

Thin-film limit formalism applied to surface defect absorption spectroscopy

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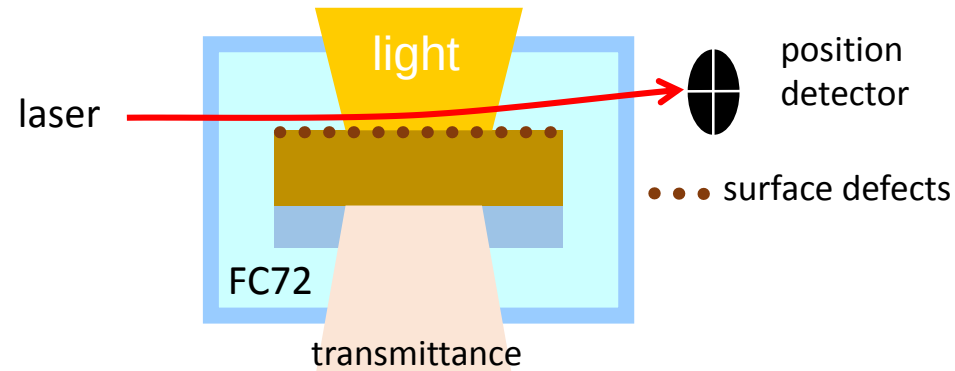
Outline

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Motivation: low absorptance spectroscopy

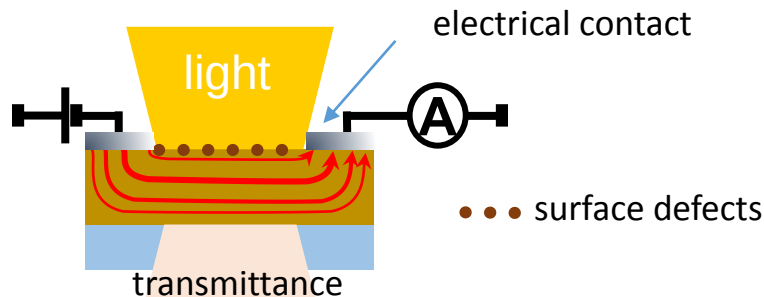
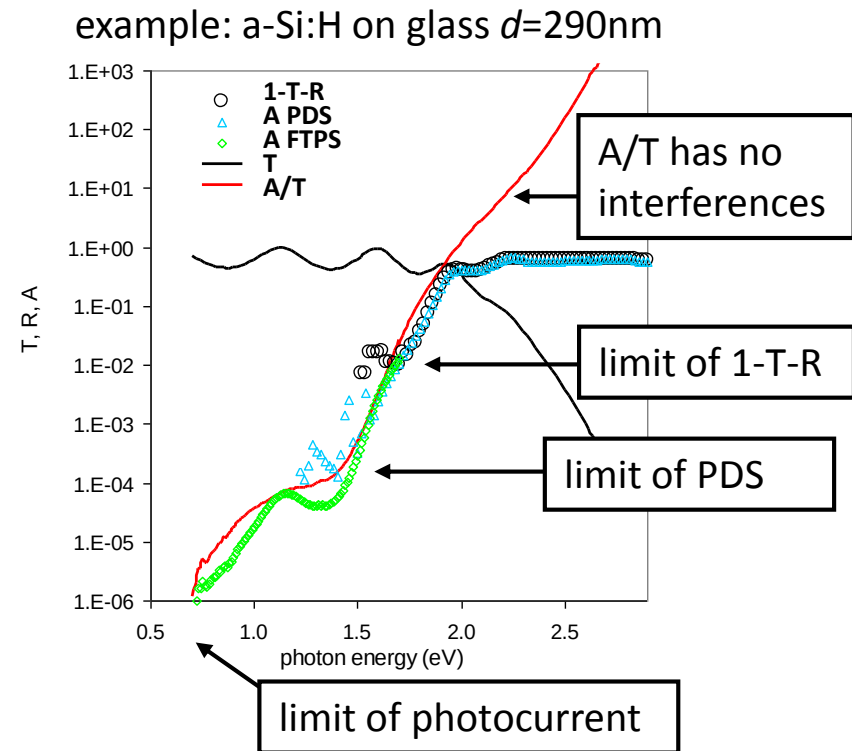
- PDS = Photothermal Deflection Spectroscopy

- non-absorbing substrates, limit 10^{-4} , absolute evaluation of A, T, R



- FTPS = Fourier-Transform Photocurrent Spectroscopy

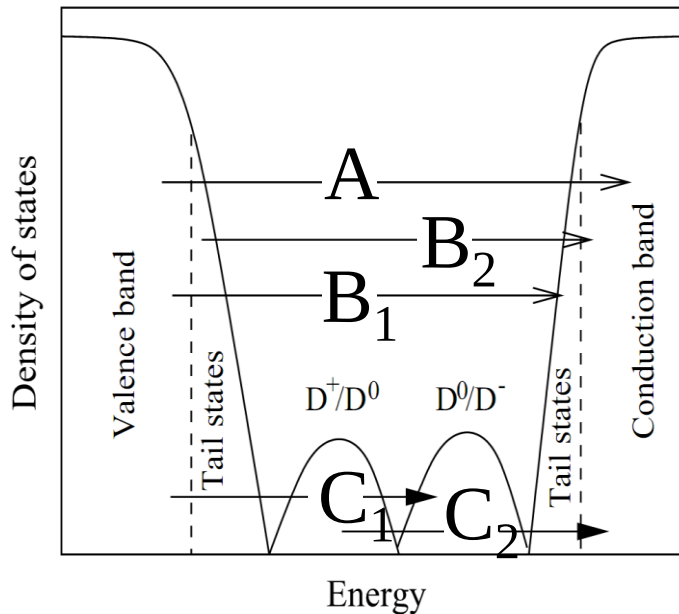
- absorbing substrates, solar cells, limit 10^{-7}



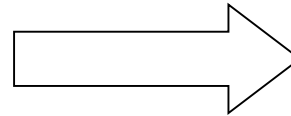
Motivation: low absorptance spectroscopy

- optical transitions in amorphous semiconductors

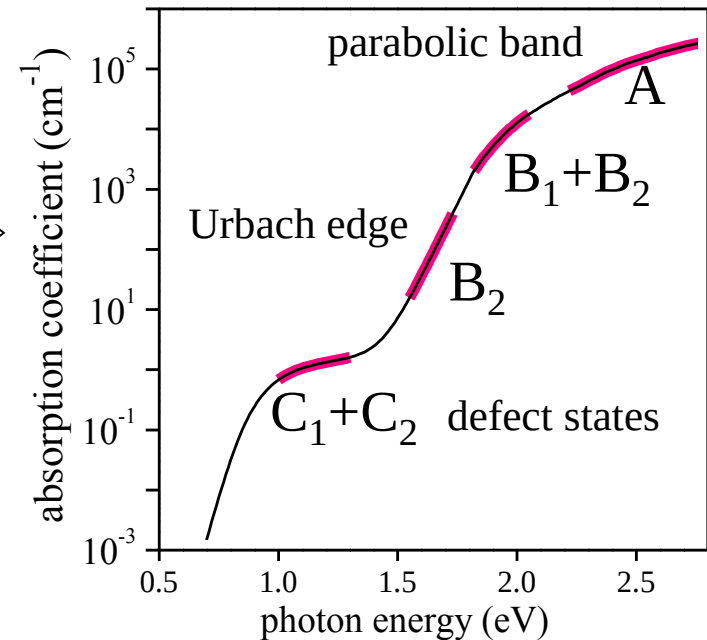
Band diagram of a-Si:H



convolution

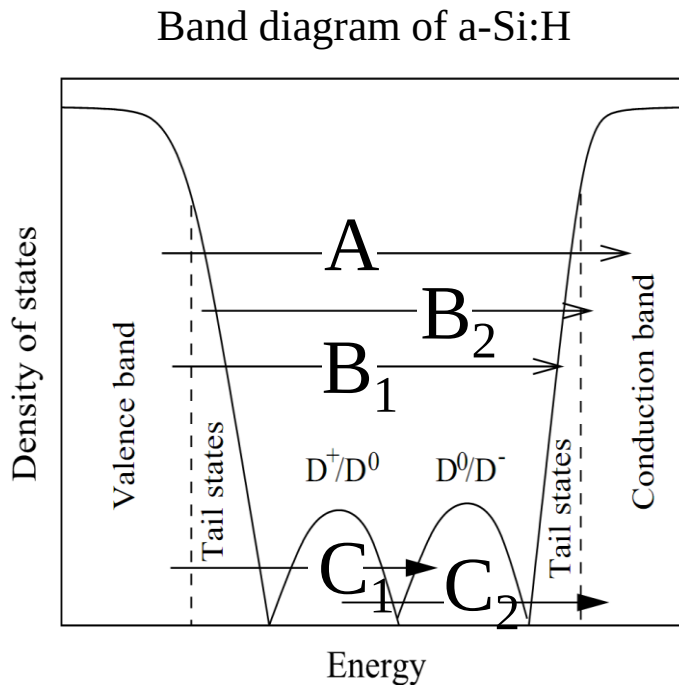
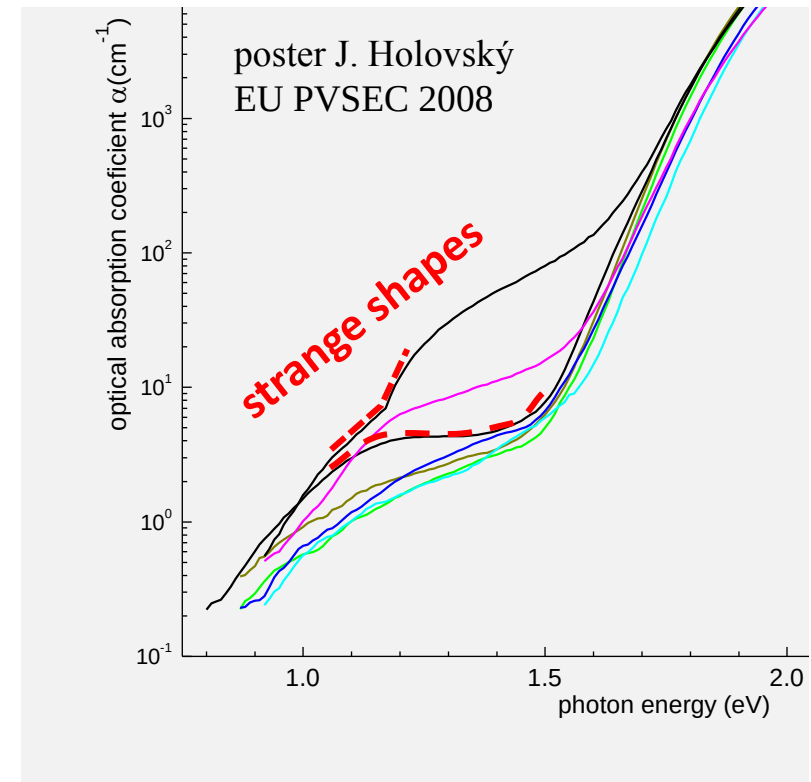


optical absorption coefficient



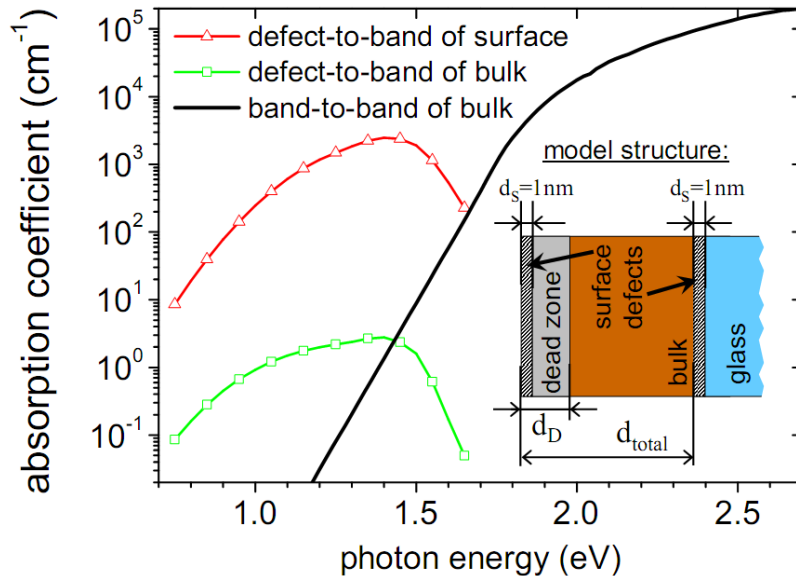
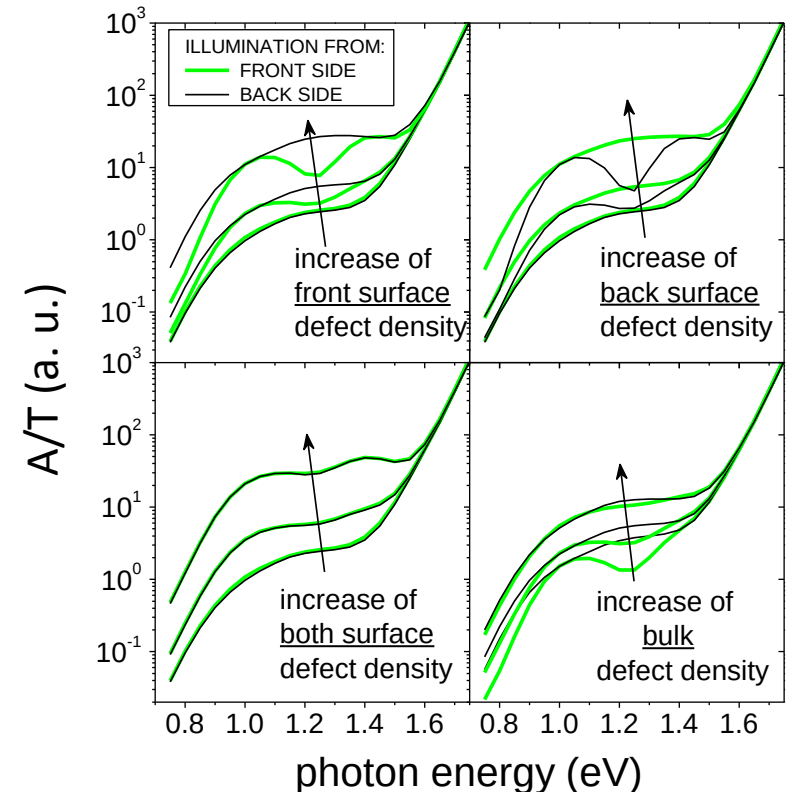
Motivation: low absorptance spectroscopy

- optical transitions in non-crystalline semiconductors



Surface defects – simulations

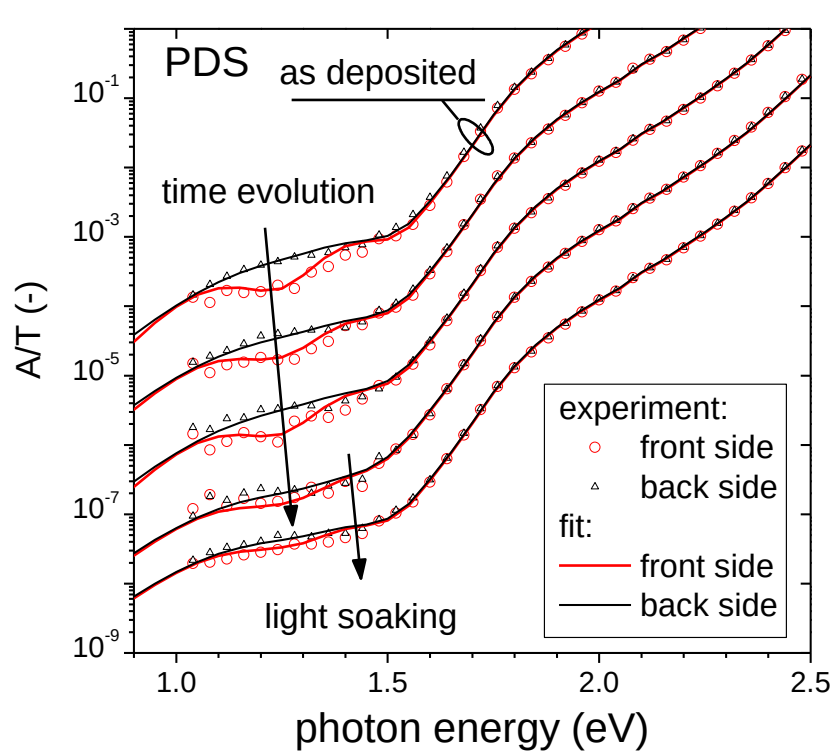
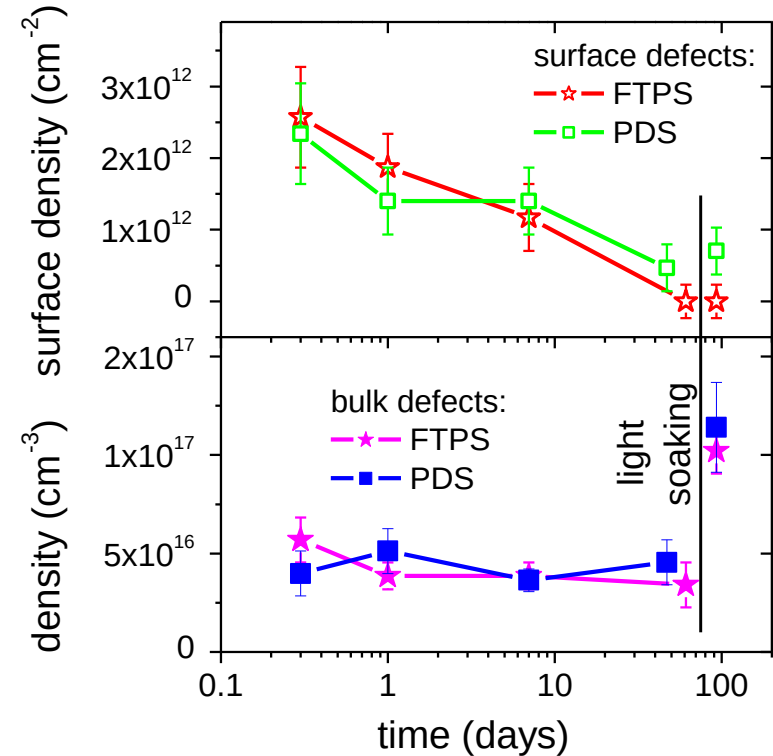
- Surface defect on illuminated side → non-vanishing interferences in A/T
- Transfer matrix simulations



J. Holovský, et al., *Time evolution of surface defect states in hydrogenated amorphous silicon studied by photothermal and photocurrent spectroscopy and optical simulation*, J. Non-Cryst. Solids. 358, (2012) 2035–2038.

Surface defects – experiment / fit

- EXPERIMENT and FIT by transfer matrix simulations



- DIFFERENT behavior of BULK defects and SURFACE defects

J. Holovský, et al., *Time evolution of surface defect states in hydrogenated amorphous silicon studied by photothermal and photocurrent spectroscopy and optical simulation*, J. Non-Cryst. Solids. 358, (2012) 2035–2038.

Summary I

- Techniques to measure very low absorptance
- If ultrathin defective layer is present on one side
→ interferences in A/T do not vanish for measurement from this side
- Ability to simulate the effect by transfer matrix method
- Lacking physical ‘common sense’ insight
- Lacking direct correction method

Thin-film limit: equations

- Everything is a function of product αdn

$$T_{\text{TFL}} = \frac{4n_0n_2}{(n_0 + n_2 + \alpha dn)^2}$$

$$A_{\text{TFL}} = \frac{4adnn_0}{(n_0 + n_2 + \alpha dn)^2}$$

$$R_{\text{TFL}} = \frac{(n_0 - n_2 - \alpha dn)^2}{(n_0 + n_2 + \alpha dn)^2}$$

- “universal curve”

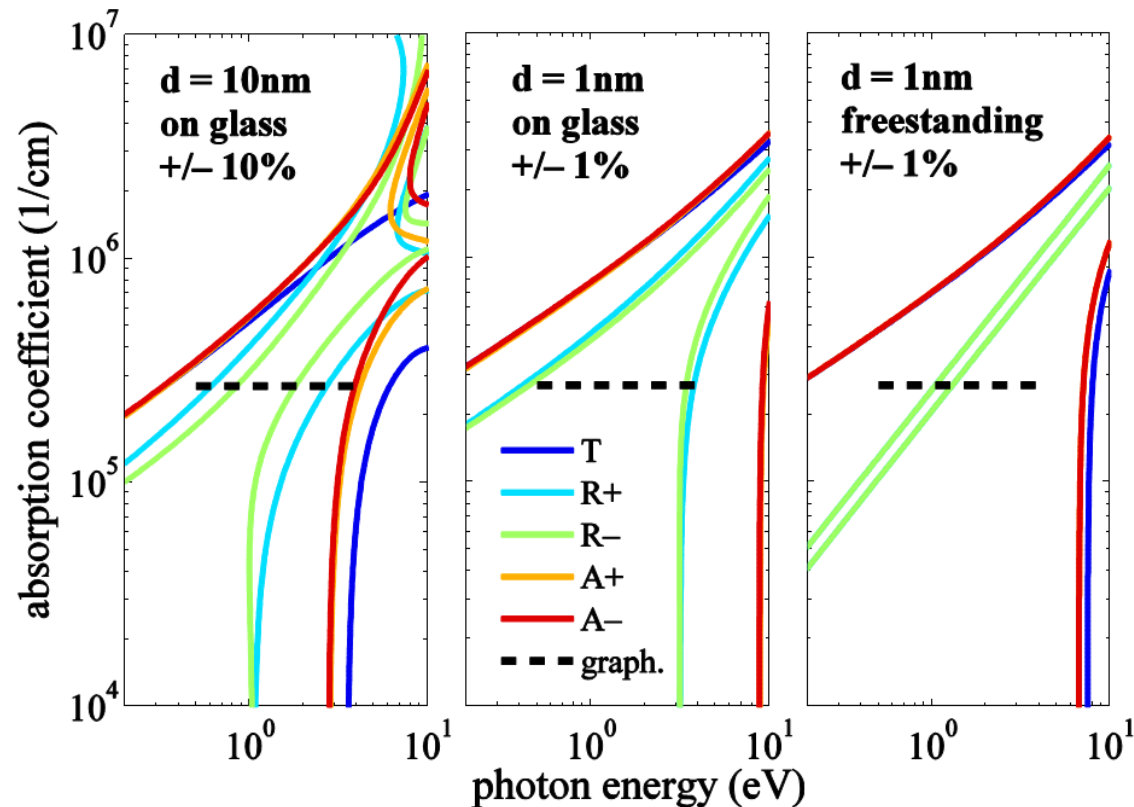
$$R_{\text{TFL}} \approx \left(1 - \sqrt{\frac{n_0 T_{\text{TFL}}}{n_2}} \right)^2$$

- ambient dependence

$$\frac{A_{\text{TFL}}}{T_{\text{TFL}}} = \frac{\alpha dn}{n_2}$$

Thin-film limit: numerical verification

- Areas where difference from rigorous calculation is $<10\%$ or 1%
 - simulation for optical parameters of graphene, different thicknesses



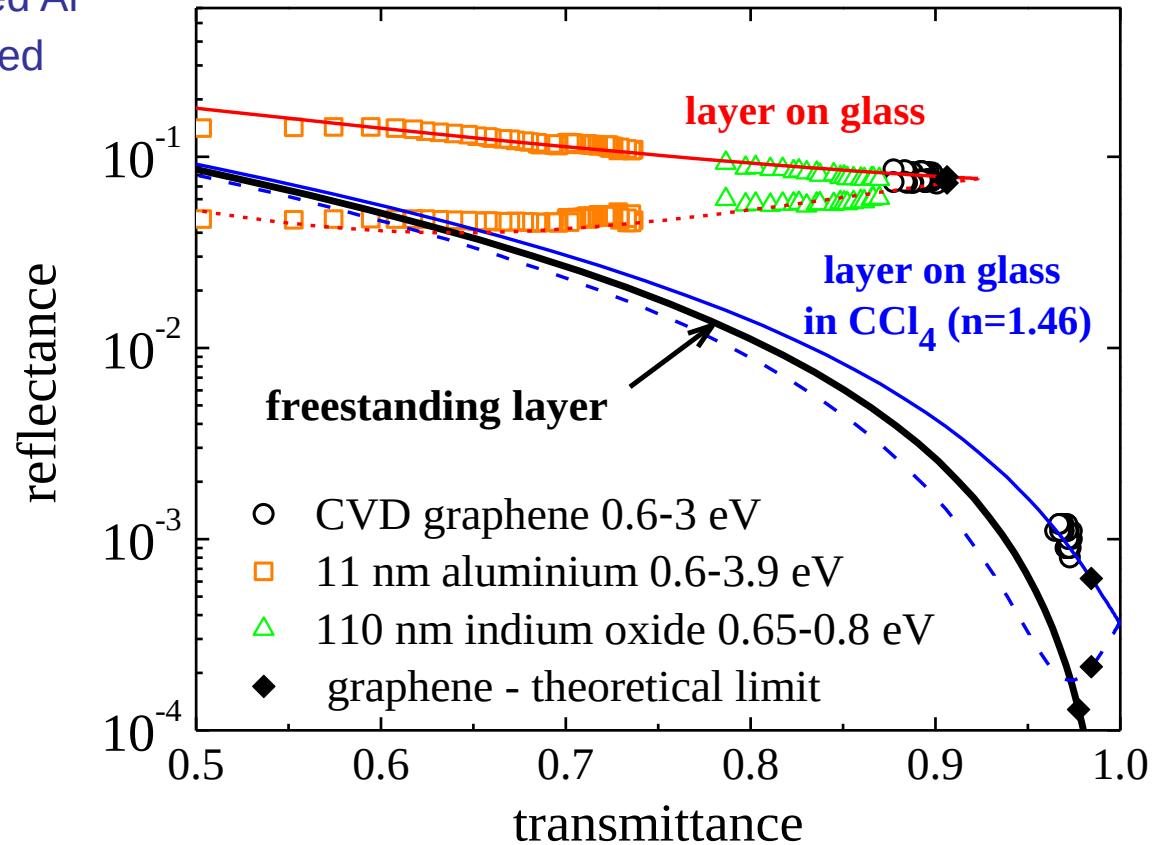
- Valid within $1\%_{\text{REL}}$ for perpendicular incidence for graphene on glass

Thin-film limit: experimental verification

- Universal relation between R and T :

- graphene
- 11 nm of evaporated Al
- doped ITO in infrared

$$R_{\text{TFL}} \approx \left(1 - \sqrt{\frac{n_0 T_{\text{TFL}}}{n_2}} \right)^2$$



Thin-film limit: consequence

- Performance of a conductive window layer

- A/T is a good parameter
- different layers with same αd

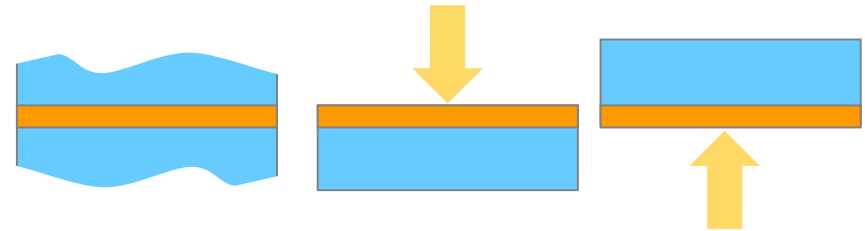
thin-film limit

$$\frac{A_{\text{TFL}}}{T_{\text{TFL}}} = \frac{\alpha d n}{n_2}$$

„thick“ film

$$\frac{A}{T} \approx \frac{e^{\alpha d} - R_2 e^{-\alpha d} - 1 + R_2}{1 - R_2}$$

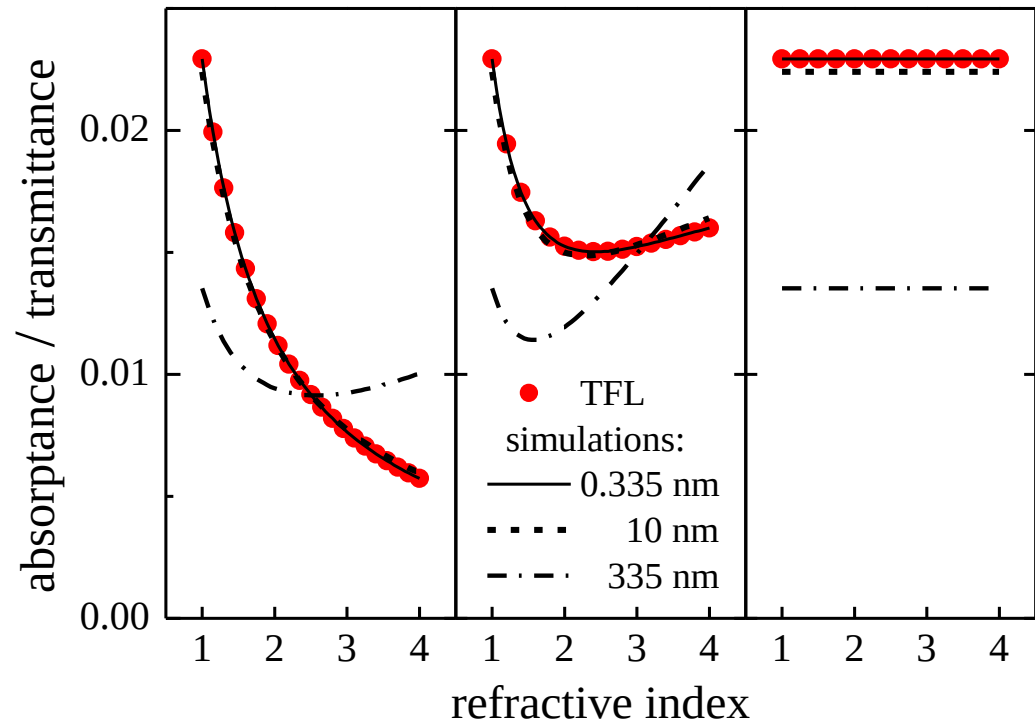
D. Ritter, K. Weiser, Optics
Commun. 57 (1986) 336–338.



embedded

substrate +

substrate –



J. Holovsky, et al., *Effect of thin-film limit on measurable properties of graphene*, in preparation

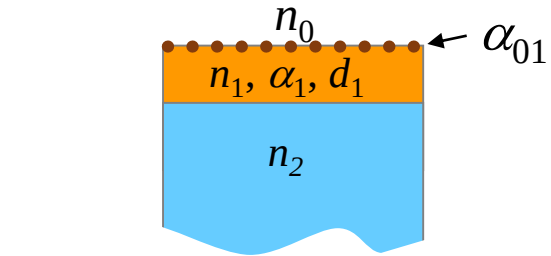
Summary II

- In the thin-film limit, all properties are given by $a \cdot d \cdot n$ product
- Absorptance can be strongly reduced by ambient refractive index
- Example of the thin-film limit: graphene on glass

Surface defects - correction

- Calculation of α_{01} for defects on top
 - after dividing by transmittance and some algebra:

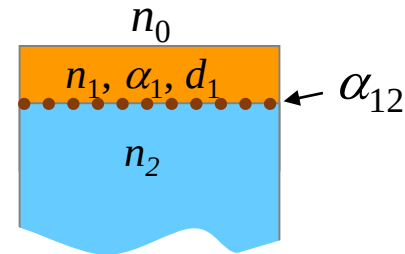
$$\underbrace{\frac{A_{\downarrow} - bA_{\uparrow}}{T_{012}}}_{\text{experiment}} \cong \alpha_{01} \underbrace{\left(\frac{|(1+r_{01})(1+r_{12}e^{2i\beta})|^2}{n_2 |t_{01}t_{12}e^{i\beta}|^2} - \frac{b}{n_0} \right)}_{\text{correction factor}} \\ \text{(calculated from uncorrected results)}$$



$$b \equiv \frac{A_{1\downarrow}}{A_{1\uparrow}} \cong \frac{(n_1^2 + n_2^2)n_0}{(n_1^2 + n_0^2)n_2}$$

- Analogically, calculation of α_{12} for defects on interface

$$\frac{A_{\downarrow} - bA_{\uparrow}}{T_{012}} \cong \alpha_{12} \left(\frac{1}{n_2} - b \frac{n_0}{n_2^2} \frac{|(1-r_{12})(1-r_{01}e^{2i\beta})|^2}{|t_{01}t_{12}e^{i\beta}|^2} \right)$$



Surface defects – correction

- Corrected spectrum A_1/T for defects on top:

$$\frac{A_{1\uparrow}}{T} \cong \frac{A_{\uparrow}}{T} - \frac{\alpha_{01}}{n_0}$$

- Analogically, corrected spectrum A_1/T for defects on interface:

$$\frac{A_{1\downarrow}}{T} \cong \frac{A_{\downarrow}}{T} - \frac{\alpha_{12}}{n_2}$$

- Absorption coefficient of bulk α is then calculated from A_1/T :

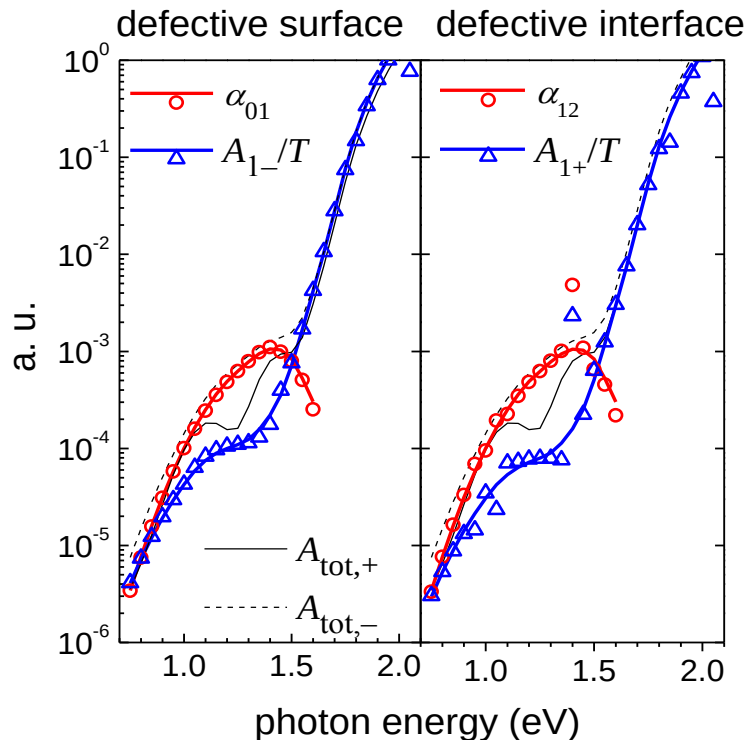
$$\alpha = \frac{1}{d} \ln \left(0.5 \left\{ (1 - R_2)(1 + A/T) + \sqrt{(1 - R_2)^2 (1 + A/T)^2 + 4R_2} \right\} \right)$$

D. Ritter, K. Weiser, Optics Commun. 57 (1986) 336–338.

Surface defects –verification

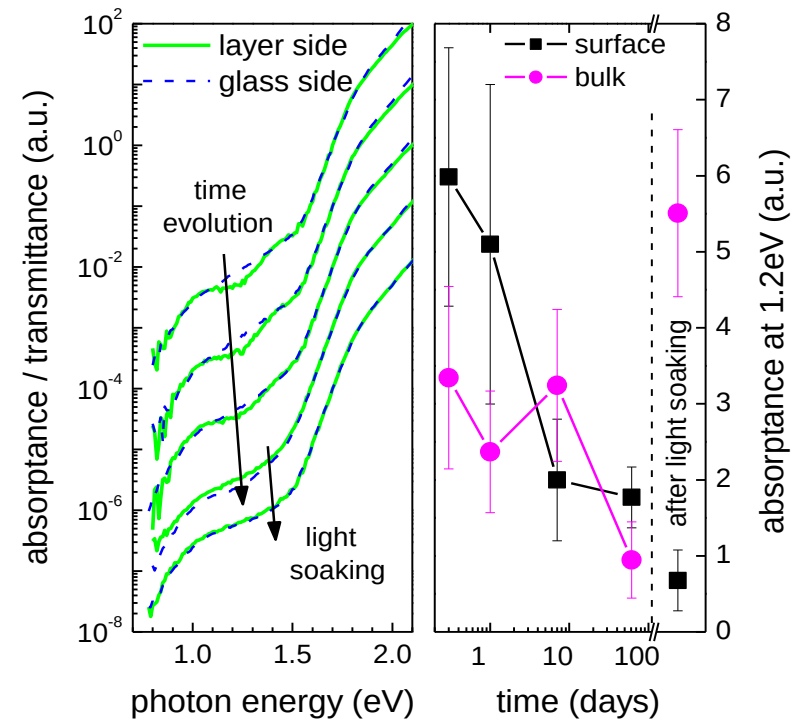
- Numerical verification

- structure: $d_1=360\text{nm}$, $n_1 = n_{\text{a-Si:H}}$
- thickness of defective layer: 3nm



- Application to measured data

- a-Si:H layer, $d_1=350\text{nm}$



- Unfortunately, the method is very sensitive to small errors

Summary III

- Explanation of interference vanishing in A/T ratio.
- Theoretical possibility to directly evaluate bulk and surface defect density separately.
- It works, but it is highly sensitive to small errors.

Acknowledgments

- 7thFP EU project „Fast-track“
- Swiss exchange program „SCIEX“