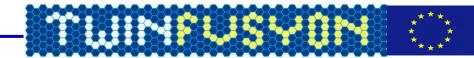


#### **Propagation of Light in Layered Materials**

#### Kurt.Hingerl@jku.at

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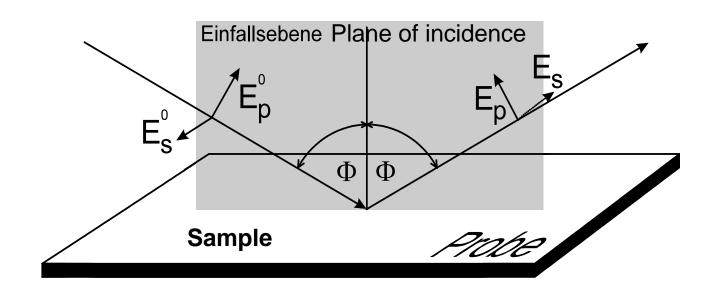
#### Contents



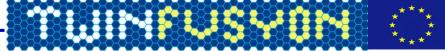
- Recapitulation of Electrodynamics
- 2 phase and 3- phase model
- Transmission (scattering) matrix,
- Virtual interface model



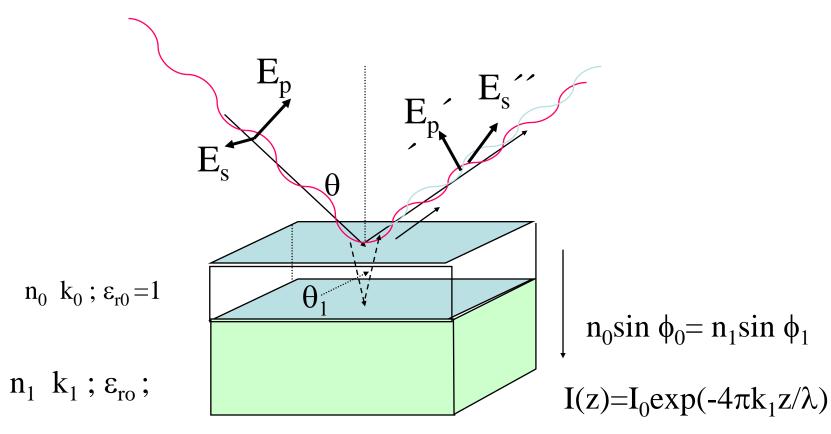
# Components of Polarization: 'senkrecht' 'parallel'



#### Recap II: Polarization, Reflection, Refraction

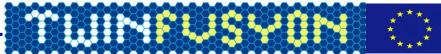






 $n_s k_s$ ;  $\varepsilon_{rs}$ 

## Maxwell's equations in vacuum and matter:



$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \qquad \nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0}$$

microscopic fields

$$\nabla \times \mathbf{B} = \mu_0 \left( \mathbf{J} + \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right) \qquad \nabla \cdot \mathbf{B} = 0$$

**E** and **H** are electric and magnetic field, **D** and **B** are displacement and magnetic induction fields; **E** and **B** are observable fields,

Bound charges and currents are put into the macroscopic fields **E B** 

$$\nabla \cdot \underline{\boldsymbol{E}} = \frac{1}{\varepsilon_0} \left( \rho_f + \rho_b \right) = \frac{\rho_f}{\varepsilon_0} - \frac{\nabla \cdot \boldsymbol{P}}{\varepsilon_0} \cdots \boldsymbol{P} = \frac{1}{\Delta V} \sum \boldsymbol{p}$$

$$\nabla \times \underline{\boldsymbol{B}} = \mu_0 \left( \boldsymbol{J}_f + \boldsymbol{J}_b + \varepsilon_0 \frac{\partial \underline{\boldsymbol{E}}}{\partial t} \right) = \mu_0 \left( \boldsymbol{J}_f + \frac{\partial \boldsymbol{P}}{\partial t} + \nabla \times \boldsymbol{M} + \varepsilon_0 \frac{\partial \underline{\boldsymbol{E}}}{\partial t} \right)$$

#### **Linear Material properties**

# 

E all fields from now on macroscopic fields <u>without</u> underline, most general linear approach

$$\mathbf{D}(\mathbf{r},t) = \varepsilon_0 \ \ddot{\varepsilon}(\mathbf{r},t) \ \mathbf{E}(\mathbf{r},t) = \varepsilon_0 \ \ddot{\varepsilon}(t) \ \mathbf{E}(\mathbf{r},t) = \varepsilon_0 \ \mathbf{E}(\mathbf{r},t) + \mathbf{P}(\mathbf{r},t) = \varepsilon_0 \ (1 + \chi(\mathbf{r},t)) \mathbf{E}(\mathbf{r},t)$$
$$\ddot{\varepsilon}(\mathbf{r},\omega) -> \ddot{\varepsilon}(\omega) -> \varepsilon(\omega)$$

$$\boldsymbol{B}(\boldsymbol{r},t) = \mu \boldsymbol{H}(\boldsymbol{r},t) = \mu_0 (1 + \chi_m) \boldsymbol{H}(\boldsymbol{r},t)$$
 for optical frequencies  $\boldsymbol{B}(\boldsymbol{r},t) = \mu_0 \boldsymbol{H}(\boldsymbol{r},t)$ 

If  $\varepsilon$  tensor- see lecture on generalized ellipsometry, if  $\varepsilon$  is a function of  $\mathbf{r}$ , then solve a more complicated diff. equation,  $\varepsilon(t)$  real => FT:  $\varepsilon(\omega) = \varepsilon(-\omega)$ 

Redefine ME in macroscopic fields:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \qquad \nabla \cdot \mathbf{D} = \rho_f$$

$$\nabla \times \mathbf{H} = \mathbf{J}_f + \frac{\partial \mathbf{D}}{\partial t} \qquad \nabla \cdot \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{D} = \rho_f$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\varepsilon = \varepsilon_0 (1 + \chi) \quad \mathbf{D} = \varepsilon \mathbf{E}$$

$$\mu = \mu_0 (1 + \chi_m) \quad \mathbf{B} = \mu \mathbf{H}$$

#### Dispersion relation and continuity at interfaces

No <u>free</u> charges or currents at optical frequencies:

$$\Delta \mathbf{E} - \mu \epsilon \frac{\partial^2 \mathbf{E}}{\partial t^2} = 0 \qquad \mathbf{E} = \mathbf{E}_0 e^{i(\mathbf{k} \Box \mathbf{r} - \omega t + \phi_e)}$$

$$\tilde{\mathbf{n}}^2 = (\mathbf{n} - i\mathbf{k})^2 = \mu \epsilon c^2 = \frac{\mu}{\mu_0} \frac{\epsilon}{\epsilon_0} \qquad k = \tilde{\mathbf{n}} \frac{\omega}{c} \quad \text{Dispersion relation: } \mathbf{k}^2 = \mu \epsilon \omega^2$$
Normal component of  $\mathbf{D} = \epsilon \mathbf{E}$  contingues

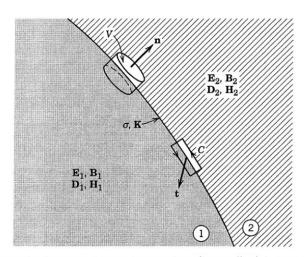


Figure I.4 Schematic diagram of boundary surface (heavy line) between different media. The boundary region is assumed to carry idealized surface charge and current densities  $\sigma$  and **K**. The volume V is a small pillbox, half in one medium and half in the other, with the normal n to its top pointing from medium 1 into medium 2. The rectangular contour C is partly in one medium and partly in the other and is oriented with its plane perpendicular to the surface so that its normal t is tangent to the surface.

$$k = \tilde{n} \frac{\omega}{c}$$
 Dispersion relation:  $k^2 = \mu \varepsilon \omega^2$ 

Normal component of  $D = \varepsilon E$  continous Normal component of **B** continous Tangential component of *E* continous Tangential component of **H=B/** $\mu$  continous

$$\iint_{S} \mathbf{D} \cdot \mathbf{n} \, d\mathbf{A} = (\mathbf{D}_{1} - \mathbf{D}_{2}) \cdot \mathbf{n} \, \Delta \mathbf{A} = \varepsilon (\mathbf{E}_{1} - \mathbf{E}_{2}) \cdot \mathbf{n} \, \Delta \mathbf{A} = \rho = 0$$

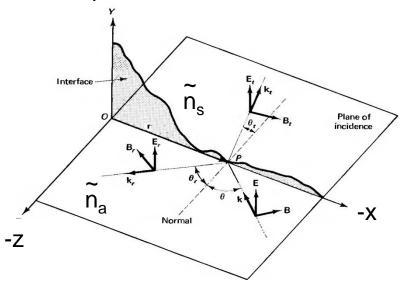
$$(\mathbf{B}_{1} - \mathbf{B}_{2}) \cdot \mathbf{n} = 0 \qquad \varepsilon (\mathbf{E}_{1} - \mathbf{E}_{2}) \cdot \mathbf{n} = 0$$

$$\iint_{C} \mathbf{E} \, d\mathbf{l} = (\mathbf{t} \times \mathbf{n}) (\mathbf{E}_{2} - \mathbf{E}_{1}) \cdot \Delta \mathbf{l} = 0 = -\iint_{S^{2}} \frac{\partial \mathbf{B}}{\partial t} \mathbf{n} \, d\mathbf{A}$$

$$\mathbf{n} \times (\mathbf{E}_{2} - \mathbf{E}_{1}) = 0 \qquad \mathbf{n} \times (\mathbf{H}_{2} - \mathbf{H}_{1}) = 0$$

#### Continuity II: waves from beneath

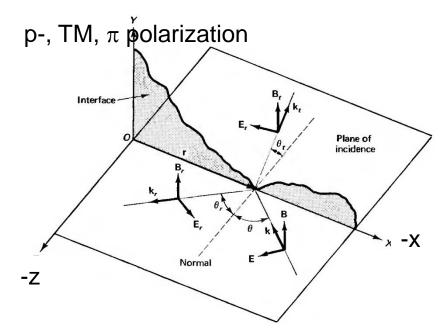
#### s-, TE, σ polarization



$$\mathbf{k} = (k_x, 0, k_z) = \tilde{n}_a \frac{\omega}{c} (\sin \theta, 0, \cos \theta)$$

$$\mathbf{k}^{r} = (k_{x}^{r}, k_{y}^{r}, k_{z}^{r}) \quad k_{x}^{r^{2}} + k_{y}^{r^{2}} + k_{z}^{r^{2}} = (\tilde{n}_{a} \frac{\omega}{c})^{2}$$

$$\mathbf{k}^{r} = (k_{x}^{t}, k_{y}^{t}, k_{z}^{t}) \quad k_{x}^{t^{2}} + k_{y}^{t^{2}} + k_{z}^{t^{2}} = (\tilde{n}_{s} \frac{\omega}{c})^{2}$$



$$\boldsymbol{E}_{\tan g} e^{ixk_x} + \boldsymbol{E}_{\tan g}^{r} e^{i(xk_x^r + yk_y^r)} = \boldsymbol{E}_{\tan g}^{t} e^{i(xk_x^t + yk_y^t)}$$

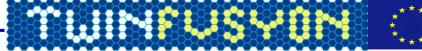
$$\boldsymbol{H}_{\mathrm{tang}} \mathrm{e}^{\mathrm{i} x k_{\mathrm{x}}} + \boldsymbol{H}^{\mathrm{r}}_{\mathrm{tang}} \mathrm{e}^{\mathrm{i} (x k^{\mathrm{r}}_{\mathrm{x}} + y k^{\mathrm{r}}_{\mathrm{y}})} = \boldsymbol{H}^{\mathrm{t}}_{\mathrm{tang}} \mathrm{e}^{\mathrm{i} (x k^{\mathrm{t}}_{\mathrm{x}} + y k^{\mathrm{t}}_{\mathrm{y}})}$$

Phases have to be the same at z=0:

$$k_{y}^{r} = k_{y}^{t} = 0, \quad k_{x}^{r} = k_{x} \quad k_{x}^{t} = k_{x}$$

$$\tilde{n}\sin\theta = \tilde{n}'\sin\theta'$$

# Fresnels formulas I : reflection for s-, TE, σ pol.



$$\begin{aligned}
\boldsymbol{E}_{y} + \boldsymbol{E}_{y}^{r} &= \boldsymbol{E}_{y}^{t} \quad (1) \\
\left(\boldsymbol{B}_{x} + \boldsymbol{B}_{x}^{r}\right) &= \frac{\mu_{a}}{\mu_{s}} \boldsymbol{B}_{x}^{t} \qquad \frac{1}{\omega} \left(\boldsymbol{k} \times \boldsymbol{E}_{y}\right)_{x} + \left(\boldsymbol{k}^{r} \times \boldsymbol{E}_{y}^{r}\right)_{x} = \frac{\mu_{a}}{\omega \mu_{s}} \left(\boldsymbol{k}^{t} \times \boldsymbol{E}_{y}^{t}\right)_{x} \quad (2) \\
\left(\boldsymbol{k}_{z} \boldsymbol{E}_{y}\right) - \left(\boldsymbol{k}_{z} \boldsymbol{E}_{y}^{r}\right) &= \frac{\mu_{a}}{\mu_{s}} \left(\boldsymbol{k}_{z}^{t} \boldsymbol{E}_{y}^{t}\right) \quad (2a) \\
\boldsymbol{E}^{t} &= \frac{2 \boldsymbol{k}_{z} \mu_{s}}{\boldsymbol{k}_{z} \mu_{z} + \boldsymbol{k}_{z}^{t} \mu_{s}} \boldsymbol{E} = \boldsymbol{t}_{s} \boldsymbol{E} \qquad \boldsymbol{E}^{r} &= \frac{\boldsymbol{k}_{z} \mu_{s} - \boldsymbol{k}_{z}^{t} \mu_{a}}{\boldsymbol{k}_{z} \mu_{z} + \boldsymbol{k}_{z}^{t} \mu_{s}} \boldsymbol{E} = \boldsymbol{r}_{s} \boldsymbol{E} \qquad \mu_{s} = \mu_{a} = 1 \end{aligned}$$

$$r_{s} = \frac{\tilde{n}_{a}\cos\theta - \tilde{n}_{s}\cos\theta}{\tilde{n}_{a}\cos\theta + \tilde{n}_{s}\cos\theta} = \frac{\sqrt{\epsilon_{a} - \epsilon_{a}\sin^{2}(\theta)} - \sqrt{\epsilon_{s} - \epsilon_{a}\sin^{2}(\theta)}}{\sqrt{\epsilon_{a} - \epsilon_{a}\sin^{2}(\theta)} + \sqrt{\epsilon_{s} - \epsilon_{a}\sin^{2}(\theta)}}$$

$$t_{s} = \frac{2\tilde{n}_{a}\cos\theta}{\tilde{n}_{a}\cos\theta + \tilde{n}_{s}\cos\theta} = \frac{2\sqrt{\varepsilon_{a} - \varepsilon_{a}\sin^{2}(\theta)}}{\sqrt{\varepsilon_{a} - \varepsilon_{a}\sin^{2}(\theta)} + \sqrt{\varepsilon_{s} - \varepsilon_{a}\sin^{2}(\theta)}}$$

## Fresnels formulas II : reflection for p-, TM, $\pi$ pol.



$$\boldsymbol{B}_{y} + \boldsymbol{B}^{r}_{y} = \frac{\mu_{a}}{\mu_{s}} \boldsymbol{B}^{t}_{y} \quad (1)$$

$$\boldsymbol{E}_{x} + \boldsymbol{E}_{x}^{r} = \boldsymbol{E}_{x}^{t} \qquad \frac{\boldsymbol{k}_{z}}{\mu_{a} \varepsilon_{a} \omega} \boldsymbol{B}_{y} - \frac{\boldsymbol{k}_{z}}{\mu_{a} \varepsilon_{a} \omega} \boldsymbol{B}_{y}^{r} = \frac{\boldsymbol{k}_{z}^{t}}{\mu_{s} \varepsilon_{s} \omega} \boldsymbol{B}_{y}^{t} (2)$$

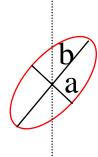
$$\boldsymbol{B}^{r} = \frac{\varepsilon_{s}\boldsymbol{k}_{z} - \varepsilon_{a}\boldsymbol{k}_{z}^{t}}{\varepsilon_{s}\boldsymbol{k}_{z} + \varepsilon_{a}\boldsymbol{k}_{z}^{t}}\boldsymbol{E} = r_{p}\boldsymbol{B} \qquad \boldsymbol{B}^{t} = \frac{2 \mu_{s}\varepsilon_{s}\boldsymbol{k}_{z}}{\mu_{a} \left(\varepsilon_{s}\boldsymbol{k}_{z} + \varepsilon_{a}\boldsymbol{k}_{z}^{t}\right)}\boldsymbol{B} = t_{p}^{B}\boldsymbol{B}$$

$$\boxed{r_{p} = \frac{\tilde{n}_{s}\cos\theta - \tilde{n}_{a}\cos\theta_{s}}{\tilde{n}_{s}\cos\theta + \tilde{n}_{a}\cos\theta_{s}} = \frac{\epsilon_{s}\sqrt{\epsilon_{a} - \epsilon_{a}\sin^{2}(\theta)} - \epsilon_{a}\sqrt{\epsilon_{s} - \epsilon_{a}\sin^{2}(\theta)}}{\epsilon_{s}\sqrt{\epsilon_{a} - \epsilon_{a}\sin^{2}(\theta)} + \epsilon_{a}\sqrt{\epsilon_{s} - \epsilon_{a}\sin^{2}(\theta)}}}$$

$$t_{p} = \frac{2\tilde{n}_{a}\cos\theta_{s}}{\tilde{n}_{s}\cos\theta + \tilde{n}_{a}\cos\theta_{s}} = \frac{2\varepsilon_{a}\sqrt{\varepsilon_{s} - \varepsilon_{a}\sin^{2}(\theta)}}{\varepsilon_{s}\sqrt{\varepsilon_{a} - \varepsilon_{a}\sin^{2}(\theta)} + \varepsilon_{a}\sqrt{\varepsilon_{s} - \varepsilon_{a}\sin^{2}(\theta)}}$$

## 2 Phase System can be solved analytically





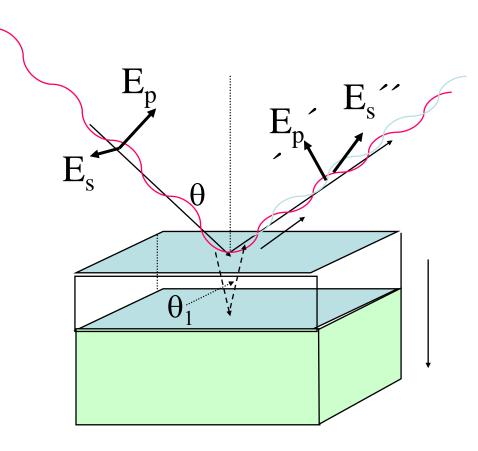
 $\Psi, \Delta$  (ellipsometric angles)

$$\rho = \frac{r_p}{r_s} = \frac{\sin^2(\theta) - \cos(\theta) \sqrt{\frac{\epsilon_s}{\epsilon_a} - \sin^2(\theta)}}{\sin^2(\theta) + \cos(\theta) \sqrt{\frac{\epsilon_s}{\epsilon_a} - \sin^2(\theta)}} =: \tan \psi e^{i\Delta}$$

$$\frac{\varepsilon_{s}}{\varepsilon_{a}} = \sin^{2}(\theta) + \sin^{2}(\theta) \tan^{2}(\theta) \frac{(1-\rho)^{2}}{(1+\rho)^{2}}$$

## 3 Phase System cannot be solved analytically

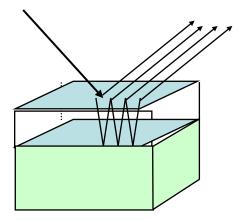
However,  $\varepsilon_a$ ,  $\varepsilon_o$ ,  $\varepsilon_s$ , and  $d_o$  by simulation respectively / fitting is always possible and highly accurate (multiple solutions).



#### The measured value is still $\rho$ !

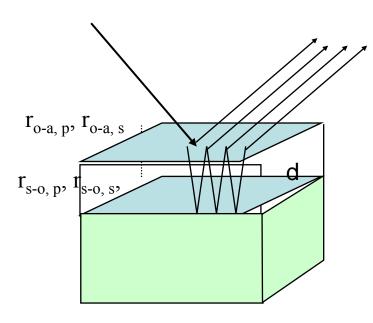
#### Techniques:

- 3 Phase system (extension to more layers by continuous fractions)
- Scattering Matrix (S-matrix)
- T-matrix



#### 3 Phase System





For both polarizations it can be shown:

$$\mathbf{r}_{o-a} = -\mathbf{r}_{a-o}$$
 $\mathbf{t}_{o-a} = (1 - \mathbf{r}_{a-o}^{2}) / \mathbf{t}_{a-o}$ 

The phase acquired by passing the overlayer back and forth:

$$Z = e^{i4\pi (d_o/\lambda)\tilde{n}_o \cos\theta_o} = e^{2i(\omega/c)\sqrt{\epsilon_s - \epsilon_a \sin^2(\theta)}}$$

For s- and p-pol therefore:

$$\begin{split} r_{all} &= r_{a-o} + t_{a-o} t_{o-a} r_{o-s} Z + t_{a-o} t_{o-a} r_{o-a} r_{o-s}^2 Z^2 + t_{a-o} t_{o-a} r_{o-a}^2 r_{o-s}^3 Z^3 + ... \\ r_{all} &= r_{a-o} + \frac{t_{a-o} t_{o-a} r_{o-s} Z}{1 - r_{o-a} r_{o-s} Z} = \frac{r_{a-o} + r_{o-s} Z}{1 + r_{a-o} r_{o-s} Z} \end{split}$$

## 3 layer: ambient / overlayer /substrate



$$\rho_{all} = \frac{r_{all,p}}{r_{all.s}} = \ tan \ \psi \ e^{i\Delta} = \frac{r_{a-o,p} + r_{o-s,p}Z}{1 + r_{a-o,p}r_{o-s,p}Z} / \frac{r_{a-o,s} + r_{o-s,s}Z}{1 + r_{a-o,s}r_{o-s,s}Z}$$

#### Thin layer expansion:

$$r_{all,p} = r_{a-s,p} \left( 1 + \frac{d \, 4\pi i (\grave{o}_{o} - \grave{o}_{s}) \cos\theta \sqrt{\grave{o}_{a}} \left( \grave{o}_{a} (\grave{o}_{o} + \grave{o}_{s}) \sin^{2}(\theta) - \grave{o}_{o} \grave{o}_{s} \right)}{\lambda_{o} \grave{o}_{o} \left( \grave{o}_{s}^{2} \cos^{2}(\theta) + \grave{o}_{a} \left( \grave{o}_{a} \sin^{2}(\theta) - \grave{o}_{s} \right) \right)} \right)$$

$$r_{\text{all,s}} = r_{\text{a-s,s}} \left( 1 - \frac{d \, 4\pi i (\grave{o}_{o} - \grave{o}_{s}) \cos(\theta) \sqrt{\grave{o}_{a}}}{\lambda_{o} \left(\grave{o}_{s} - \grave{o}_{a}\right)} \right)$$

$$\left\langle \epsilon \right\rangle = \frac{\varepsilon_{s}}{\varepsilon_{a}} + d\frac{4\pi i\sqrt{\varepsilon_{a}}}{\lambda} \frac{\varepsilon_{s} \left(\varepsilon_{s} - \varepsilon_{o}\right) \left(\varepsilon_{o} - \varepsilon_{a}\right)}{\varepsilon_{o} \left(\varepsilon_{s} - \varepsilon_{a}\right)} \sqrt{\frac{\varepsilon_{s}}{\varepsilon_{a}} - \sin^{2}\phi_{a}} \right\}$$

#### Contents

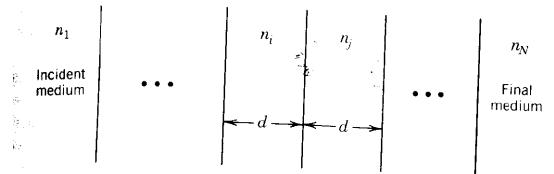


- Recapitulation of Electrodynamics
- 2 phase and 3- phase model
- Transmission (scattering) matrix,
- Virtual interface model

### Transmission and Scattering matrices:



4 layers: recursive fractions: 
$$\frac{\mathbf{r}_{a-o,p} + \mathbf{r}_{o-s,p} \mathbf{Z}}{1 + \mathbf{r}_{a-o,p} \mathbf{r}_{o-s,p} \mathbf{Z}}$$



For s- as well as for p- polarization:

$$\boldsymbol{E}_{rj} = \boldsymbol{E}_{ri}'\boldsymbol{t}_{ij} + \boldsymbol{E}_{lj}\boldsymbol{r}_{ji}$$

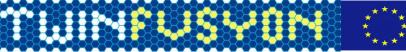
$$E'_{li} = E_{lj}t_{ji} + E'_{ri}r_{ij}$$

Using the realtions for the Fresnel coefficients:

Instead: use linear relationship, including the phases: Light is impinging on the structure with N layers from the left. The ith layer is the one left of the jth. Fields on the left side of each layer are unprimed, on the right side are primed:

 $E_{rj}$  is the rightward propagating field on the left side of the jth layer (but on the right side of the interface),  $E'_{lj}$  is the leftward propagating field in the jth layer.

# Transmission and Scattering matrices II:



$$E'_{li} = \frac{1}{t_{ij}} \left( E_{lj} + r_{ij} E_{rj} \right)$$

$$E'_{ri} = \frac{1}{t_{ij}} \left( r_{ij} E_{lj} + E_{rj} \right)$$

$$\textbf{E'}_{i} = \begin{pmatrix} E'_{li} \\ E'_{ri} \end{pmatrix}, \textbf{E}_{j} = \begin{pmatrix} E_{lj} \\ E_{rj} \end{pmatrix}, \quad \textbf{H}_{ij} = \frac{1}{t_{ij}} \begin{pmatrix} 1 & r_{ij} \\ r_{ij} & 1 \end{pmatrix}$$

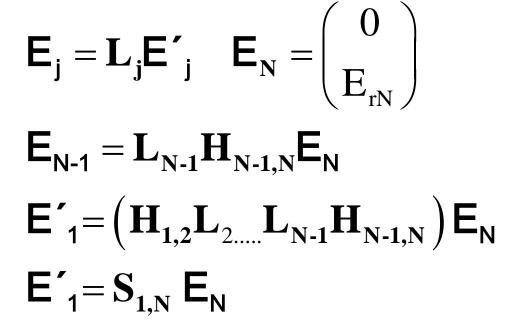
Propagation within one layer:

$$E_{rj}^{\prime} = E_{rj}^{\phantom{\dagger}} e^{i\beta_j}^{\phantom{\dagger}} = E_{rj}^{\phantom{\dagger}} e^{2\,i\,(\omega/c)\sqrt{\epsilon_s^{\phantom{\dagger}} - \epsilon_a^{\phantom{\dagger}} \sin^2(\theta)}}$$

$$E_{lj} = E_{lj}^{\prime} e^{i\beta_j} = E_{lj}^{\prime} e^{2\,i\,(\omega/c)\sqrt{\epsilon_s - \epsilon_a sin^2(\theta)}}$$

$$\mathbf{L}_{\mathbf{j}} = \begin{pmatrix} e^{i\beta_{\mathbf{j}}} & 0 \\ 0 & e^{i\beta_{\mathbf{j}}} \end{pmatrix}$$

#### Transmission and Scattering matrices III:



Matrix S contains all combined effects of arbitrary many layers including multiple reflections. Per definition, it is related to the total reflection and transmission coefficient

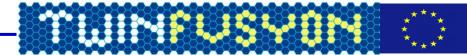
$$\begin{pmatrix}
E'_{11} \\
E'_{r1}
\end{pmatrix} = \begin{pmatrix}
S_{11} & S_{12} \\
S_{21} & S_{22}
\end{pmatrix} \begin{pmatrix}
0 \\
E_{rN}
\end{pmatrix}$$

$$= \begin{pmatrix}
S_{12}E_{rN} \\
S_{22}E_{rN}
\end{pmatrix}$$

$$r_{1N} = \frac{E'_{11}}{E'_{r1}} = \frac{S_{12}}{S_{22}}$$

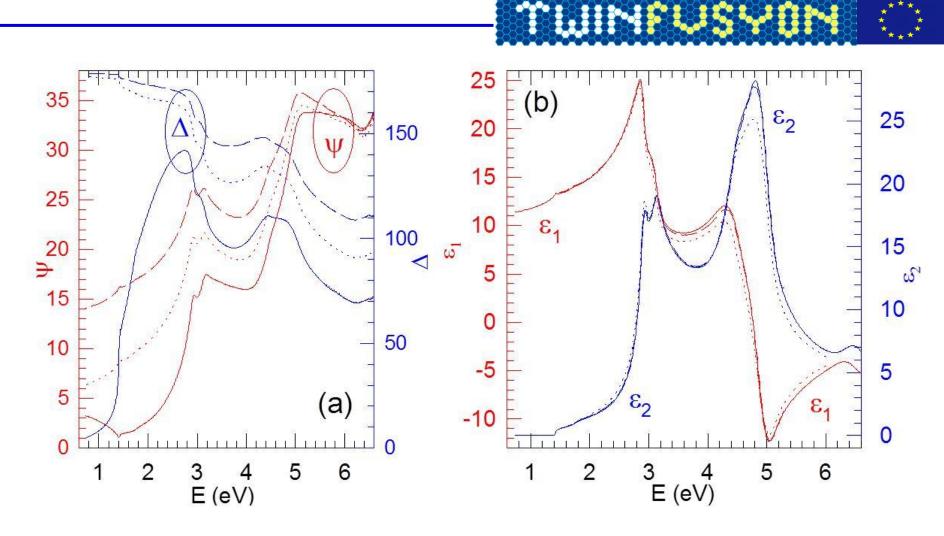
$$t_{1N} = \frac{E_{rN}}{E'_{r1}} = \frac{1}{S_{22}}$$

#### **Example: Optical Constants of GaAs:**



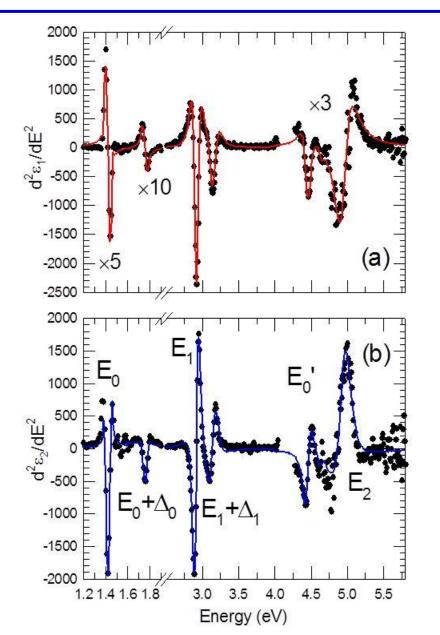
- Below the band gap (0.04 to 1.4 eV):
  - Absorption coefficient from transmission measurements (bulk)
  - Refractive index from prism refraction measurements
  - Both are very accurate, see Blakemore (JAP 53, R123, 1982).
- Near gap (1.2 to 1.8 eV):
  - n from reflection measurements of bulk samples
  - k from transmission measurements through thin films
  - Good accuracy, see Sell (1974) and Sturge (1962)
- Above the band gap (2 to 6 eV):
  - Kramers-Kronig transform of reflectance data is not accurate.
  - Spectroscopic Ellipsometry: Aspnes and Studna (1984): Rotatinganalyzer ellipsometer
  - Rotating- compensator ellipsometer

#### Dielectric Function of Bulk GaAs at 300 K



- (a) Ellipsometric angles at three angles of incidence (65, 70, 75 degrees).
- (b) Differences between solid and dotted: oxide coverage (5A).

#### Critical-point parameters of Bulk GaAs at 300 K



# 

- Derivatives related to band structure and critical points (CPs)
- Critical-point parameters:

A: amplitude

*E*: transition energy

Γ: broadening

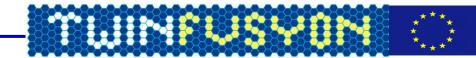
φ: phase angle

n: dimension of CP

- Solid lines show fit to data using analytical lineshapes.
- Good agreement with Lautenschlager *et al.* (1987).

$$\varepsilon(\hbar\omega) = A(\hbar\omega)^{-2} \exp(i\phi)(\hbar\omega - E + i\Gamma)^{n}$$

#### Contents



- Recapitulation of Electrodynamics
- 2 phase and 3- phase model
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- Virtual interface model

#### Virtual Interface Model: Thin layer expansion



During growth /etching we have a time dependent signal: either  $r_{all}(t)$  or  $<\epsilon>(t)$ ;

Is it possible –assuming we know the growth rate- to determine the dielectric function of the currently growing layer with dielectric function  $\varepsilon_o$  for any "*virtual*" substrate? Answer ... Dave Aspnes 1992, 1993, JOSA 10(5), 974

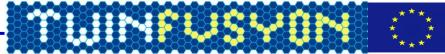
Exact: 
$$r_{\text{all,s}} = r_{\text{a-s,s}} \left( 1 - \frac{d \, 4\pi i (\grave{o}_{o} - \grave{o}_{s}) \cos(\theta) \sqrt{\grave{o}_{a}}}{\lambda_{o} \left( \grave{o}_{s} - \grave{o}_{a} \right)} \right) = > \grave{o}_{o} = \grave{o}_{s} - \frac{i \Delta r_{s} (\grave{o}_{a} - \grave{o}_{s}) \lambda_{o}}{4\pi \sqrt{\grave{o}_{a}} \cos(\theta)}$$

Approximation: 
$$\langle \varepsilon \rangle = \frac{\varepsilon_{s}}{\varepsilon_{a}} + d \frac{4\pi i \sqrt{\varepsilon_{a}}}{\lambda} \frac{\varepsilon_{s} (\varepsilon_{s} - \varepsilon_{o})(\varepsilon_{o} - \varepsilon_{a})}{\varepsilon_{o} (\varepsilon_{s} - \varepsilon_{a})} \sqrt{\frac{\varepsilon_{s}}{\varepsilon_{a}} - \sin^{2} \phi_{a}}$$

$$\varepsilon_{o} = \xi \pm (\xi^{2} - \langle \varepsilon \rangle \varepsilon_{a})^{1/2},$$

$$\xi = \frac{1}{2} (\langle \epsilon \rangle + \epsilon_a) + \frac{i \lambda (\langle \epsilon \rangle - \epsilon_a) \langle \epsilon \rangle'}{8 \pi \langle n_z \rangle \langle \epsilon \rangle}.$$

#### The Role of Surfaces and Interfaces



# "God made solids, but surfaces were the work of the Devil." Wolfgang Pauli

- Material Science: Function strongly dependent on the surface/ interface properties: for sensors, semiconductor devices, etc.
- Broken symmetry -> dimers, image charges, modification of bulk properties, surface stress and surface strain!
- Intrinsic effects: band bending, surface phonons, surface plasmons,
- "Dirt effects:" roughness, diffusion, steps, Quantum dots
- When you can't avoid it; HOW can you control/monitor it?