = \frac{\beta}{(1-\alpha^2)^{1/2}};$$

where P is polarizer azimuth in RAE or analyzer azimuth in RPE

Alpha is α parameter for reflectance ellipsometry
Beta is β parameter for reflectance ellipsometry
Alpha_T is α parameter for transmission ellipsometry
Beta_T is β parameter for transmission ellipsometry

2. Rotating Compensator ellipsometry (RCE)

The time –dependent signal collected from the detector can be expressed in the following form:

$I(t) = I_0\{1 + a_2\cos(2ft) + b_2\sin(2ft) + a_4\cos(4ft) + b_4\sin(4ft)\}$;

where f is the frequency of compensator rotation.

For the case of isotropic system parameters a_2, b_2, a_4, b_4 can be easily expressed as a function of azimuth angle of Polarizer (P), Analyzer (A), retardation of compensator (δ) and Δ, Ψ parameters. For a simple case of P=45, A=0 equations are as follows:

$a_0 = 1 - 0.5(1 + \cos\delta)\cos\Psi$

$a_2 = 0;$

$b_2 = \sin\delta\sin 2\Psi\sin\Delta / a_0$

$a_4 = -0.5(1 - \cos\delta)\cos 2\Psi / a_0$

$b_4 = 0.5(1 - \cos\delta)\sin 2\Psi\cos\Delta / a_0$

A2 –a_2 parameter for reflectance ellipsometry
B2 – a_4 parameter for reflectance ellipsometry
A4- a_2 parameter for reflectance ellipsometry
B4- b_4 parameter for reflectance ellipsometry
A2_T –a_2 parameter for transmission ellipsometry
B2_T – a_4 parameter for transmission ellipsometry
A4_T- a_2 parameter for transmission ellipsometry
B4_T- b_4 parameter for transmission ellipsometry

Conventions

1. Delta convention

Some measurement systems (e.g. RAE) can distinguish between 0-180deg and 180-360 deg Delta bidrants. In this case Delta is only defined in 0-180 deg. range TFCompanion supports both 0-180deg and 0-360 deg. Convention.

2. Sign convention

There are several conventions in Delta calculation that depends on whether optical constant are represented in n+ik or n-ik form and the sign of reflectance used for substrate.

TFCompanion follows Azzam convention by using internally dielectic constant in the form ε_1-iε_2. The consequence of using this convention is that Δ_{Azzam} =180deg for reflection from bare substrate.

Beaglehole convention set Δ_{bil} =0deg for reflection from bare substrate.

Δ_{bil}=180-Δ_{Azzam}

TFCompanion supports both Azzam and Beaglehole conventions that can be selected in configuration defaults setup.

Note. Aspnes convention uses **ε_1+iε_2** convention and Δ_{bil}=-Δ_{Aspnes} ; Aspnes convention is currently not supported