Dielectric function measurement of emerging semiconductors

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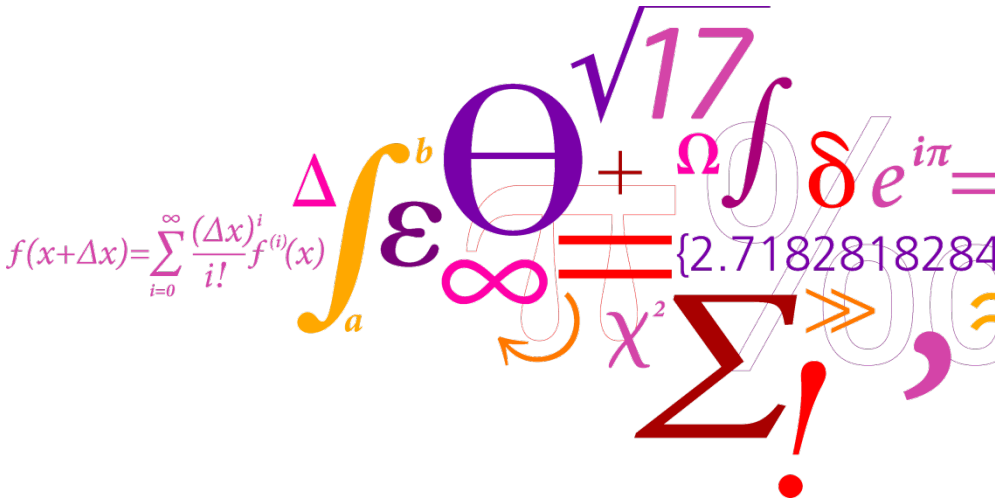


DTU Nanotech
Department of Micro- and Nanotechnology

Dielectric function of semiconductors

Which semiconductors?

- Thin–film sulfide semiconductors for solar cells

Why ellipsometry?

- Band gap and absorption coefficient are crucial for solar energy materials
- By comparing the experimental and calculated dielectric function, much can be learned about the electronic properties of those materials

Ellipsometry measurement issues?

- Those sulfides for solar cells must be:
  - deposited on a metal back contact
  - annealed in a sulfur atmosphere

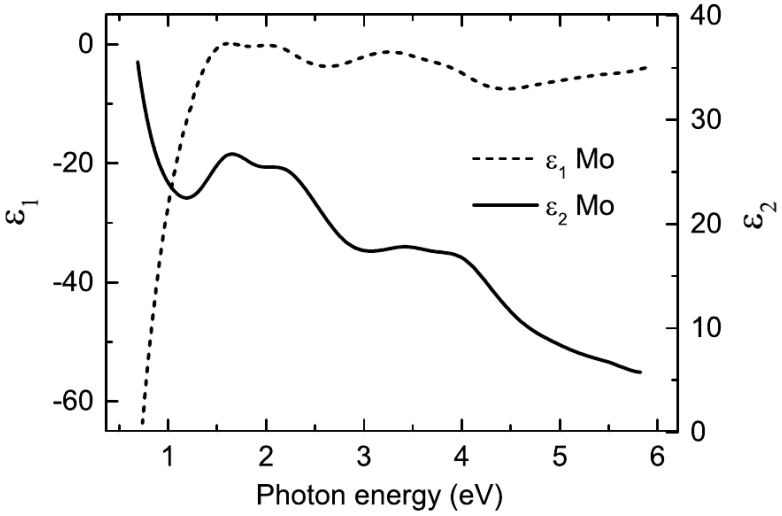
  ➔ Problem 1: **Multi-layered substrate**

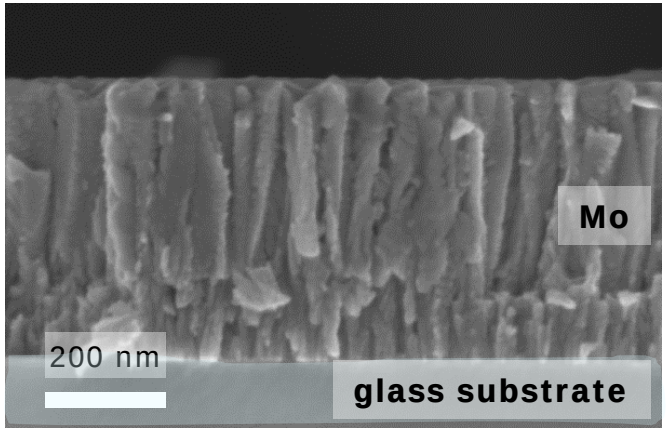
  ➔ Problem 2: **Changes in properties** of all layers upon annealing

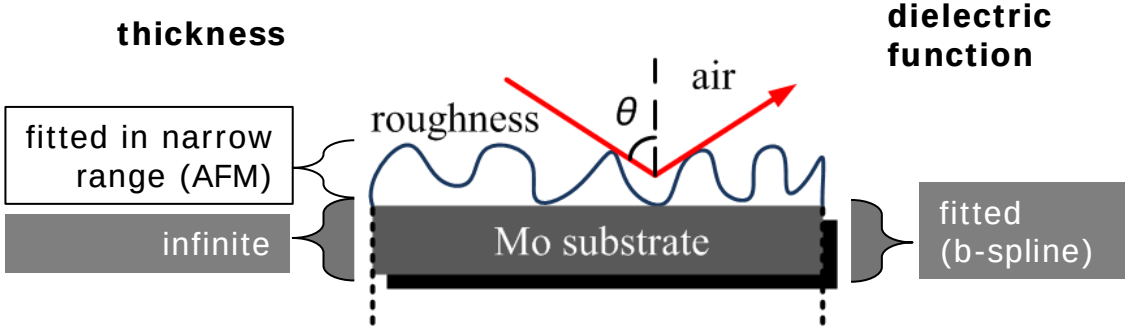
Case study: Cu_2SnS_3 (CTS)

Step 1: back contact dielectric function

- Grow Mo on glass (sputtering)
- Anneal it in a N_2 atmosphere (to reproduce sulfur annealing but without MoS_2 formation)
- 1st ellipsometry measurement





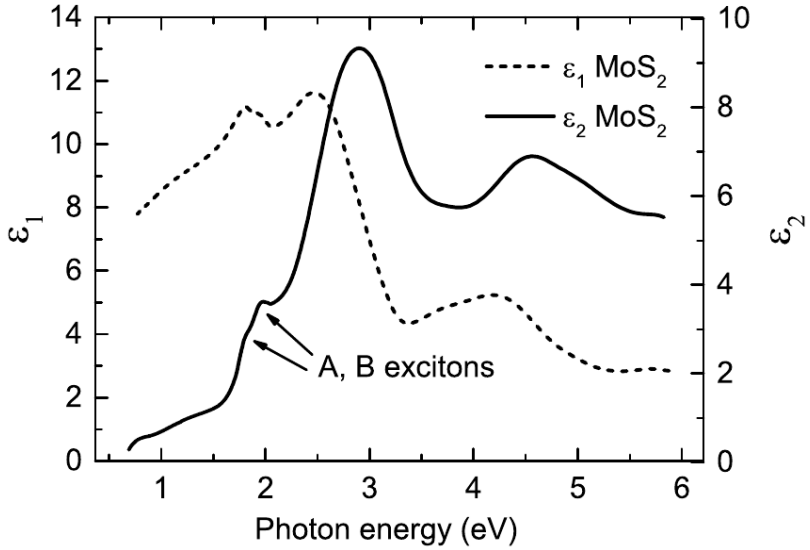


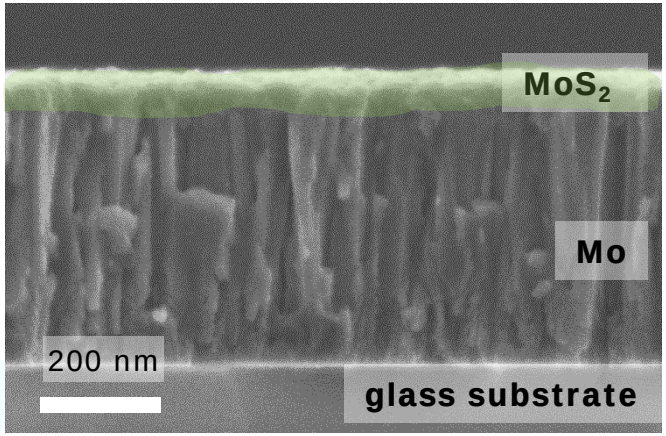
A. Crovetto et al., *Solar Energy Materials and Solar Cells*, **154**, 121–129 (2016)

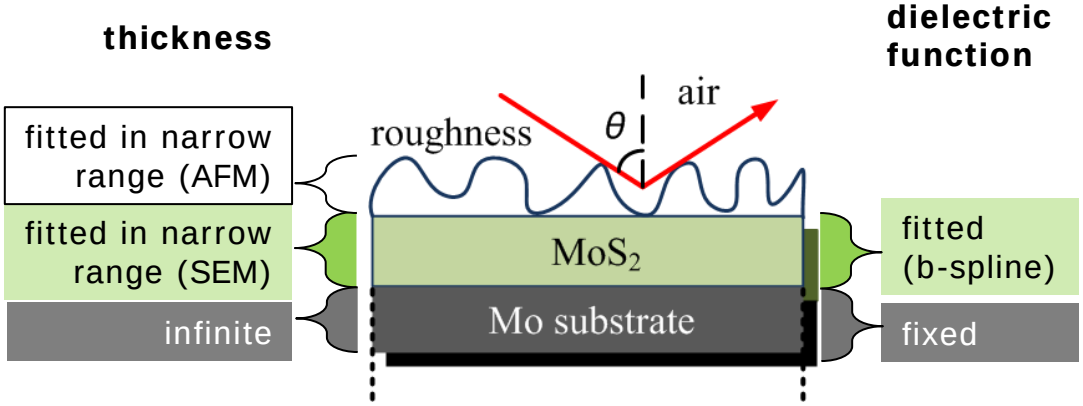
Case study: Cu_2SnS_3 (CTS)

Step 2: dielectric function of MoS_2 on Mo

- Anneal Mo in a **sulfur + N_2** atmosphere to form MoS_2
- 2nd ellipsometry measurement





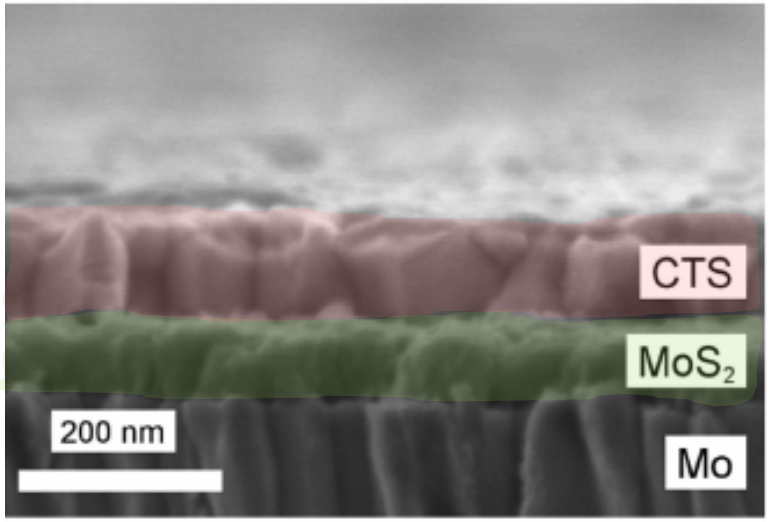


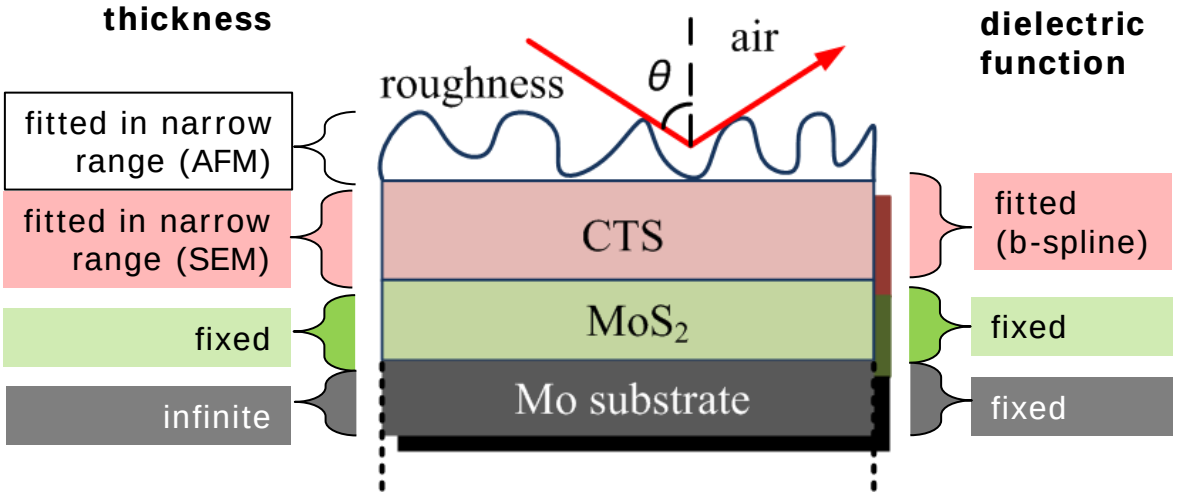
A. Crovetto et al., *Solar Energy Materials and Solar Cells*, **154**, 121–129 (2016)

Case study: Cu_2SnS_3 (CTS)

Step 3: measure the dielectric function of Cu_2SnS_3 on MoS_2/Mo

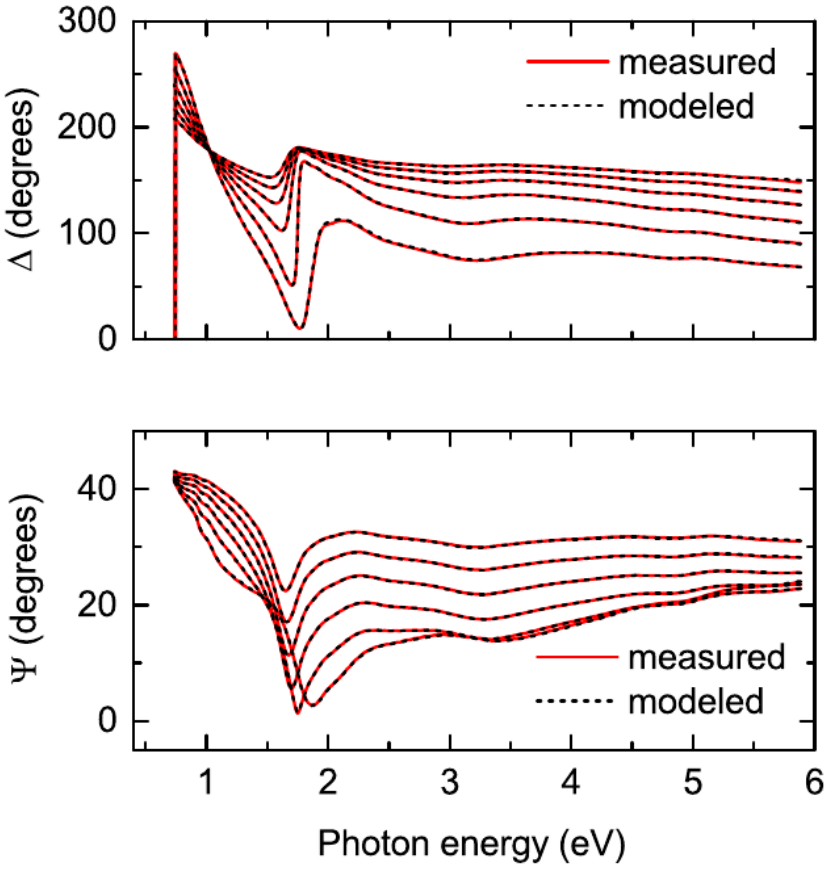
- Deposit a **thin layer** of Cu_2SnS_3 on Mo (to keep roughness low)
- Anneal Cu_2SnS_3 in a **sulfur + N_2** atmosphere
- 3rd ellipsometry measurement

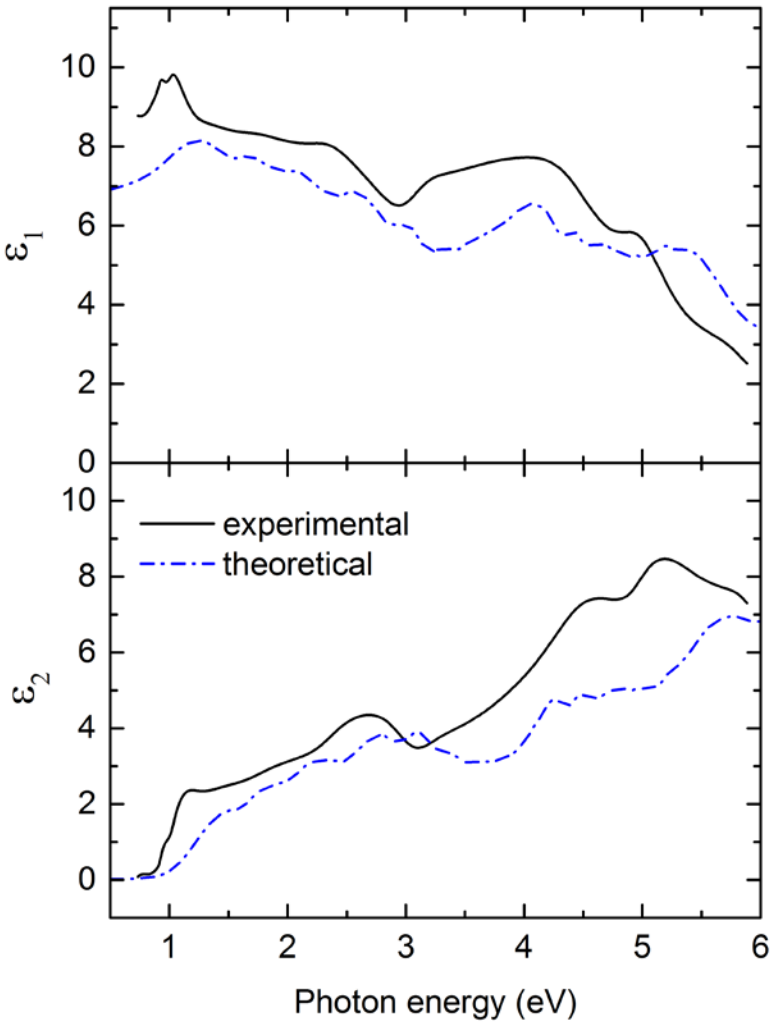




A. Crovetto et al., *Solar Energy Materials and Solar Cells*, **154**, 121–129 (2016)

Case study: Cu_2SnS_3 (CTS)



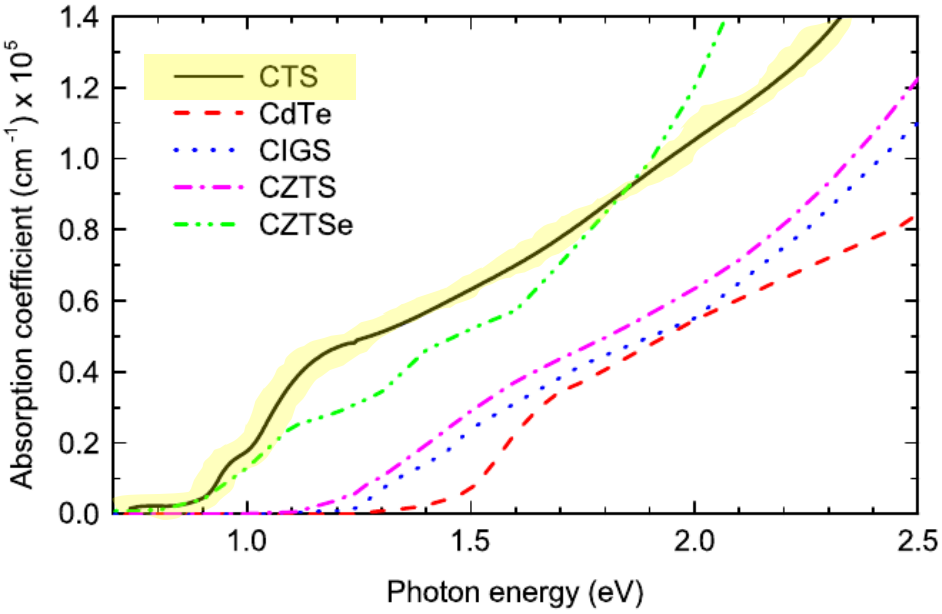


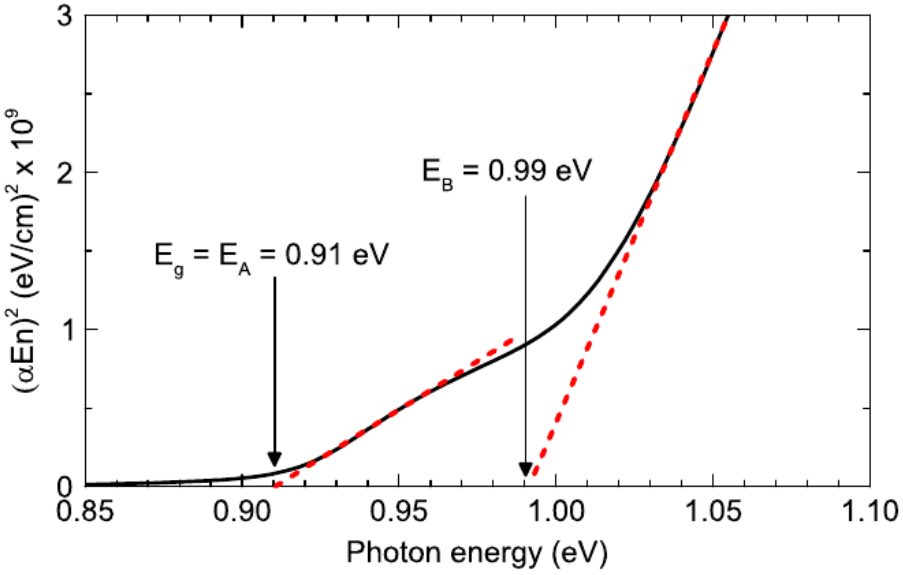
Theoretical calculation by Rongzhen Chen/Clas Persson (KTH, Stockholm - University of Oslo)

A. Crovetto et al., *Solar Energy Materials and Solar Cells*, **154**, 121–129 (2016)

Case study: Cu_2SnS_3 (CTS)

Two interesting findings:



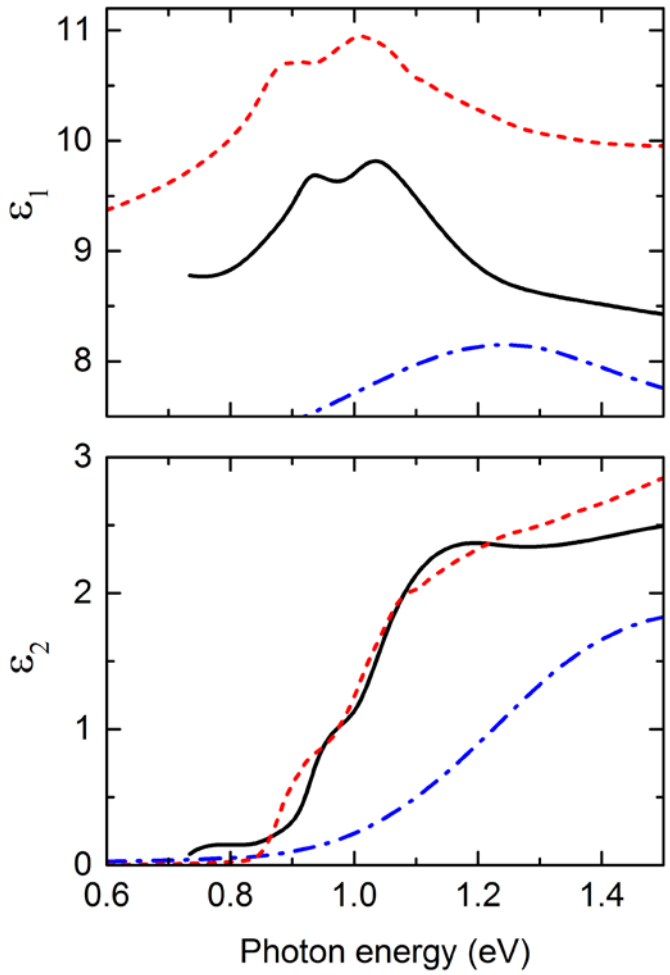


1. Absorption coefficient of CTS is larger than in "competing" materials

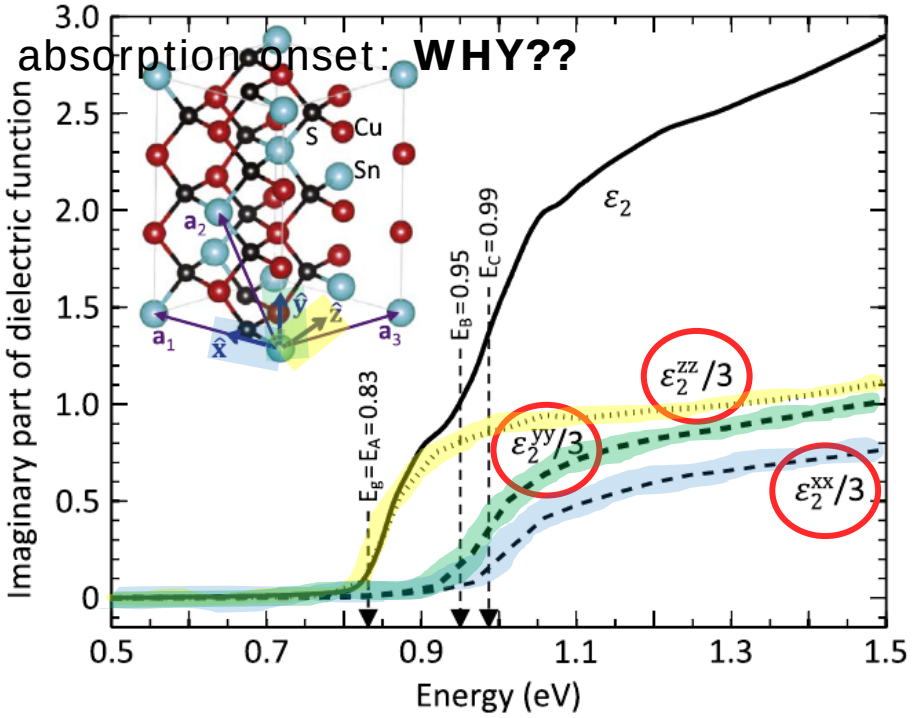
2. Double absorption onset!

A. Crovetto et al., *Solar Energy Materials and Solar Cells*, **154**, 121–129 (2016)

Case study: Cu_2SnS_3 (CTS)



Double absorption onset: **WHY??**



experimental

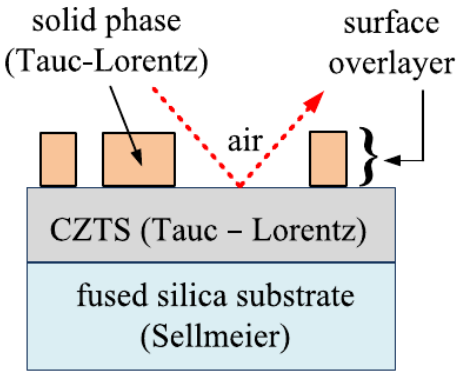
theoretical (HSE): accurate model BUT coarse **k**-sampling

theoretical (PBE+U): less accurate model BUT denser **k**-sampling

A. Crovetto et al., *Solar Energy Materials and Solar Cells*, **154**, 121–129 (2016)

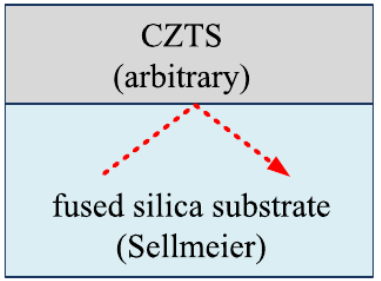
Other ellipsometry activities

non-ideal films

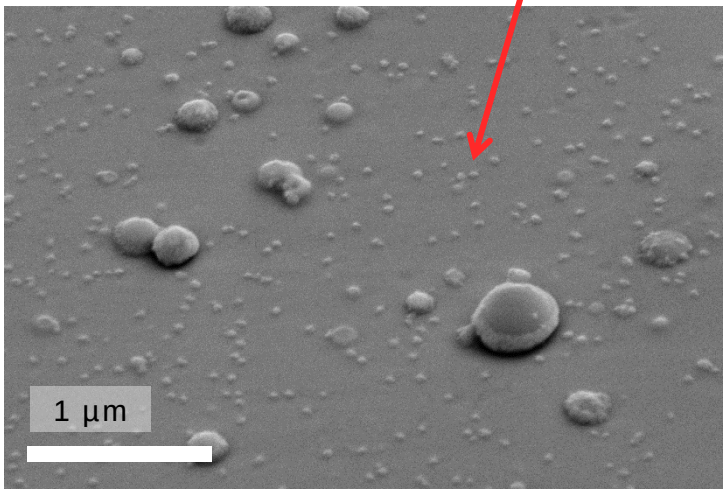


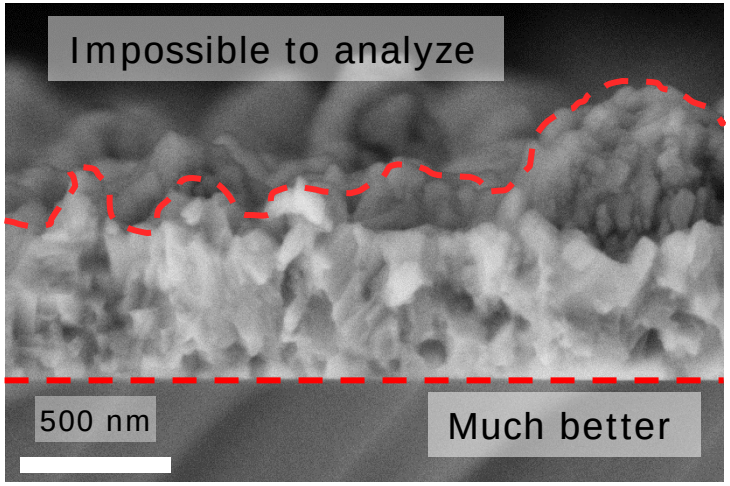
CuS_2 phases

(based on their dielectric function)



What are these?





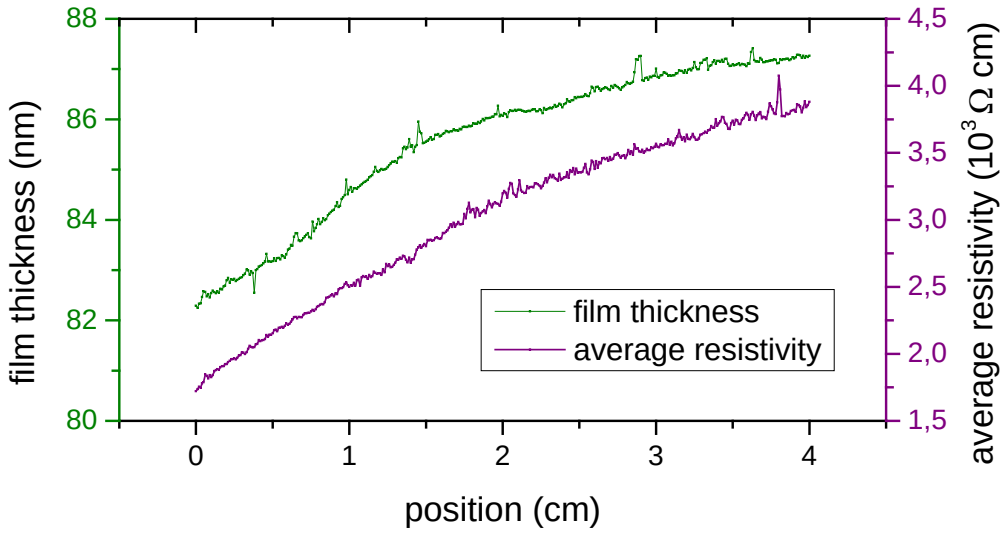
A. Crovetto et al., *Thin Solid Films*, **582**, 203–207 (2015)

Other ellipsometry activities

resistivity mapping

Resistivity of a thin film: (sheet resistance) * (thickness)

Four-point probe **Ellipsometry**



A. Crovetto et al., *Journal of Physics D: Applied Physics*, **49**, 295101 (2016)

Other ellipsometry activities

optical measurement of carrier density & mobility

Material: **ZnO:Al** thin films

➔ **transparent conductor** (degenerately doped high-band gap semiconductor)

Resistivity of a thin film: $\frac{1}{(\text{constant}) * (\text{carrier density}) * (\text{mobility})}$

Four-point probe + ellipsometry

Hall measurement

ellipsometry

derived

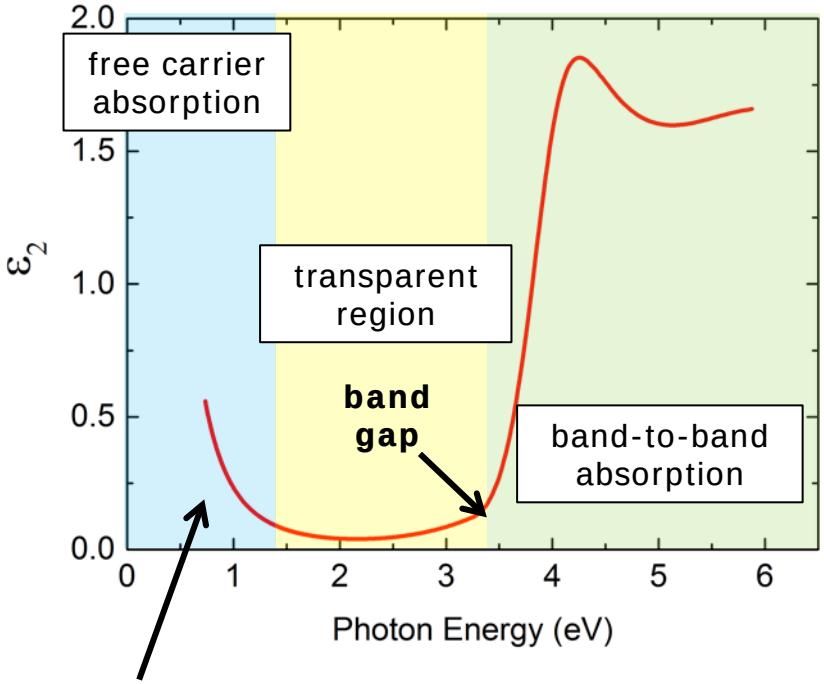
Optical way
Traditional way

A. Crovetto et al., *Journal of Physics D: Applied Physics*, **49**, 295101 (2016)

Other ellipsometry activities

optical measurement of carrier density & mobility

Dielectric function (imaginary) of **ZnO:Al**



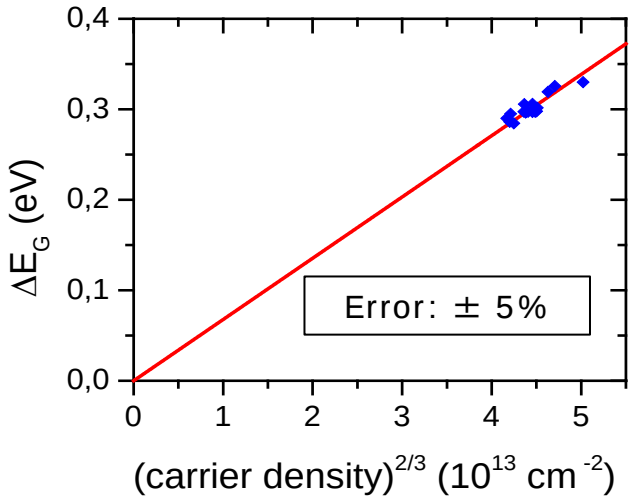
Fitting this region with e.g. Drude model…

…**carrier density** and **mobility**

Alternative method:

Burstein-Moss effect

The band gap increases proportionally to (carrier density)$^{2/3}$



A. Crovetto et al., *Journal of Physics D: Applied Physics*, **49**, 295101 (2016)

Summary of activities

- **Dielectric function** determination of new thin-film semiconductors
  - Learning about their electronic properties
- **Phase analysis** of ”non-ideal” thin films
- Thickness **mapping** (for its own sake and for resistivity mapping)
- All-optical determination of **electrical properties** of transparent conductive materials