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Controlling growth rate and band-gap by combining in situ measurements and reflectance model for molecular beam epitaxy fabrication

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Motivations

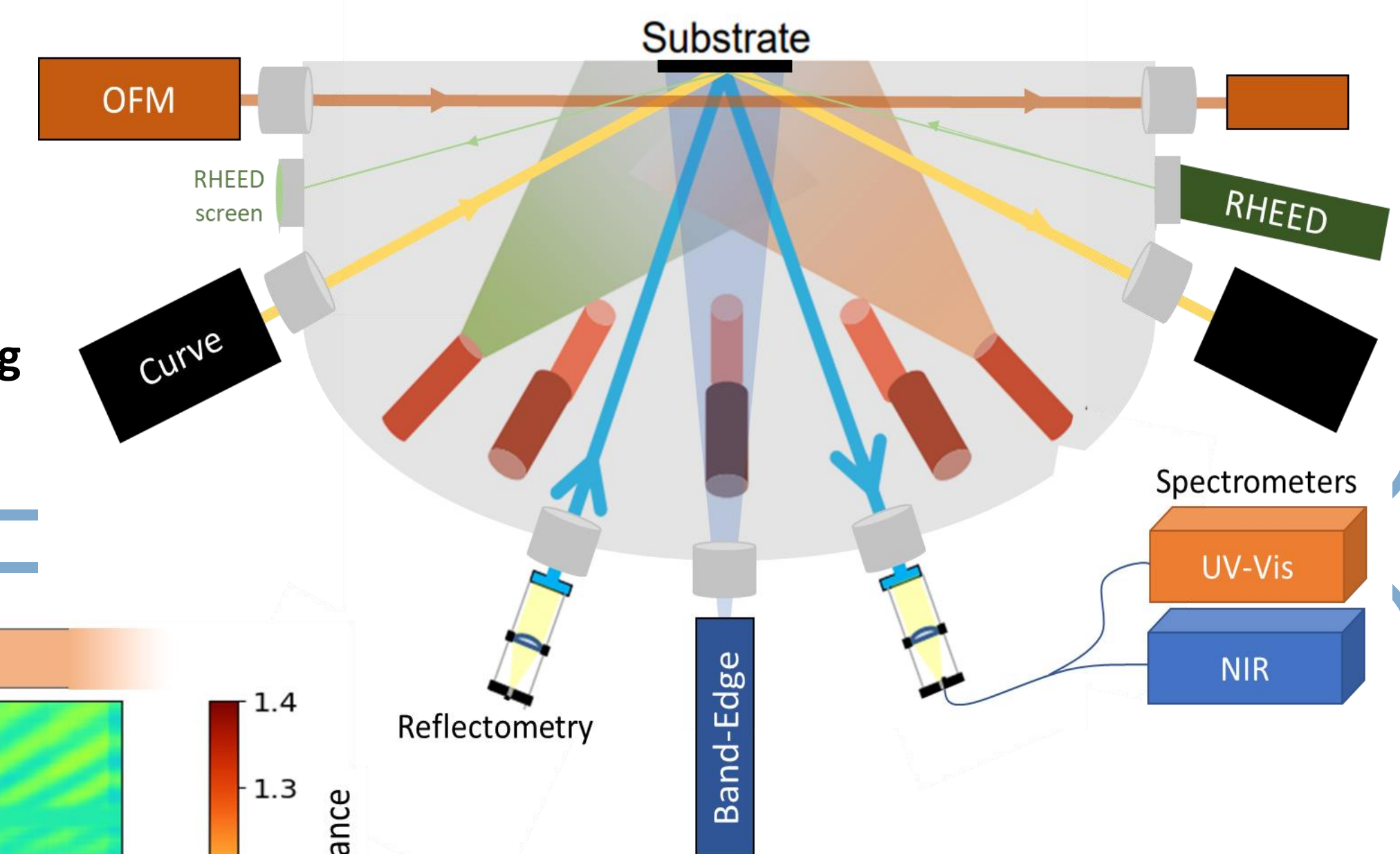
Better control over epitaxy process is a key element for the realization of high efficiency solar cells, and more generally, complex multilayer semiconductor structures. However, no universal practical tool has been implemented to date.

With EpiCentre, joint lab with Riber, we're working on combining *in-situ* measurements in molecular beam epitaxy (MBE) to achieve advanced materials growth control in real time.

In-situ tools:

- Reflection high-energy electron diffraction (RHEED)
- Optical flux monitoring (OFM)
- Spectroscopic reflectometry
- Curvature measurement
- Band-edge measurement

- ✓ Surface morphology
 - ✓ Cells fluxes
 - ✓ Growth rates
 - ✓ Compositions
 - ✓ Substrate temperature
- Feed-back control
Optical constants
Band-gap, Doping



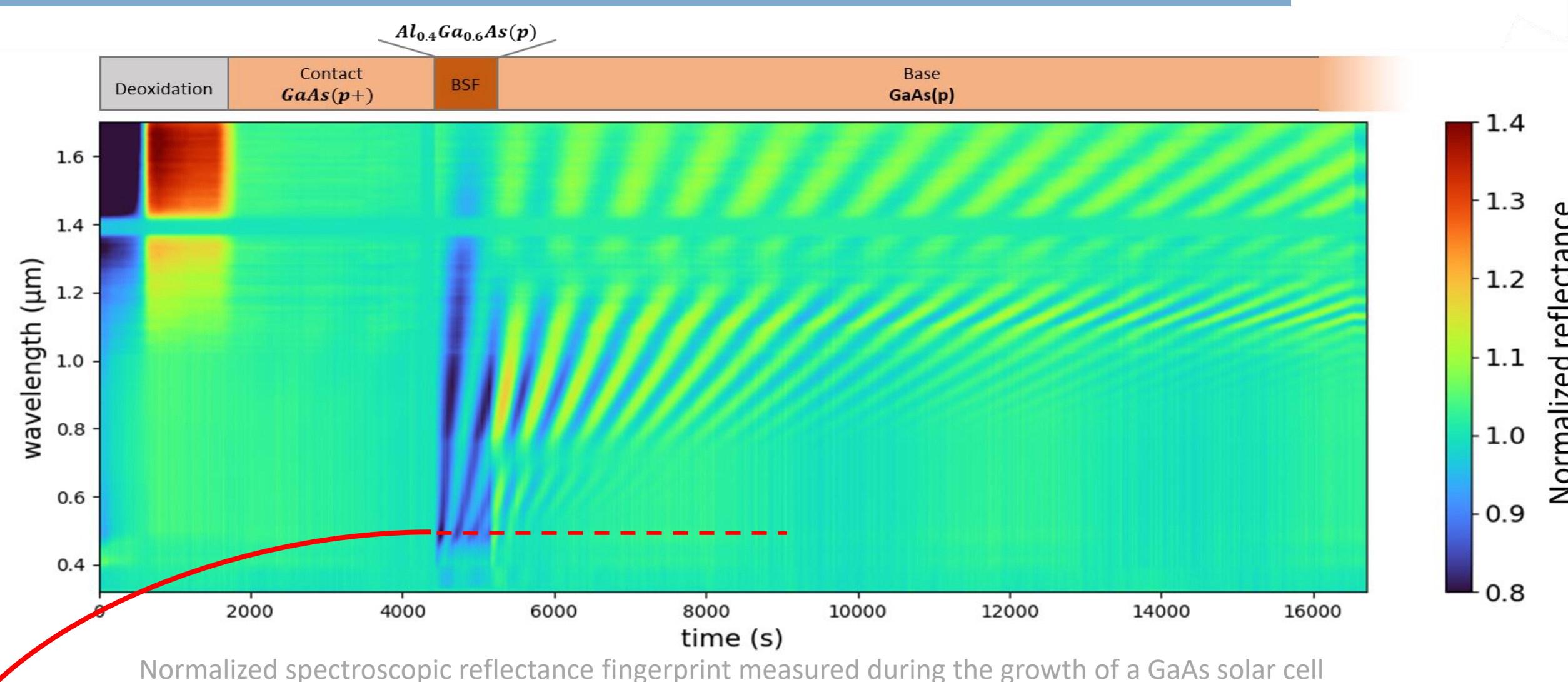
In-situ spectroscopic reflectance

Goal: Deduce layer thickness from spectroscopic reflectance measurement

Problem: Reflectance response depend on multiple parameters

- Optical indices dispersion
 - Temperature
 - Composition (alloy and doping)
- Thickness of the layer

How to separate those contributions to deduce materials parameters in real time ?



Model Fitting

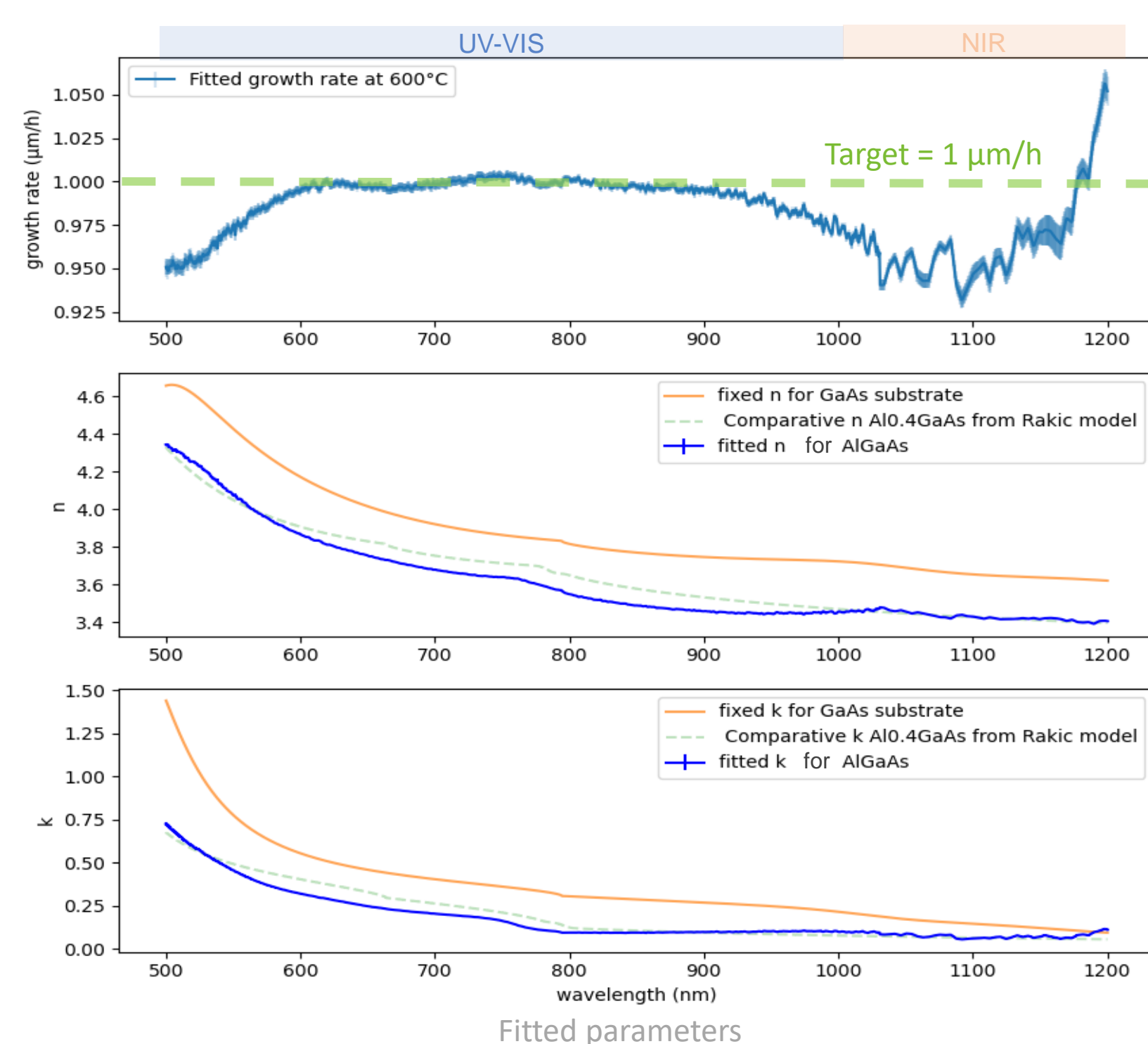
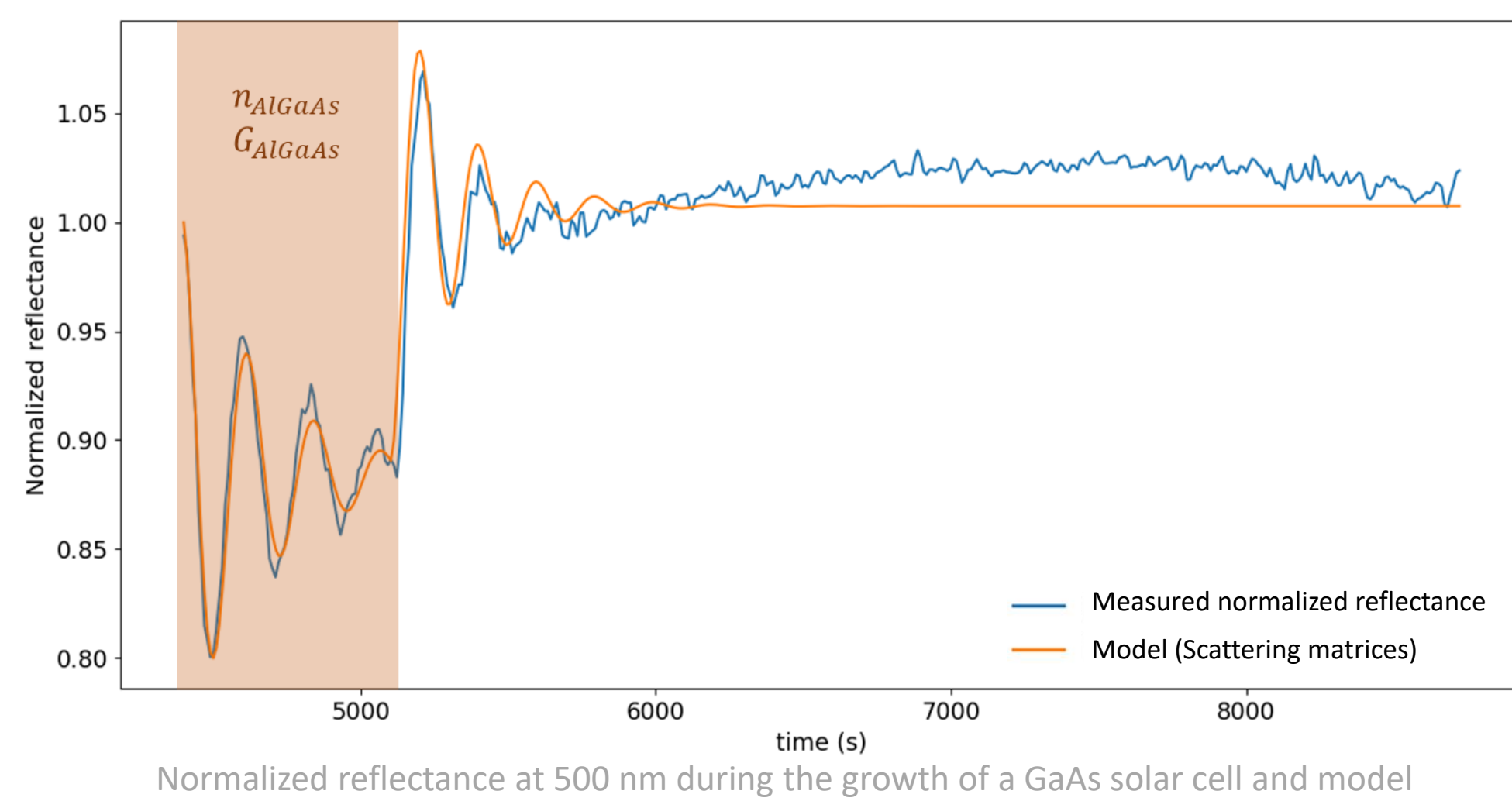
Fitting over one wavelength:

- Virtual substrate model [1]

$$r(t) = \frac{r_{\infty} + r_1 e^{-i4\pi \frac{NGt}{\lambda}}}{1 + r_2 e^{-i4\pi \frac{NGt}{\lambda}}}$$

Fitted results :

- Optical indices, n_{AlGaAs}
- Growth rate, G_{AlGaAs}



Repeat over wavelength range:

- Optical indices dispersion with wavelength

Problems:

- Substrate hypothesis: fitting results are really dependent on the optical indices model for substrate
- $$n_{substrate} = f(T, doping)$$

➔ Experimental measurement

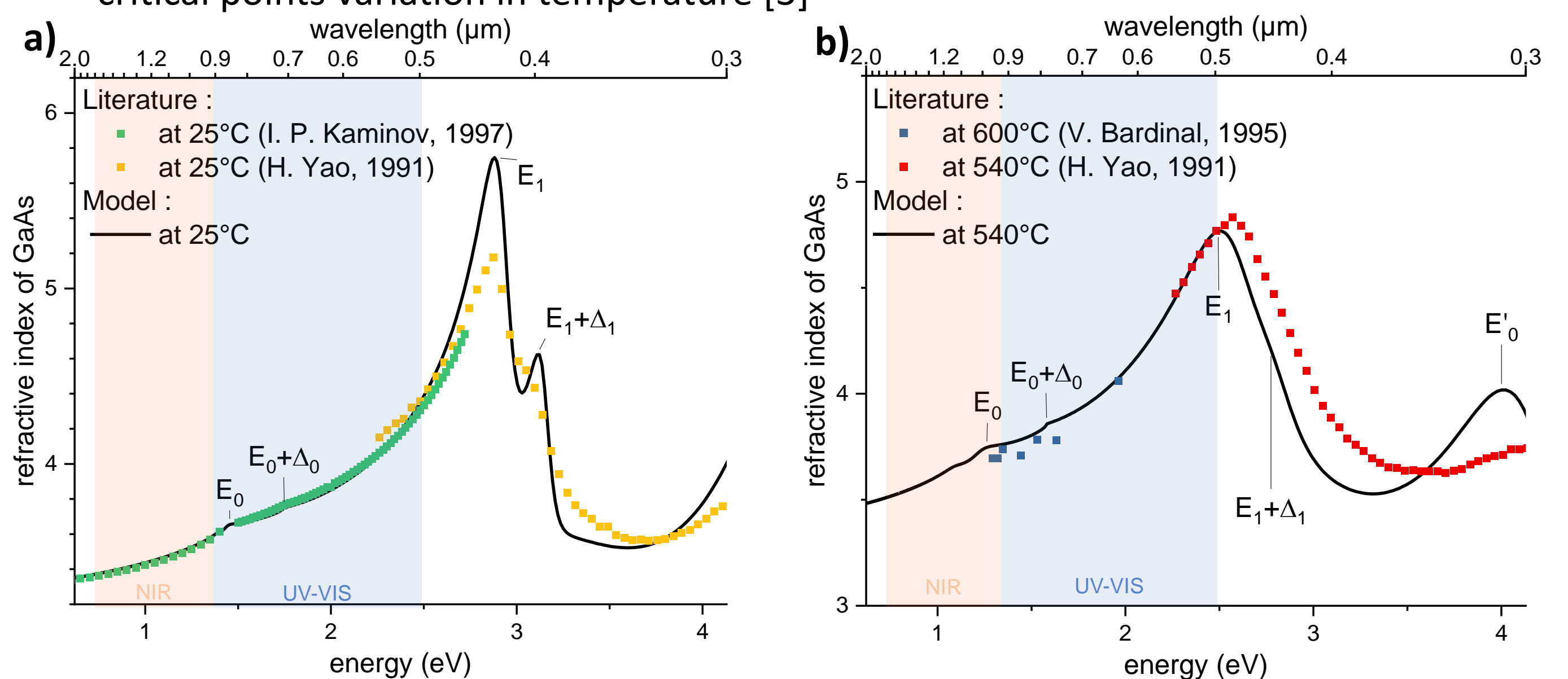
- Fitting requires growth of thick layer:

$$d_{layer} > \frac{\lambda}{2n} \quad (1 \text{ period})$$

High temperature $Al_xGa_{1-x}As$ optical indices

Theoretical model for GaAs based on literature:

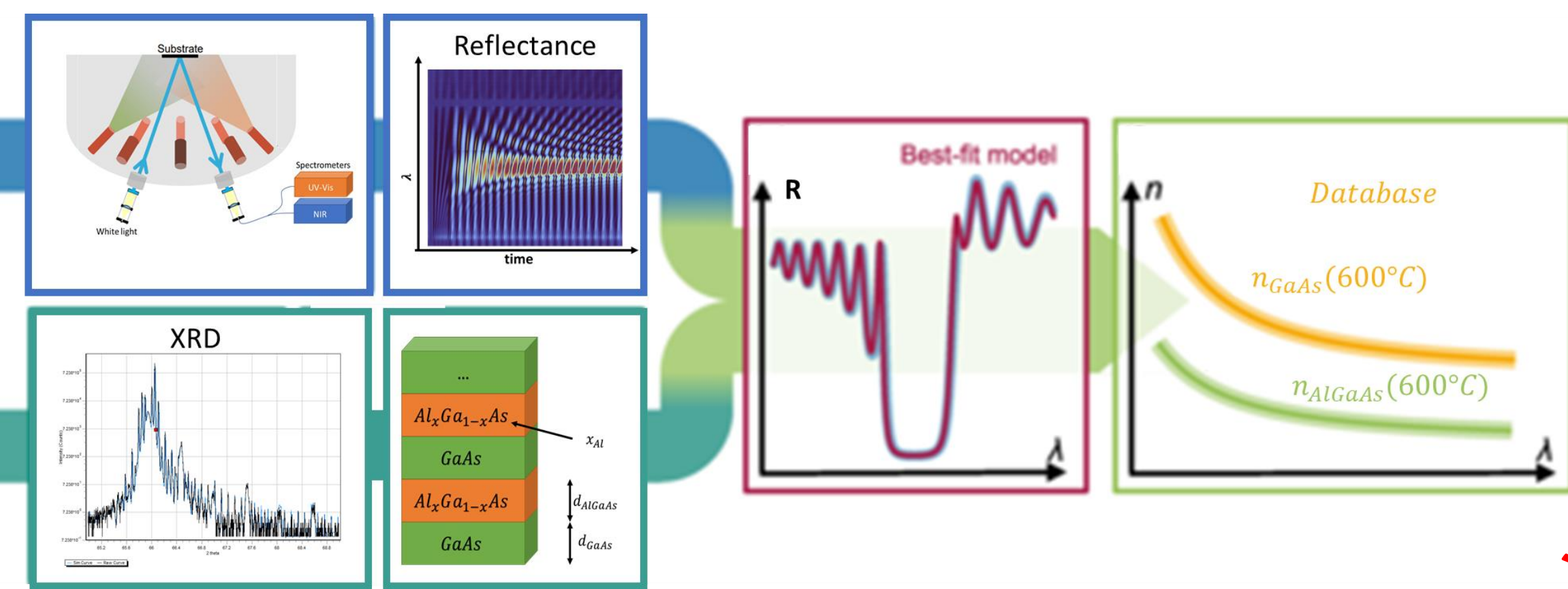
- Rakić's model [2]
- critical points variation in temperature [3]



Optical indices dispersion of GaAs computed with our model at a) 25°C and b) 540°C, compared to measurements from literature.

Experimental:

Using fitting model complemented with ex-situ thickness measurement (XRD), we extract optical indices at growth temperature that we use to refine our n, k model.



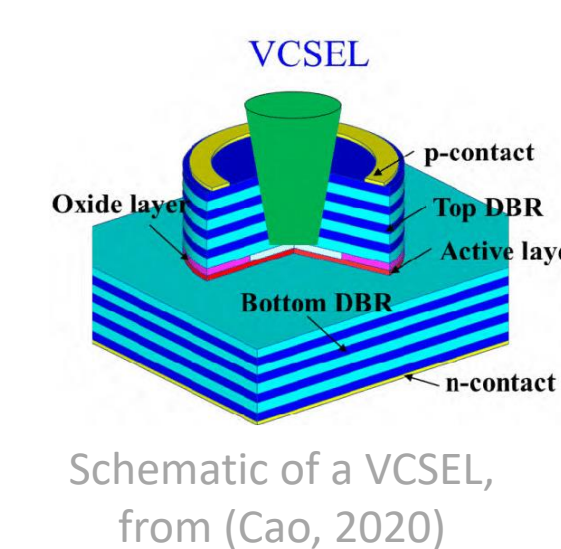
Proposed experimental plan to measure optical indices at high temperature in our MBE reactor. Inspired by (Perner et al., 2023)

Work In Progress

Perspectives

- Combining in-situ measurements:
 - Using $n(\lambda, T)$ database to deduce growth rate from reflectance measurement
 - With in-situ curvature measurement to extract alloy composition

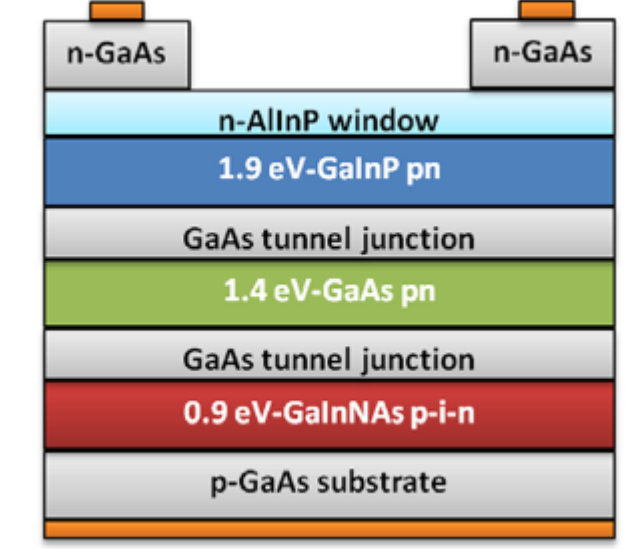
Feed-back control on the process parameters for complex multilayers (VCSEL)



Schematic of a VCSEL, from (Cao, 2020)

- Development of in-situ curvature measurement and applications:
 - Auto-matching: composition control of alloy for lattice match applications

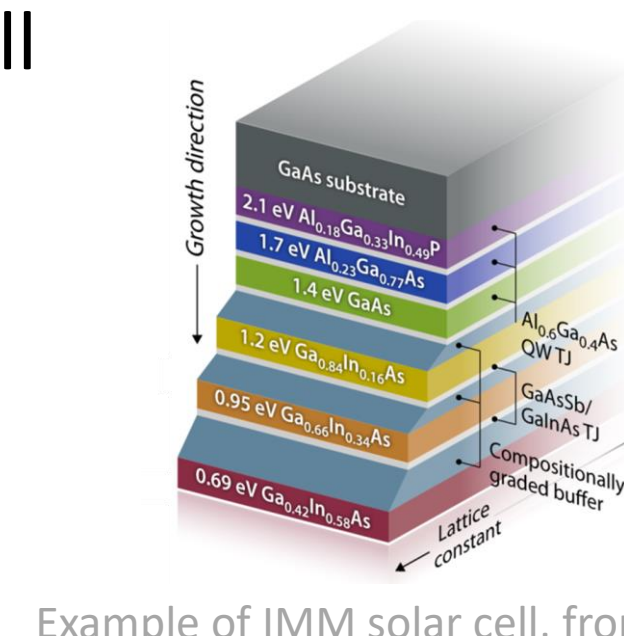
Development of $InGaAsN$ material for solar cell for spatial applications [4,5]



Schematic of 3 junctions solar cell with $InGaAsN$ sub-cell lattice matched on GaAs, from [5]

- Strain monitoring during the growth of metamorphic heterostructures

Inverted metamorphic multijunction [6]



Example of IMM solar cell, from [10]

More informations



References:

- [1] W. G. Breiland et K. P. Killeen, « A virtual interface method for extracting growth rates and high temperature optical constants from thin semiconductor films using *in situ* normal incidence reflectance », *Journal of Applied Physics*, vol. 78, n° 11, p. 6726-6736, déc. 1995, doi: [10.1063/1.360496](https://doi.org/10.1063/1.360496).
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- [4] M. Levillayer et al., « As-Grown InGaAsN Subcells for Multijunction Solar Cells by Molecular Beam Epitaxy », *IEEE Journal of Photovoltaics*, vol. 11, n° 5, p. 1271, 2021, doi: [10.1109/JPHOTOV.2021.3093048](https://doi.org/10.1109/JPHOTOV.2021.3093048).
- [5] A. Aho et al., « Composition dependent growth dynamics in molecular beam epitaxy of GaInAs solar cells », *Solar Energy Materials and Solar Cells*, vol. 124, p. 150-158, mai 2014, doi: [10.1016/j.solmat.2014.01.044](https://doi.org/10.1016/j.solmat.2014.01.044).
- [6] J. F. Geisz et al., « Six-junction III-V solar cells with 47.1% conversion efficiency under 143 Suns concentration », *Nat Energy*, vol. 5, n° 4, p. 326-335, avr. 2020, doi: [10.1038/s41560-020-0598-5](https://doi.org/10.1038/s41560-020-0598-5).