UV-Vis Optical Analysis Report

Optical gap (Tauc), Urbach energy, absorption and optical constants from T and R spectra

1 Comparison of samples

Sample	Eg (eV)	Eu (meV)	n(550 nm)
Sample 0	4.268 ± 0.015	144.8 ± 3.9	1.465
Sample 15	4.265 ± 0.016	162.3 ± 4.4	1.683

Comparison with reference values

Sample	Parameter	Reference	This tool	Difference	Verdict
Sample 0	Eg, Origin	4.26 eV	4.268 ± 0.015 eV	+0.0081 (+0.2 %)	**agrees ± unc.**
Sample 0	Eg, first Python tool	4.397 eV	4.268 ± 0.015 eV	-0.129 (-2.9 %)	**close**
Sample 0	Eu, first Python tool	4365 meV	144.8 ± 3.9 meV	-4.22e+03 (-96.7 %)	**differs**
Sample 15	Eg, Origin	4.26 eV	4.265 ± 0.016 eV	+0.0049 (+0.1 %)	**agrees ± unc.**
Sample 15	Eg, first Python tool	4.403 eV	4.265 ± 0.016 eV	-0.138 (-3.1 %)	**close**
Sample 15	Eu, first Python tool	3127 meV	162.3 ± 4.4 meV	-2.96e+03 (-94.8 %)	**differs**

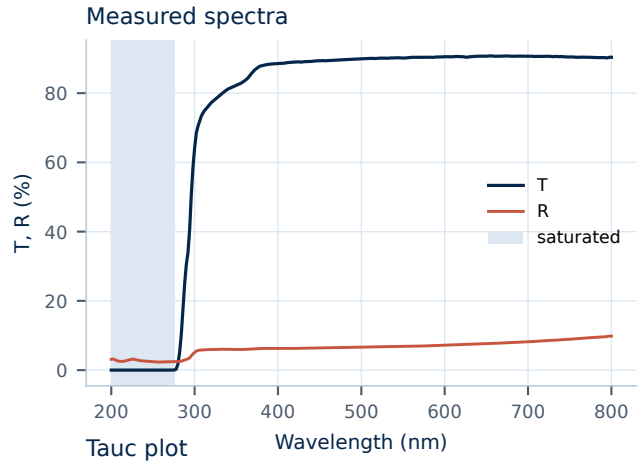
The first tool fitted ln α on the transparent region (about 2–3.3 eV), not on the tail below the edge; its Eu values are not physical.

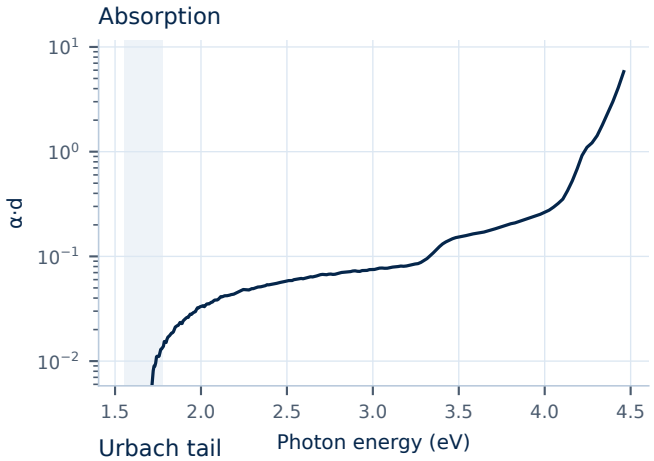
2 Sample: Sample 0

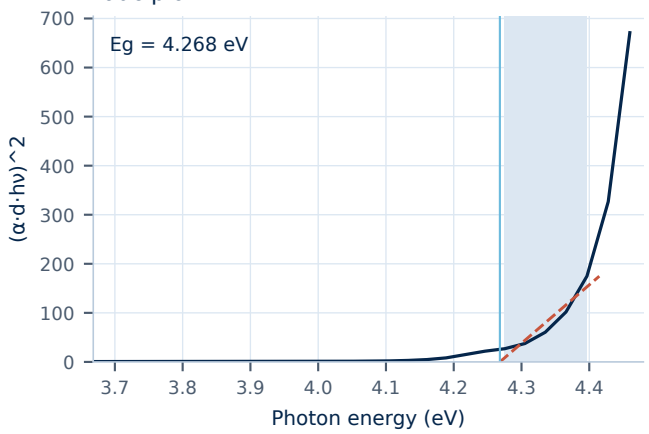
Source	Film on quartz slide; T and R measured 200–800 nm (data analysed with Dr. Mostafa El
Data	301 points, 200–800 nm, T and R
Film thickness	not given
Substrate	quartz / fused silica
Transition	direct (m = 2)

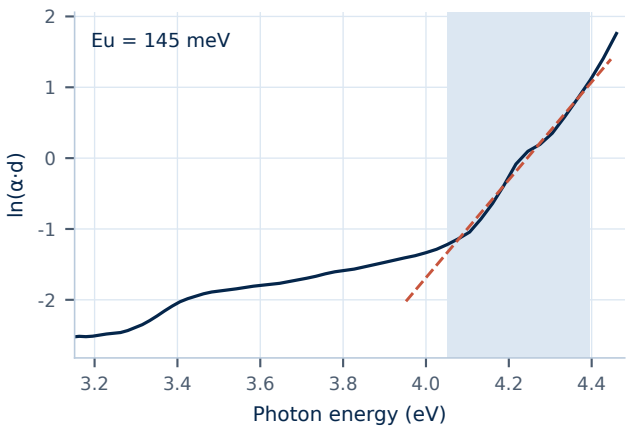
Results

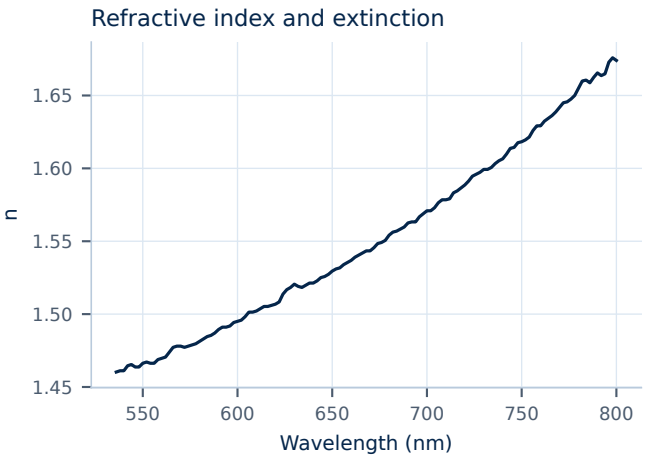
Quantity	Value	Method
Eg	4.268 ± 0.015 eV	Tauc (direct), 4.28–4.40 eV, R^2 = 0.9009
Eu	144.8 ± 3.9 meV	ln α, 4.05–4.40 eV, R^2 = 0.9919
n(550 nm)	1.465	from R, film-on-substrate (n_sub = 1.46)











3 Processing steps

- 301 points, 200–800 nm, T and R
- R in percent, converted to a fraction
- T in percent, converted to a fraction
- absorption: r-corrected
- baseline: αd = -0.0860 in 698–800 nm subtracted
- 39 saturated points left out (λ ≤ 276 nm)
- Tauc: direct transition, m = 2, window automatic
- Urbach: window automatic

4 Warnings

- no part of the edge is straight enough; Eg comes from the straightest window and is approximate
- Tauc fit R^2 = 0.901: the window is not straight
- R is below the bare substrate (6.8 % for n = 1.46) at 46 % of the transparent wavelengths: there n cannot be found from R (film index below the substrate, a different substrate, or R not measured as total reflectance)
- n from R rises with wavelength (+0.081 per 100 nm) in the transparent region, the opposite of normal dispersion: the measured R probably includes the substrate or back surface, so n from R is not reliable for this sample
- the spectrum is saturated above 4.46 eV, so only the foot of the edge is measured; Eg is approximate and probably too low (a thinner film would show the whole edge)
- no film thickness: Eg and Eu are given; α, k, ε and σ need the thickness

Refractive index from Eg by empirical relations (indicative only)

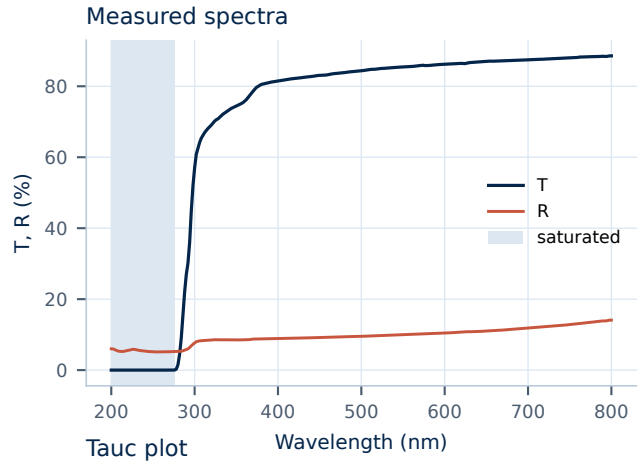
`Moss: 2.17  Ravindra: 1.44  Hervé–Vandamme: 2.04`

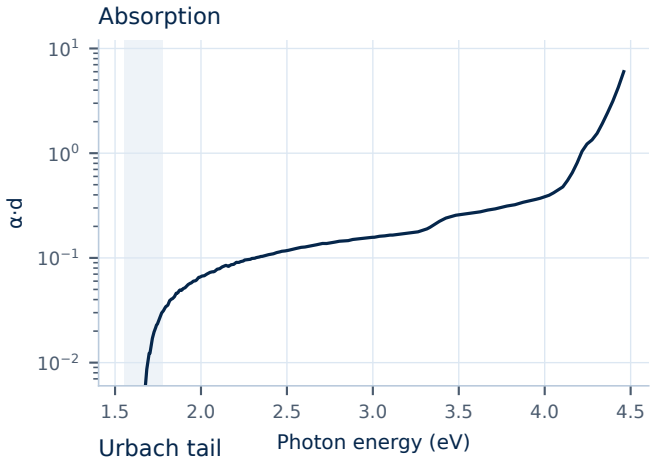
5 Sample: Sample 15

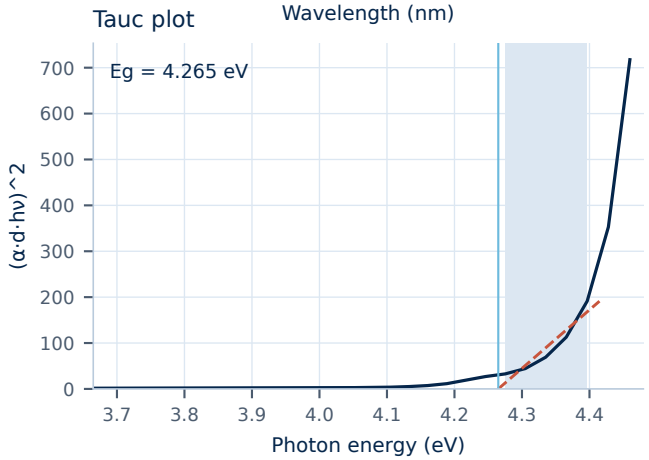
Source	Film on quartz slide; T and R measured 200–800 nm (data analysed with Dr. Mostafa El
Data	301 points, 200–800 nm, T and R
Film thickness	not given
Substrate	quartz / fused silica
Transition	direct (m = 2)

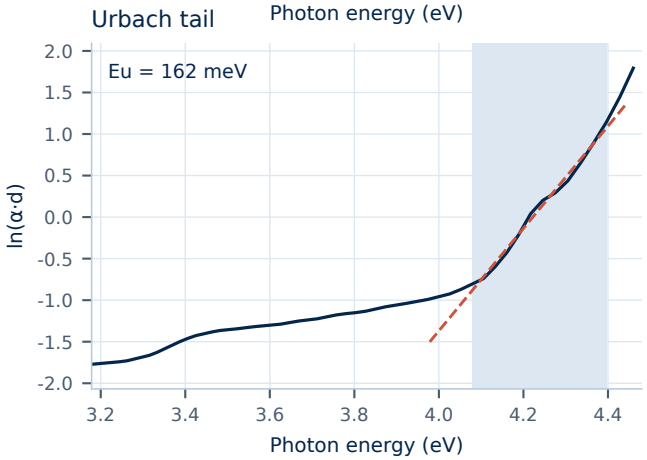
Results

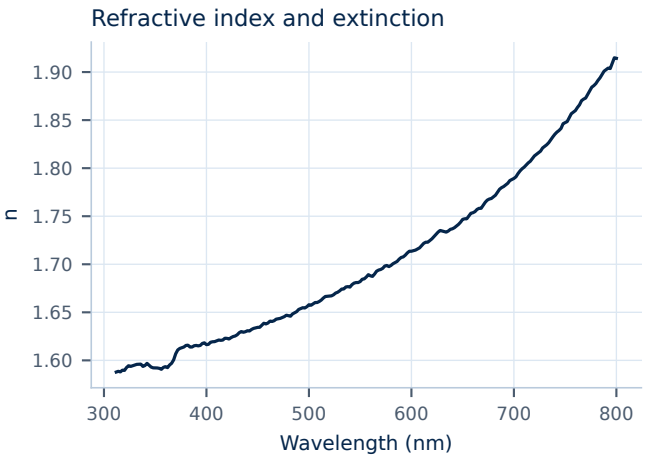
Quantity	Value	Method
Eg	4.265 ± 0.016 eV	Tauc (direct), 4.28–4.40 eV, R^2 = 0.9015
Eu	162.3 ± 4.4 meV	ln α, 4.08–4.40 eV, R^2 = 0.9927
n(550 nm)	1.683	from R, film-on-substrate (n_sub = 1.46)











6 Processing steps

- 301 points, 200–800 nm, T and R
- R in percent, converted to a fraction
- T in percent, converted to a fraction
- absorption: r-corrected
- baseline: αd = -0.1467 in 698–800 nm subtracted
- 39 saturated points left out (λ ≤ 276 nm)
- Tauc: direct transition, m = 2, window automatic
- Urbach: window automatic

7 Warnings

- no part of the edge is straight enough; Eg comes from the straightest window and is approximate
- Tauc fit R^2 = 0.901: the window is not straight
- n from R rises with wavelength (+0.063 per 100 nm) in the transparent region, the opposite of normal dispersion: the measured R probably includes the substrate or back surface, so n from R is not reliable for this sample
- the spectrum is saturated above 4.46 eV, so only the foot of the edge is measured; Eg is approximate and probably too low (a thinner film would show the whole edge)
- no film thickness: Eg and Eu are given; α, k, ε and σ need the thickness

Refractive index from Eg by empirical relations (indicative only)

`Moss: 2.17  Ravindra: 1.44  Hervé–Vandamme: 2.04`

8 How to read the results

Eg

The optical gap, from the straight part of the Tauc plot extrapolated to zero. It depends on the transition type chosen (direct or indirect) and not on the thickness.

Eu

The width of the exponential tail just below the edge. Typical films give tens to a few hundred meV; a larger value means more disorder or defects. It does not depend on the thickness. A value close to Eg means the window is not on the tail.

Saturation

Where the transmittance sits at the detector floor the points are not a measurement. They are shaded in the spectra and left out of every fit.

α, k, ε, σ

These scale with 1/thickness, so they are given only when the film thickness is entered.

n

From the reflectance in the transparent region only, for a film on a substrate of known index. It is valid when R is the total reflectance of the film and its substrate; the tool warns when the data do not allow it.

Verdict: "agrees ± unc." when the difference is within twice the combined uncertainty; otherwise "agrees" up to 2 %, "close" up to 5 %, "differs" above.

This report was produced by the Phy-Lab UV-Vis Optical Analyzer. More tools at phy-lab.com.