Investigation of hydrogenated silicon nitride thin films

Report on Phd activity of 2019/2020-1 semester

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Motivation

Microtechnology, solar cells

(PE)CVD method

Si_3N_4:H thin films

Tunable optical properties

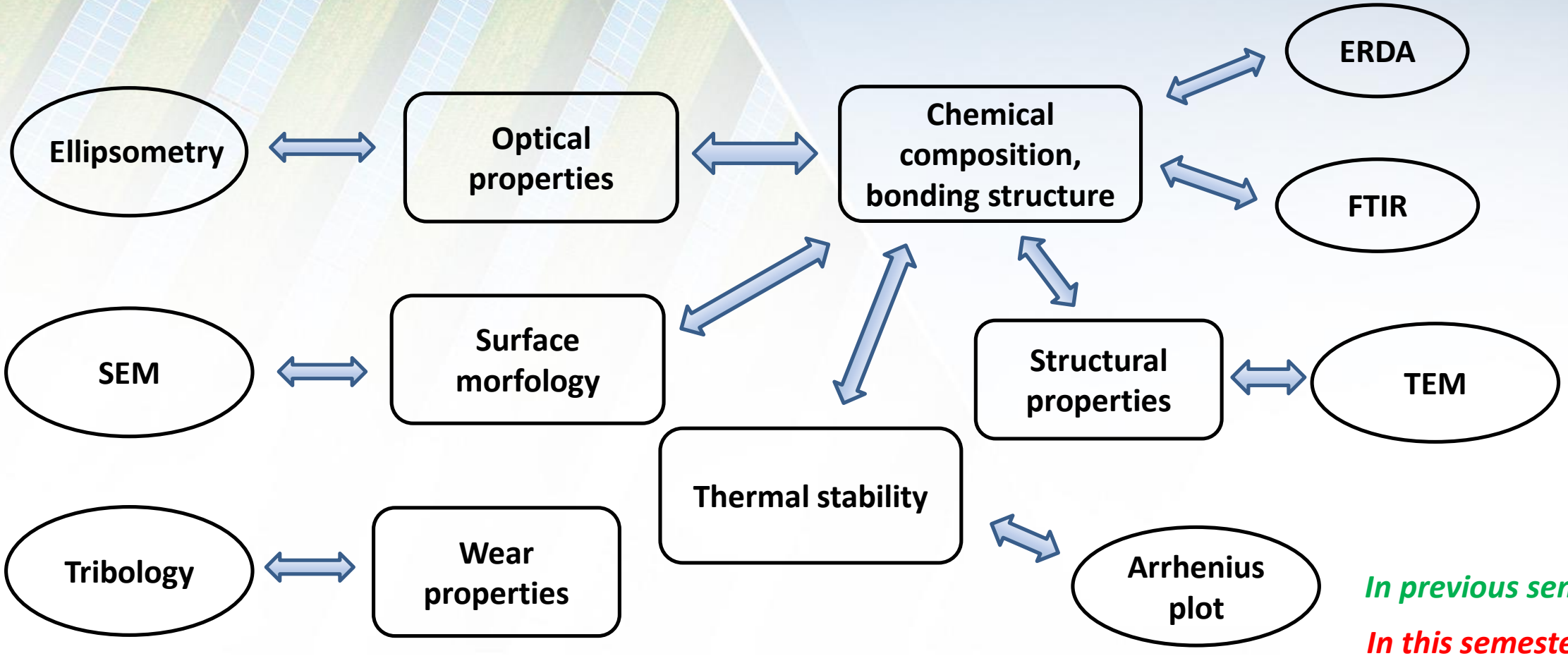
Antireflection effect

Good surface passivation effect

Radio Frequency (RF) sputtering as alternative method

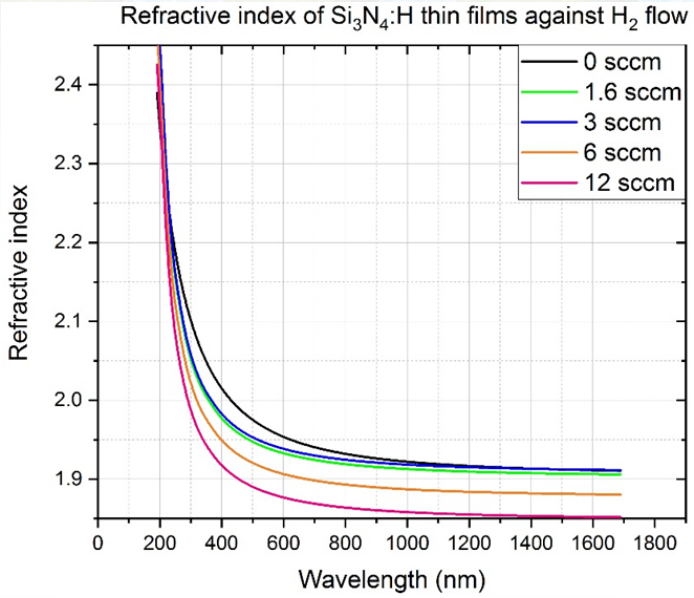
- Cost saving method
- Easy to scale up
- Low deposition temperature
- Avoid of toxic gases

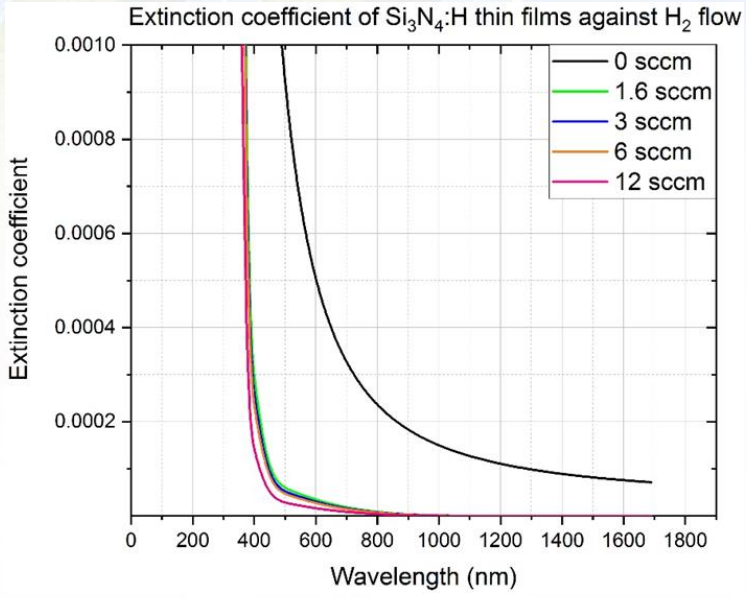
Overview of performed measurements



Previous results 1/2

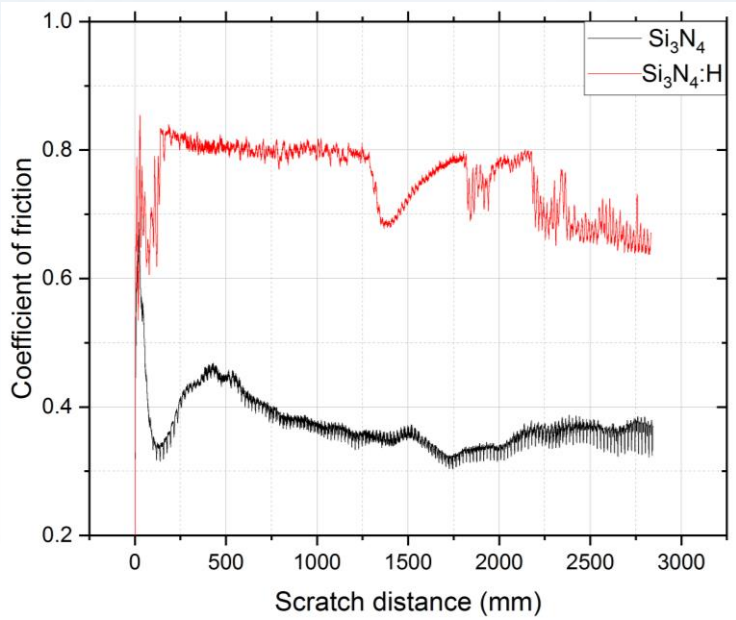
Optical properties





Refractive index and extinction coefficient are decreased while hydrogen flow is increased

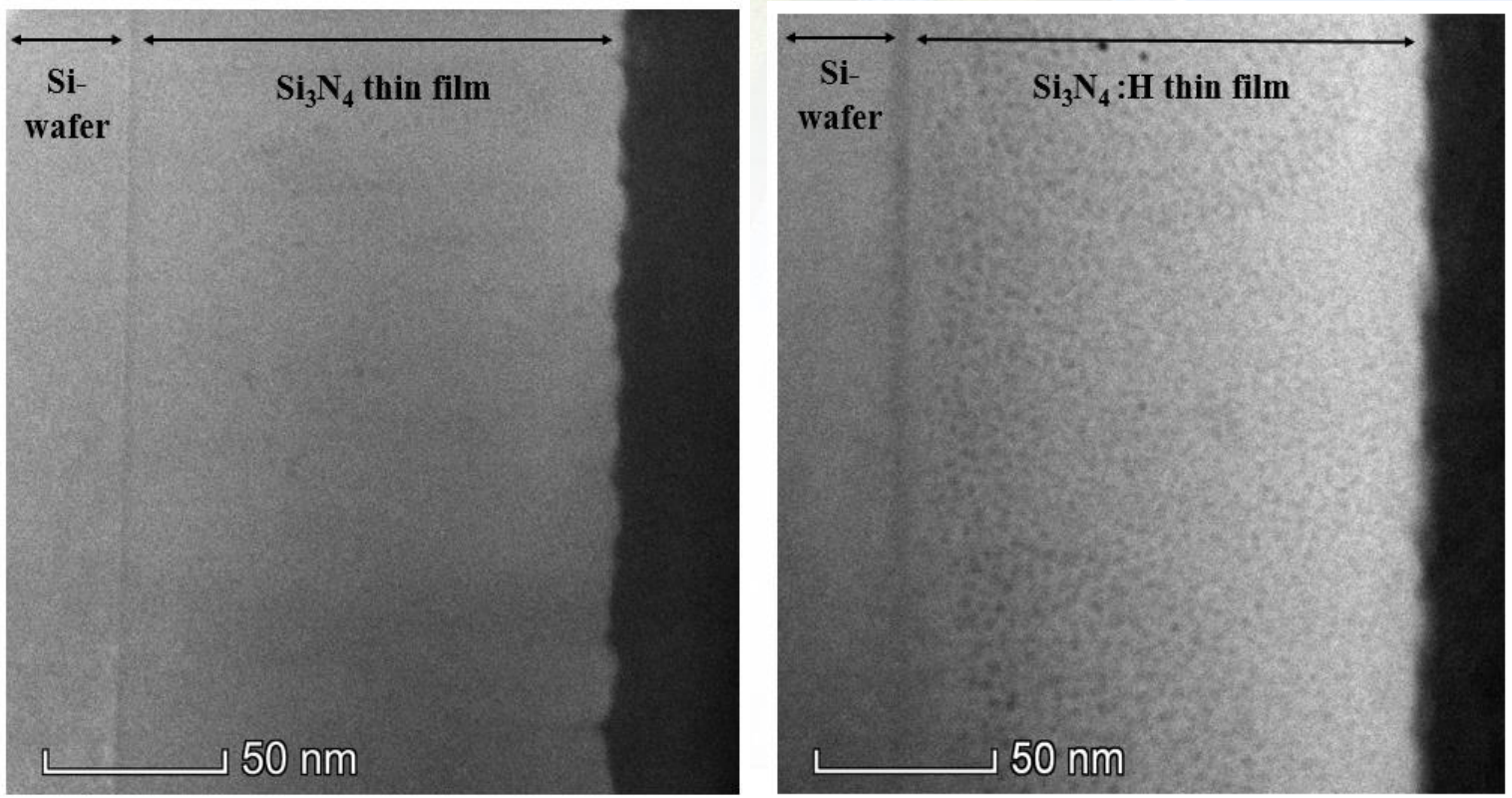
Wear properties



Presence of hydrogen increases the coefficient of friction of the thin film

Previous results 2/2

Structural properties – TEM HAADF pictures

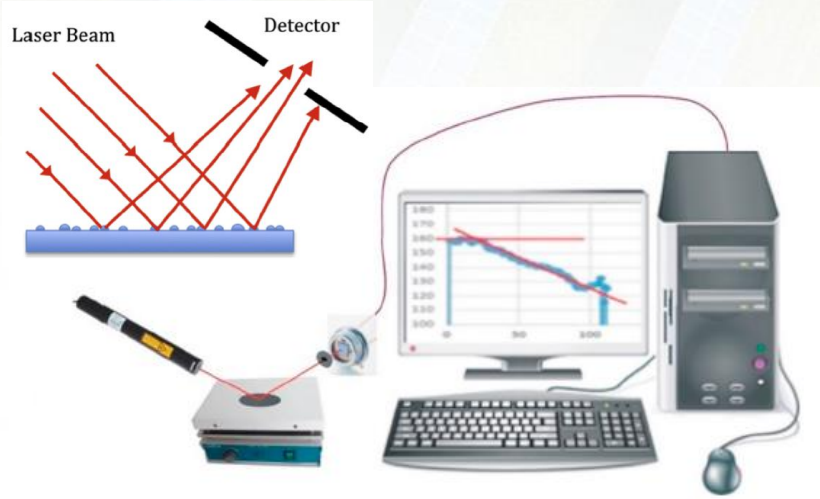


The films are amorphous, no crystalline phase is visible

Hydrogenated layer (right) is more porous then hydrogen free one (left)

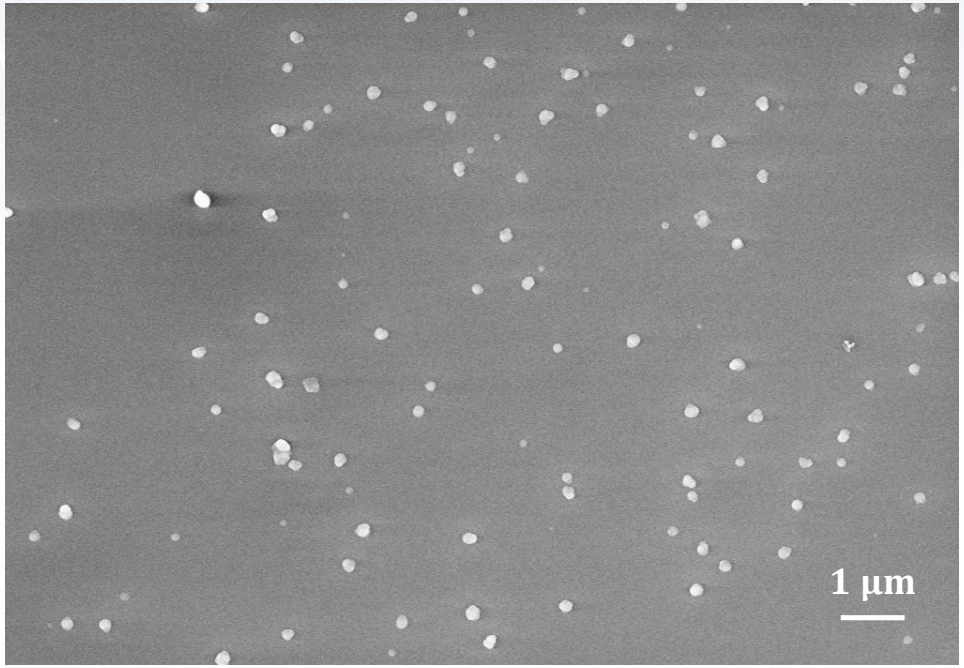
Annealing

H_2 release from Si_3N_4:H thin films upon annealing

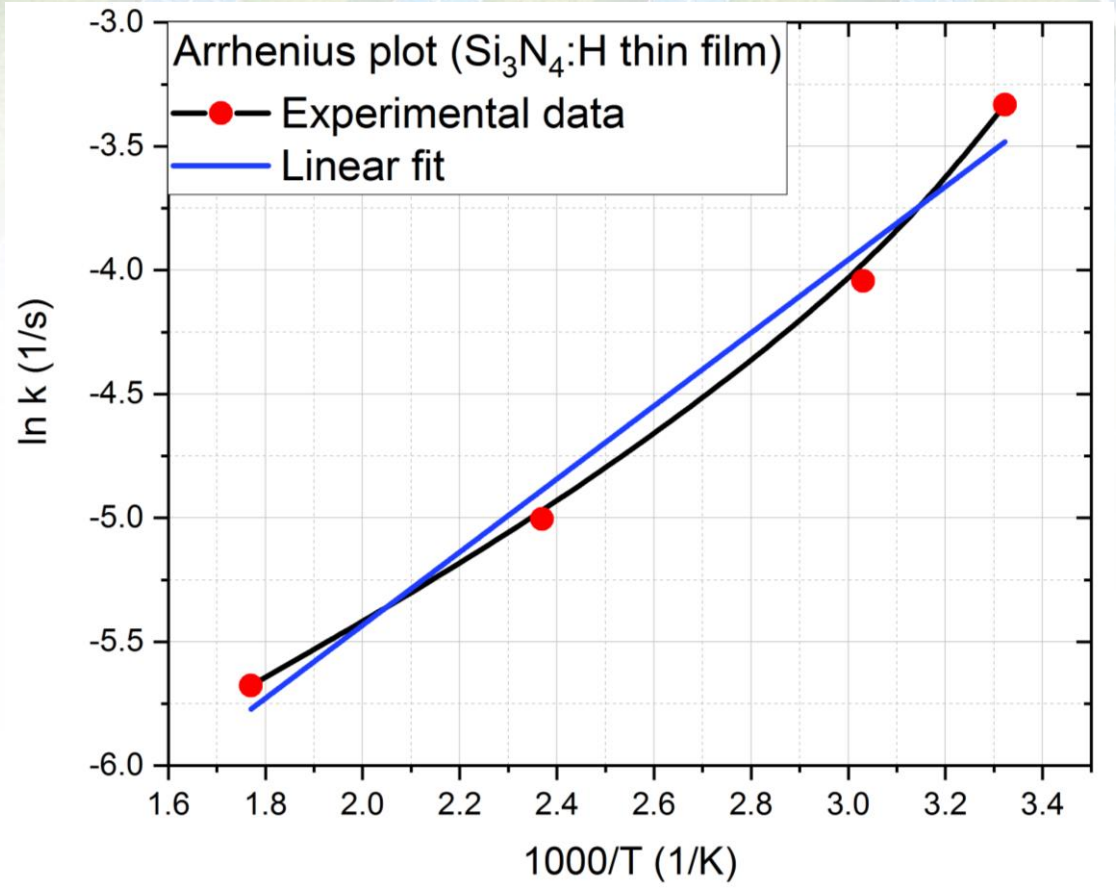


Optical method for detemining the onset of the phenomena

SEM picture of surface of annealed Si_3N_4:H thin film



Arrhenius-method



Arrhenius-equation

$$\underbrace{k = A \cdot e^{-\frac{E_a}{RT}} \qquad k = \frac{1}{t}}$$

$$ln\frac{1}{t} = lnA - \frac{E_a}{RT}$$

$$\boldsymbol{E_a \approx 12.26\ \frac{kJ}{mol}}$$

k: rate constant

A: pre exponential factor

R: universal gas constant

T: abolute temperature

t: ellapsed time

Ea: activation energy

Bond dissociation energies:

$H - N$: 314 $\frac{kJ}{mol}$

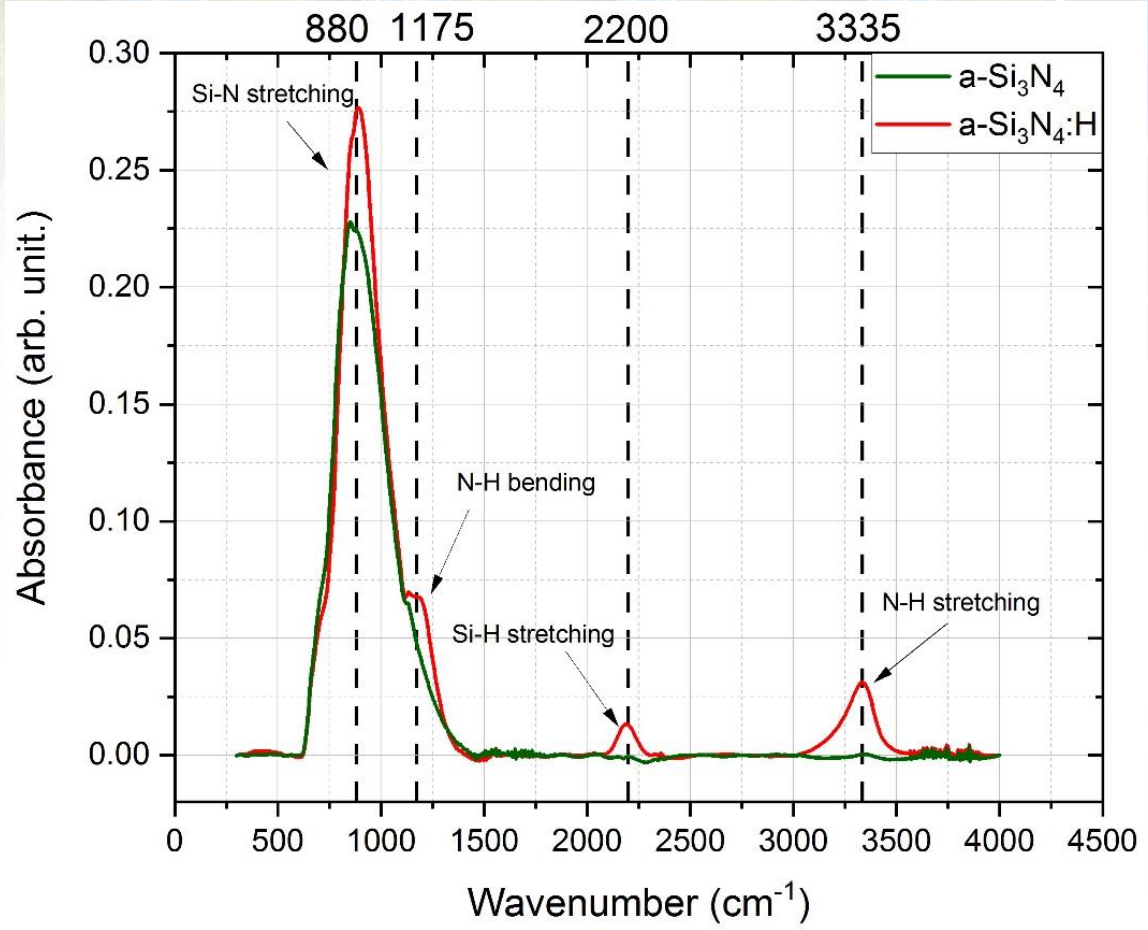
$H - Si$: 298 $\frac{kJ}{mol}$

Constant

Measured

Questionable

Infrared spectroscopy



Quantitative analysis

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Lanford-Rand-method

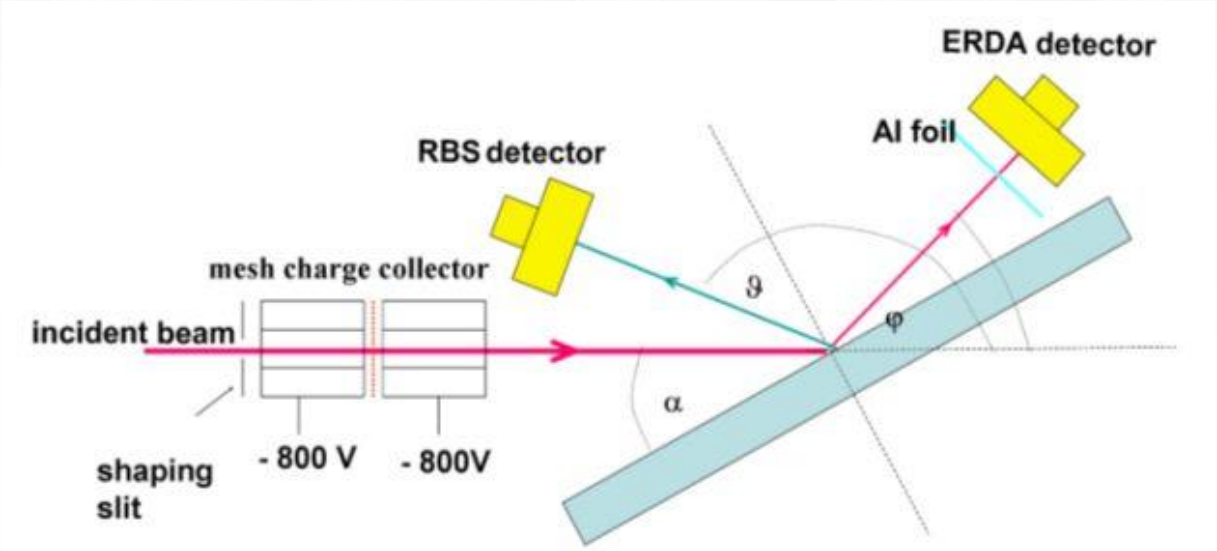
$$C_{Y-H} = \frac{A_{Y-H}}{ln10 \cdot \sigma_{Y-H}}$$

N-H	Si-H
$3.49 \cdot 10^{20} \frac{1}{cm^3}$	$0.61 \cdot 10^{20} \frac{1}{cm^3}$

This method is only sensitive for bound hydrogen

FTIR vs. ERDA

Schematic Overview of
Elastic Recoil Detection Analysis



Hydrogen concentration

Bound – FTIR	Total – ERDA
$4.1 \cdot 10^{20}\ \frac{\text{atoms}}{\text{cm}^3}$	$9.6 \cdot 10^{21}\ \frac{\text{atoms}}{\text{cm}^3}$

Less than 5% of total hydrogen atoms are bonded to silicon or nitrogen atoms

Hydrogen mainly exists in the film in *molecular* form

Conclusions

Hydrogen is in the film dominantly in moleculer form

- Increased porosity and decreased density (TEM)
- Hydrogen releases at low temperature
  - Blistering of the sample surface (SEM)
  - Low activation energy (Arrhenius-method)

Subjects, publications

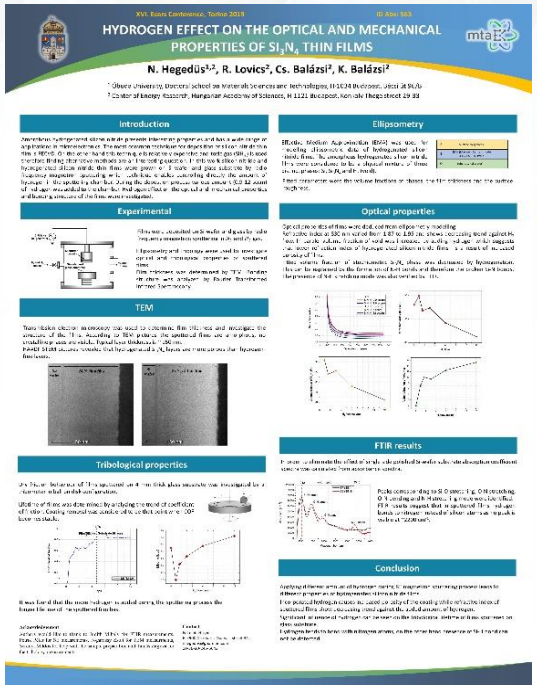
- Subjects:
  - Mechanical properties of engineering ceramics (Dr. Ján Dusza)
  - Material structure and fracture mechanism of engineering ceramics (Dr. Ján Dusza)

- Publications:
  - Writing publications is in progress about the presented results and a review on hydrogenated silicon nitride thin films

Presentations

Poster presentation

XVI. Conference and Exhibition of the European Ceramic Society



Oral presentation

2nd Fine Ceramic Day

Science Society of Silicate Industry

Plans for the next semester

- Preparation of first publication with IF
- Explain the results with theoretical model
- Investigate the influence of the process parameters on the ratio of bound/unbound hydrogen content in the film

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- Dr. Péter Petrik[2] (SE-measurements)
- Dr. Zsolt Zolnai[4] (ERDA-measurements)
- Tamás Zagyva[1] (Tribology-measurements)

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Thank you for your attention!

Thank You