Optical metrology for energy production

Dr. Nasim Rezaei
Material modelling scientist
Company presentation

Outline

- Motivation
  - Scope, financial aspects

- Who are we?
  - History, markets, approach

- Light ↔ Electricity
  - LEDs, Solar cells and transistors

- Reflectometry, deflectometry and pyrometry

- Case studies

- Conclusions

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Interesting fact, 1: solid-state lighting

Electricity production 2010

<table>
<thead>
<tr>
<th>Lighting</th>
<th>Rest</th>
</tr>
</thead>
<tbody>
<tr>
<td>19</td>
<td>81</td>
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→ 2651 TWh

Electricity production 2021

<table>
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<tr>
<th>Lighting</th>
<th>Rest</th>
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<tr>
<td>16.5</td>
<td>83.5</td>
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→ 2900 TWh

Solid-state lighting (SSL)

Thanks to the increase in efficiency and yield of SSL:

For 800 lm

- Incandescent lamp: 60 W
- LED: 7-10 W

The rebound effect? Not there yet 😊

** https://www.takethreelighting.com/lumen-watt-comparison.html
Interesting fact, 1

Lighting is not neutral in terms of human health → Wavelength matters!

- Filtering harmful wavelengths
- Specific applications, e.g. UV for medical use
- Uniformity

[*] IEA, Global residential lighting sales share by technology in the Net Zero Scenario, 2010-2030, IEA, Paris

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Interesting fact, 2: Photovoltaic technology

PV plays a major role in energy transition
- Consistent costs, technical performance and accessibility
- Faster permitting procedures

Interesting fact, 2: Thin-film PV

~%5 of the PV market is covered by thin-film solar cells *

* Fraunhofer ISE: Photovoltaics Report, updated: 21 February 2023
Interesting fact 2: Future of thin-film PV

Perovskites are expected to change the equation soon!

- Only affordable PV technology proven to surpass Si efficiency
- Si hitting physical limits
- Tandem production lines can be added to the existing Si lines


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Interesting fact, 2

Economic value of metrology: Example thin film solar cells (simplified)

[1] Up to absorber:
- $\approx 38\%$ of total cost
- $\approx 7.6$ M€ / year
- 95% efficient

[2] From absorber to flasher:
- $\approx 23\%$ of total cost
- $\approx 4.6$ M€ / year
- 100% efficient

1. Late detection $\rightarrow$ 380,000 €/year
   + 230,000 €/year loss

2. Early detection $\rightarrow$ 380,000 €/year loss $\rightarrow$ +Investment cost = 100,000 €

230% return of investment after one year

* Zentrum für Sonnenenergie- und Wasserstoff-Forschung (ZSW), www.zsw-bw.de
** K. A. W. Horowitz et al., NREL/PR-6A20-64507, 2015
The importance of in-situ metrology

On the road to higher performance, higher yield and lower cost ...

→ Metrology helps you to understand – metrology can be your dictionary!

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- Reflectometry, deflectometry and pyrometry

- Case studies

- Conclusions
Metrology company founded 1999 in Berlin

- 24 years old
- 85 employees
- >3500 systems sold
- Spin-off of TU Berlin
- Operating worldwide
- Member of Nynomic group

Our business: Process-integrated optical metrology
Our markets: Semiconductor and thin-film industry & academia incl. lighting, laser, PV, glass coating …
Company overview

Integrated metrology for various industries and markets

Laser

LED

Functional glass

Power devices

Photovoltaics

MEMBER OF THE NYNOMIC GROUP

Image credits: see last slide
Company presentation

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Light ⇔ Electricity in simple words

Solar cells

Front contact

- n-type

- p-type

- Back contact

LEDs

(in)visible photon

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Light ↔ Electricity in simple words

Insulated gate bipolar transistors (IGBT)


What needs to be taken care of...

CIGS solar cell [*]

Deep UV LED[**]

- Composition
- Temperature
- Curvature and strain
- Surface roughness

~50 + 200 nm

~50 nm

< 2.5 μm

~500 μm

p-GaN cap
p-AlGaN SPSEL
p-AlGaN EBL

(In)AlGaN MQWs

n-AlGaN

$Al_xGa_{1-x}N$ transition

AlN base

substrate

* Zentrum für Sonnenenergie- und Wasserstoff-Forschung (ZSW), www.zsw-bw.de
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Reflectometry

- **Interference is:**
  - Constructive at $2nd_1 = m\lambda$
  - Destructive at $2nd_1 = (m+1/2)\lambda$

- $$r = \frac{r_{01} + r_{12}e^{-2i\beta}}{1 - r_{10}r_{12}e^{-2i\beta}}$$ where $$\beta = 2\pi \frac{d_1}{\lambda} n_1 \cos \varphi_1$$

- **Reflectance**, $R = |r|^2$

- **Light source**
  - White light
  - Monochromatic

- **Fabry-Perot oscillations**
  - Spectral
  - Temporal (growth oscillations)
Reflectometry

- Fabry-Perot oscillations
  - Temporal (growth oscillations)
- Information on film thickness (growth rate) and refractive index

3 parameters:

- \( R \) level \( \rightarrow \) refractive index \( n \& k \)
- damping \( \rightarrow \) ext. coefficient \( k \)
- frequency \( \rightarrow \) growth rate \( r \)

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Deflectometry: curvature basics

concave
upwards
positive curvature

convex
downwards
negative curvature
Deflectometry: curvature basics

Concave

Flat

Convex
Why does it happen?

- Uneven temperature
- Lattice mismatch
- Thermal expansion mismatch
Curvature parameters and implications

Curvature \( k = \frac{1}{R} \)
Curvature parameters and implications

Curvature $k = 0.1 \, \text{[km}^{-1}]$

- $R = 10000 \, \text{m}$
- $W = 2''$
- $\delta = 0.0323 \, \mu \text{m}$
Curvature parameters and implications

Curvature $k = 0.1 \text{ km}^{-1}$

- $R = 10000 \text{ m}$
- $W = 4''$
- $\delta = 0.129 \mu\text{m}$
Curvature parameters and implications

- Curvature $k = 100 \text{ [km}^{-1}]$

- Why does it matter?
  - Temperature uniformity $\rightarrow$ performance uniformity
  - Avoid cracking
  - Avoid complications further down the chain, e.g. in lithography

![Diagram showing curvature parameters](image-url)

- $R = 10 \text{ m}$
- $W = 2''$
- $\delta = 32.3 \text{ [\mu m]}$
Deflectometry

- Incident beam
- Reflected beam

- Concave
- Flat
- Convex

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Deflectometry: Aspherical bowing

- Spherical
- Parabolic
- Hyperbolic
Solution: 3-point measurement
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Pyrometry: how does it work?

Plank’s equation for black body*:

\[ I = \frac{2}{h^4 c^3} \cdot \frac{(\hbar \omega)^5}{e^{\frac{\hbar \omega}{k_B T}} - 1} \]

Normal materials:

\[ I = \varepsilon \cdot \frac{2}{h^4 c^3} \cdot \frac{(\hbar \omega)^5}{e^{\frac{\hbar \omega}{k_B T}} - 1} \]

Pyrometry: why 950 nm?

- Epitaxy deals with **surface** chemistry.
- Lower photon energies $\rightarrow$ transparency regime $\rightarrow$ susceptor temperature.
- Higher energies $\rightarrow$ not enough intensity
- 950 nm best choice for most applications
- For transparent substrates (SiC), even shorter wavelength is used.
Pyrometry: emissivity correction

- Conservation of energy
  - $\alpha + r + t = 1$
  - Opaque semiconductor: $\alpha + r = 1$

- Kirchhoff’s law: $\alpha (\lambda, T) = \varepsilon (\lambda, T) \Rightarrow \varepsilon = 1 - r$

![Graph showing reflectance and pyrometry at 950nm](image)

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in-situ metrology for MOCVD of UV-LED structures

Schematic layer stack of UV-LED

- p-contact layer
- polarization doping layer
- electron blocking layer
- triple quantum well
- n-contact layer
- base layer
- substrate

In-situ data

Growth time
In-situ data of 230 nm UV LED (wafer #1, center)

- Heating | AlN Buffer | n-AlGaN layer | active zone | AlGaN HIL | GaN | Cooling

- Reflectance 365nm
- Reflectance 405nm
- Reflectance 633nm
- Reflectance 950nm

- In-situ data: a treasure trove of information about each layer and each wafer

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Feed-back control of pocket temperature

Run A and B (identical recipe):
①: Same heater temperature
②: Correcting for difference: lowering process temperature in Run B
③: Same pocket temperature established as in Run A

Same effect in 2nd half of run

Heater temperature
Pocket temperature

Run A
Run B
Feed-back control of pocket temperature

Run A and B (identical recipe):

①: Same heater temperature

Run B shows higher pocket temperature

②: Correcting for difference: lowering process temperature in Run B
Feed-back control of pocket temperature

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Feed-back control of pocket temperature

Run A and B (identical recipe):
①: Same heater temperature
Run B shows higher pocket temperature
②: Correcting for difference: lowering process temperature in Run B
③: Same pocket temperature established as in Run A
Same effect in 2nd half of run
Two runs with comparable recipe and similar looking in-situ data

But different template \(\rightarrow\) significantly different strain development during AlN growth

Result: Strong difference in wafer curvature during growth of MQW
Uniformity of LED emission can already be predicted

In-situ curvature measurement

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In-situ curvature measurement

Electroluminescence maps

Wafer A

Far-UVC LED on HTA-AlN/Sapphire template

Longer emission $\lambda$ in center

$\kappa_{AZ} = -96 \, \text{km}^{-1}$

Peak wavelength [nm]

- 231
- 231.4
- 231.8
- 232.2
- 231.6
- 233
- 233.4
- 231.8
- 234.2

Wafer B

Far-UVC LED on MOVPE-AlN/Sapphire template

Shorter emission $\lambda$ in center

$\kappa_{AZ} = 97 \, \text{km}^{-1}$
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- **Case study 2, solar cells**

- **Conclusions**
Metrology for high-efficiency photovoltaics: perovskite formation
Metrology for high-efficiency photovoltaics: perovskite formation

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Metrology for high-efficiency photovoltaics: perovskite formation

... during spin-coating

3CAT, Triple Cation Complex; Spin Coating @ 4000 RPM; 180s
Metrology for high-efficiency photovoltaics: perovskite formation

Spin-coating

3CAT, Triple Cation Complex; Spin Coating @ 4000RPM; 180s

Initial absorption edge of solution

Precursor solution at rest

Vanishing of interferences due to full consumption of solution.

Perovskite surface too rough for constructive interference

Onset of rotation

Shift of absorption edge during spin coating of precursor solution

C. Camus et al., Proceedings of the 47th IEEE PVSC, 2020
Metrology for high-efficiency photovoltaics: perovskite formation

Annealing

Band gap shifts from ~450nm to 725 during annealing.
Metrology for high-efficiency photovoltaics: CIGS bandgap

Approximated onset of absorption ≈ effective band gap determined by CIGS composition

Transient @ \( \lambda = 1050 \) nm

Spectrum @ \( t = 1750 \) sec

Approximated onset of absorption ≈ effective band gap determined by CIGS composition
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Interpreting etching as “inverted epitaxy”
End point detection possible using interface signatures.
Etching monitoring: GaN/Si HEMT (high electron mobility transistor)

- Atomic layer etching into AlGaN layer
- Target (remaining) thickness: 5, 10 and 15 nm

Typical (simplified) GaN/Si HEMT layer structure:
- GaN cap or p-GaN
- AlGaN
- AlN interlayer
- GaN epitaxial
- GaN buffer
  GaN/AlGaN thin interlayers and/or SL for strain-engineering and defect reduction
- Silicon substrate

Target (remaining) thickness: 5, 10 and 15 nm
Etching monitoring: GaN/Si HEMT (high electron mobility transistor)

8 ALE runs with different target thicknesses

- Target = 5nm
- Target = 10nm
- Target = 15nm

Fully removed AlGaN layer

TEM
- ex-situ
- destructive

K. Haberland et al.; Photonics West conference (2023)
Conclusions

- Integrated optical metrology, indispensable for high-yield energy production.
- Reflectometry for refractive index, growth/etch rate, etc.
- Deflectometry for wafer bowing quantification.
- Pyrometry for in-situ temperature control.
Thank you!

Knowledge is key

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Figure 4: Results of rebound effect on the average US-household annual electricity use for lighting. Original data from [HIC-15] modified by G. Zissis.

Figure 4 shows the impact of the rebound effect under 2 scenarios – Scenario 1: Individual households don’t use more light as the cost of lighting decreases but population growth and increasing in housing size over time result in increase of energy demand for lighting; Scenario 2: Energy use increases over time because individual households demand more light as the cost of lighting decreases and lit areas increase as a result of population and housing area growths. Both scenarios show that the LED “effect” will vanish somewhere in between 2065 and 2070. This is not acceptable; solutions are then necessary to solve the issue. One potential solution consists on switching to smart human-centric lighting driven by both “application efficiency” and quality of light. This just means that next gen lighting systems should provide the “Right Light” with the best efficiency and quality, when and where it is needed.