Model dielectric function of amorphous materials including Urbach tail

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Outline

- Applications of model
- Tauc-Lorentz model
- Urbach tail extension
- Fitting results
- Formula for Urbach tail part

Motivation

For analysis of measured ellipsometric parameters of sample, we need good specification of material parameters of the sample. Optical parameters of amorphous materials are often modeled using Tauc-Lorentz model published by Jellison and Modine, which is easy to implement and only five parameters are fitted. But this model doesn't describe well absorption tail near absorption band part of spectra.

Presented model extents TL model by including Urbach tail, which is described by exponential decreasing of absorption. This model gives better fits of data from ellipsometric, reflectance and especially transmission measurements.

Applications of the model

Model discussed in this presentation is suitable for following amorphous materials:

- semiconductors
  - gallium arsenide
  - gallium aluminum arsenide
  - arsenic sulfide
  - amorphous silicon
- dielectrics
  - silicon nitride
  - silicon oxide and optical glasses

Tauc-Lorentz model (Jellison, Modine)

- imaginary part of dielectric function

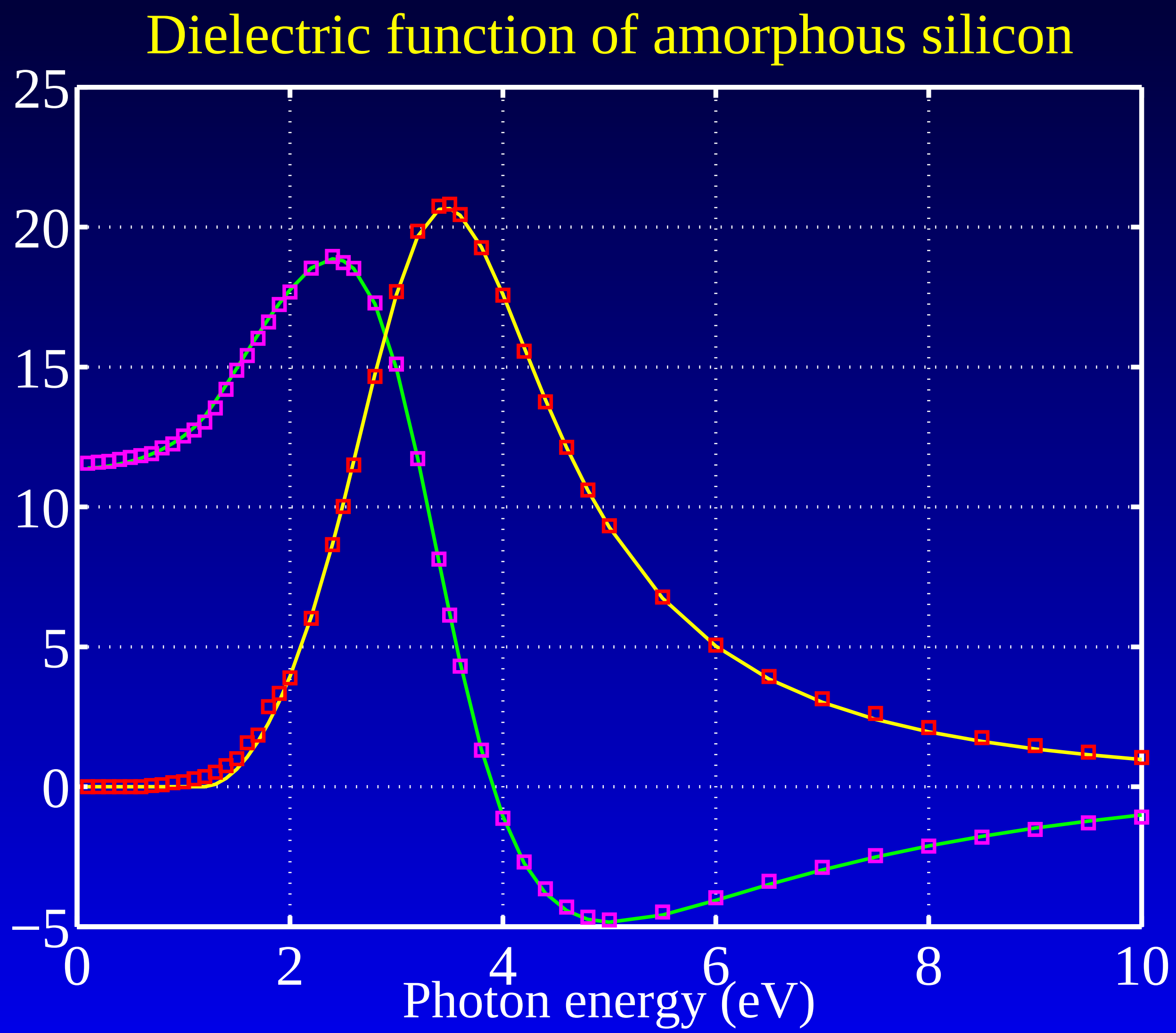
$$\epsilon_2(E) = \begin{cases} \frac{AE_0C(E-E_g)^2}{E[(E^2-{E_0}^2)^2+C^2E^2]}, & E > E_g \\ 0, & E \leq E_g \end{cases}$$

- real part of dielectric function (Kramers-Krönig relations)

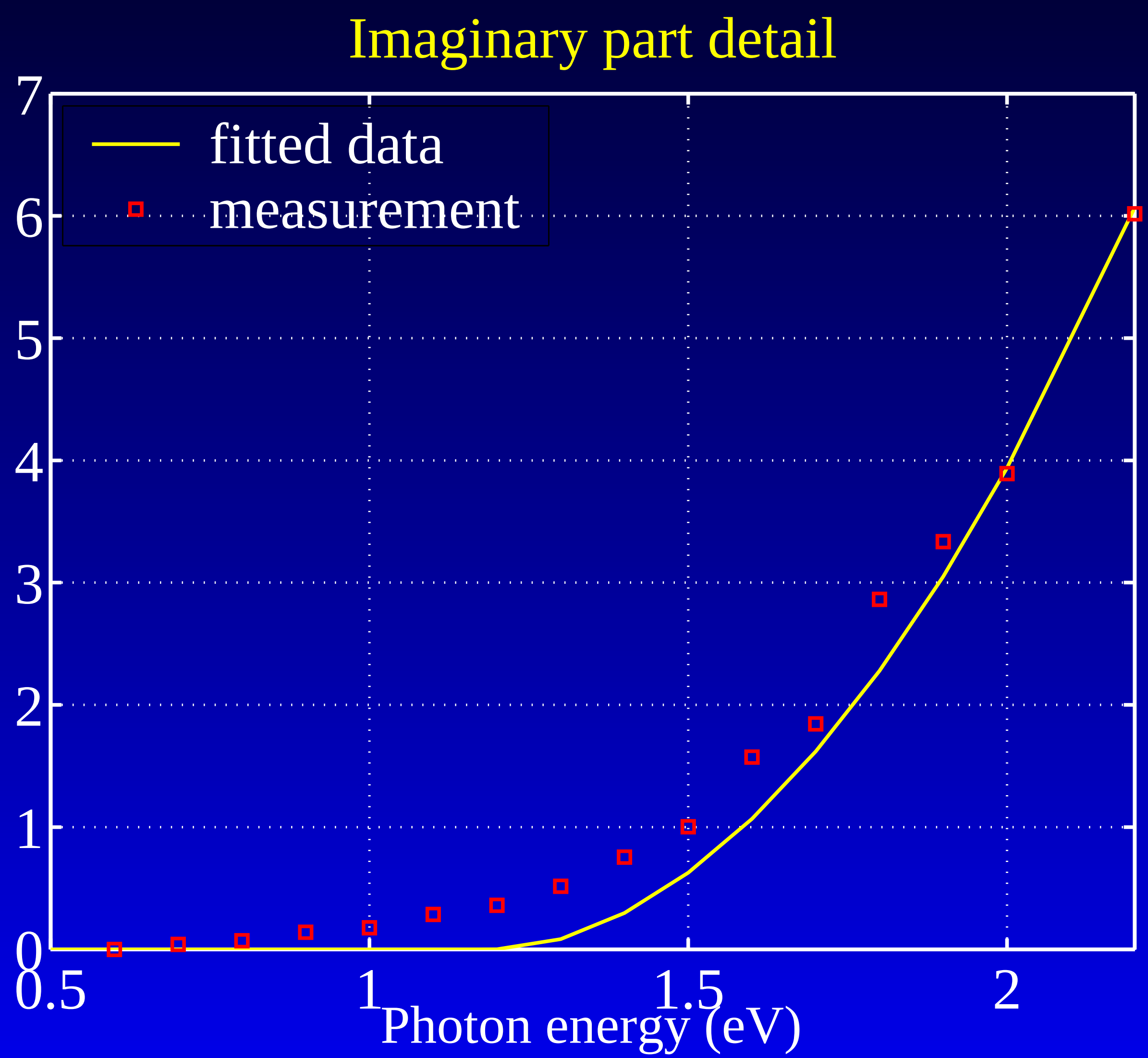
$$\epsilon_1(E) = \epsilon_{1,\infty} + (C.P.) \int\limits_0^\infty \frac{\epsilon_2(\xi)\xi}{\xi^2 - E^2}\, \mathrm{d}\xi$$

- expect zero imaginary part below absorption edge (E_g)
- ϵ_1 can be expressed analytically - Jellison, APL 69 (1996)
- five parameters for fitting $(A, E_0, C, E_g, \epsilon_{1,\infty})$

Tauc-Lorentz model



Tauc-Lorentz model detail



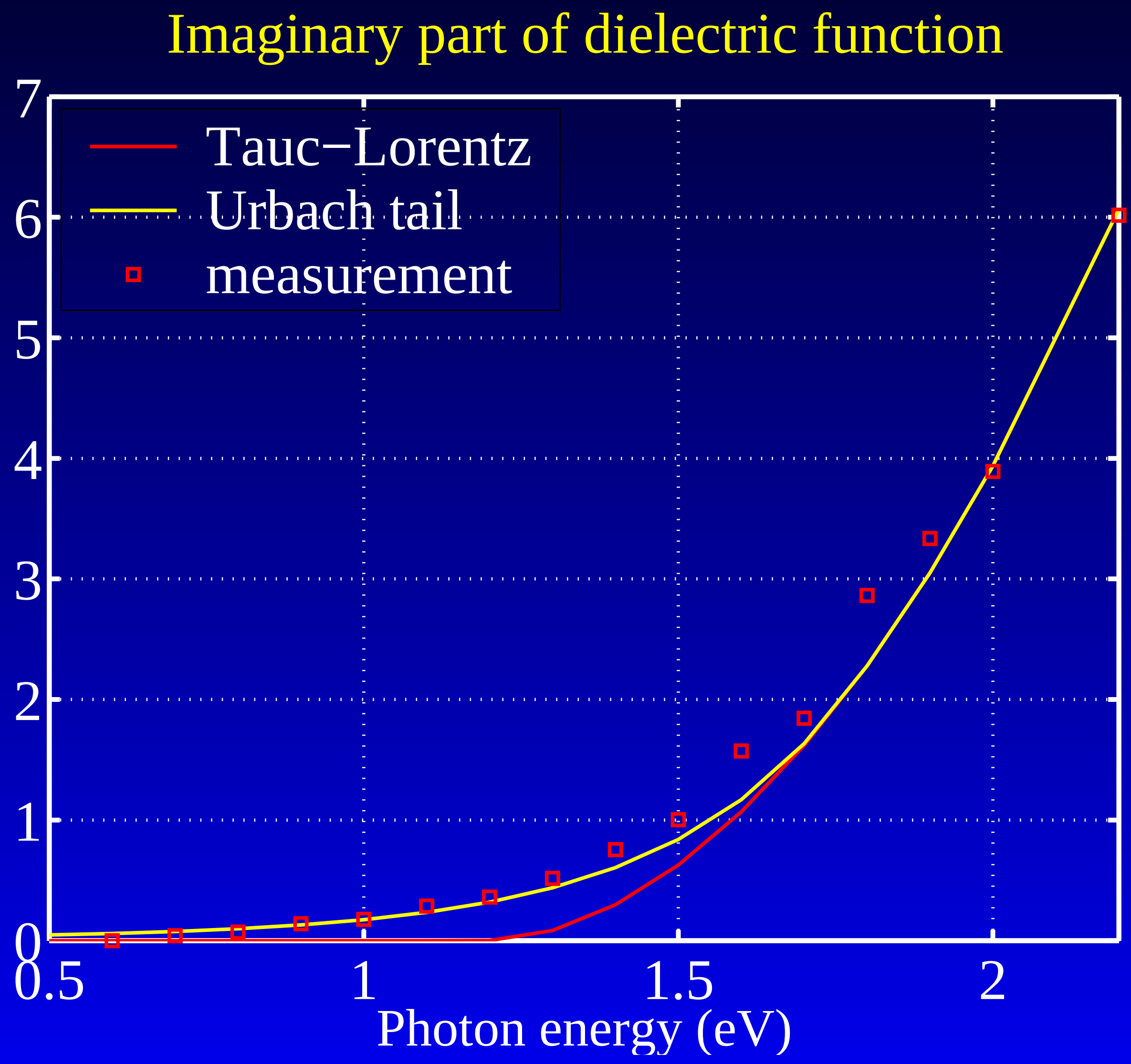
Tauc-Lorentz-Urbach model

- imaginary part of dielectric function

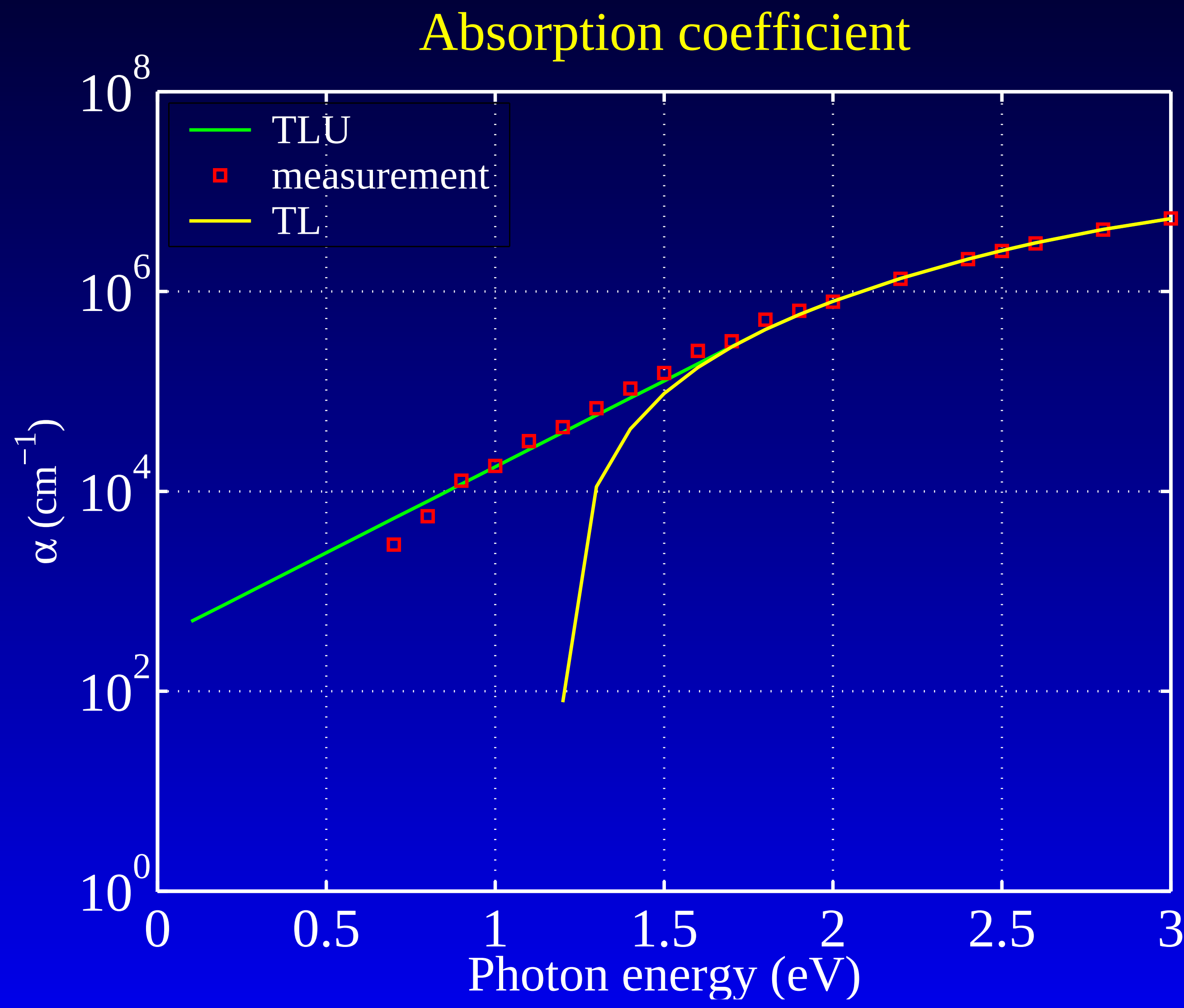
$$\epsilon_2(E) = \begin{cases} \frac{AE_0C(E-E_g)^2}{E[(E^2-{E_0}^2)^2+C^2E^2]}, & E > E_c \\ \frac{A_u}{E}\exp\left(\frac{E}{E_u}\right), & E \leq E_c \end{cases}$$

- A_u, E_u chosen so that ϵ_2 is continuous including first derivation at E_c ($E_g < E_c$)
- real part of dielectric function cannot be expressed as elementary function, but part from UT can be expressed as infinite sum of elementary functions
- energy $E = E_c$ is solved as special case
- only one more parameter for fitting (E_c)

Tauc-Lorentz-Urbach model detail



Logarithmic plot of absorption



Formula for TLU model

Real part of dielectric function expressed with help of:

- exponential integrals

$$\epsilon_{1,UT}(E) = \frac{A_u}{E\pi}\left\{\exp\left(-\frac{E}{E_u}\right)\left[Ei\left(\frac{E}{E_u}\right) - Ei\left(\frac{E_c+E}{E_u}\right)\right] + \right.$$
$$\left. + \exp\left(\frac{E}{E_u}\right)\left[Ei\left(\frac{E_c-E}{E_u}\right) - Ei\left(-\frac{E}{E_u}\right)\right]\right\}$$

- sum of elementary functions

$$\epsilon_{1,UT}(E) = \frac{A_u}{E\pi}\sum_{n=1}^{\infty}\frac{1}{{E_u}^n \cdot n \cdot n!}\left\{\exp\left(-\frac{E}{E_u}\right)[E^n - (E+E_c)^n] + \right.$$
$$+ \left. \exp\left(\frac{E}{E_u}\right)[(E_c-E)^n - (-E)^n]\right\} +$$
$$+ \frac{A_u}{E\pi}\exp\left(-\frac{E}{E_u}\right)[\ln|E| - \ln|E+E_c|]$$
$$+ \frac{A_u}{E\pi}\exp\left(\frac{E}{E_u}\right)[\ln|E-Ec| - \ln|E|]$$

Conclusions

- Tauc-Lorentz-Urbach model is more accurate than often used Tauc-Lorentz model
- presented model gives better fits for ellipsometric and transmission measurements
- evaluating Urbach tail part with sum is faster, but cannot be used for high value of E/E_u ratio
- from Urbach tail we could deduce information about defects

Publications

- J. Pistora, M. Foldyna, T. Yamaguchi, J. Vlcek, D. Ciprian, K. Postava, F. Stanek, Magneto-Optical Phenomena in Systems with prism Coupling, in Photonics, Devices, and Systems II, M. Hrabovsky, D. Senderakova, P. Tomanek, Eds., Proc. of SPIE Vol. 5036(2003) 299–304.
- O. Zivotsky, K. Postava, M. Foldyna, T. Yamaguchi, J. Pistora, Magneto-optics of systems containing non-coherent propagation in thick layers, in Photonics, Devices, and Systems II, M. Hrabovsky, D. Senderakova, P. Tomanek, Eds., Proc. of SPIE Vol. 5036(2003) 336–341.
- D. Lukas, D. Ciprian, J. Pistora, K. Postava, M. Foldyna, Multilevel Solvers for 3-Dimensional Optimal Shape Design with an Application to Magnetostatics, ISMOT 2003, Ostrava (in print).
- M. Foldyna, K. Postava, J. Bouchala, J. Pistora, T. Yamaguchi, Model dielectric function of amorphous materials including Urbach tail, ISMOT 2003, Ostrava (in print).
- M. Foldyna, D. Ciprian, J. Pistora, K. Postava, R. Antos, Reconstruction of grating parameters from ellipsometric data, ISMOT 2003, Ostrava (in print).
- K. Postava, J. Pistora, T. Yamaguchi, M. Foldyna, M. Lesnak, Magneto-optic vector magnetometry for sensor applications, Sensors and Actuators (in print).
- J. Pistora, T. Yamaguchi, M. Foldyna, J. Mistrik, K. Postava, M. Aoyama, Magnetic sensor with prism coupler, Sensors and Actuators (in print).