Urbach tail extension of Tauc-Lorentz model dielectric function

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Abstract. A generalization of the Tauc-Lorentz model dielectric function of amorphous semiconductors and dielectrics is presented in which the exponential Urbach tail is included. The generalized parametrization of the optical functions includes only six fitting parameters. The real part of the dielectric function is calculated using analytical Kramers-Krönig dispersion relations. The model is applied to hydrogenated amorphous silicon.

1 INTRODUCTION

Effective processing of spectroscopic measurements requires data fitting to a simple parameterization of the material optical functions. Jellison and Modine [1] derived an effective parameterization for optical functions of amorphous materials based on a combination of the Tauc band edge and the Lorentz oscillator function. The Tauc-Lorentz (TL) parameterization has become standard and widely used model dielectric function for amorphous semiconductors and dielectrics [2–5]. However, the Tauc-Lorentz model does not include Urbach tail effects, i.e., defect induced absorption exponentially decreasing from absorption edge. Amorphous materials exhibit absorption edge which is considerably less sharp and which consequently tails well into the gap and which invariably obeys an exponential dependence on photon energy (see details in Ref. 6).

In this paper we propose extended Tauc-Lorentz model by inclusion of the exponential Urbach tail. In our model we ensure continuous first derivate of the dielectric function. Consequently, the model is based only on six fitting parameters. In the following section we introduce the expression for the real and imaginary part of dielectric function and in Section 3 we introduce application of the model to amorphous silicon data.

2 THEORY

We propose a generalization of the Tauc-Lorentz parameterization by inclusion of the exponential Urbach tail. Proposed approach gives fast computation using analytical Kramers-Krönig integration. The imaginary part of the complex dielectric function $\epsilon = \epsilon_1 - i\epsilon_2 = (n - ik)^2$ is defined by

$$\epsilon_2(E) = \begin{cases} \dfrac{1}{E} \dfrac{AE_0C\,(E-E_g)^2}{\left(E^2-E_0^2\right)^2 + C^2E^2} & E \geq E_c \\ \\ \dfrac{A_u}{E} \exp\left(\dfrac{E}{E_u}\right) & 0 < E < E_c \end{cases} , \tag{1}$$

where the first term ($E \geq E_c$) is identical with the Tauc-Lorentz function [2] and the second term ($0 < E < E_c$) represents the exponential Urbach tail. E_g, A, E_0, and C denote the band gap energy, the amplitude, the Lorentz resonant frequency, and the broadening parameter, respectively. A_u and E_u are chosen with respect to continuity of the optical function including first derivate. This leads to the relations

$$E_u = (E_c - E_g) \left[2 - 2E_c\,(E_c - E_g)\, \frac{C^2 + 2\left(E_c^2 - E_0^2\right)}{C^2E_c^2 + \left(E_c^2 - E_0^2\right)^2} \right]^{-1}, \tag{2}$$

$$A_u = \exp\left(-\frac{E_c}{E_u}\right) \frac{AE_0C\,(E_c - E_g)^2}{\left(E_c^2 - E_0^2\right)^2 + C^2E_c^2}. \tag{3}$$

The real part ϵ_1 of the dielectric function is obtained using analytical integration of the Kramers-Krönig (KK) relation

$$\epsilon_1(E) = \epsilon_{1,\infty} + \frac{2}{\pi}\,(C.P.) \int_0^\infty \frac{\xi\epsilon_2(\xi)}{\xi^2 - E^2} d\xi, \tag{4}$$

where $(C.P.)$ denotes the Cauchy principal value of the integral. As a result, the real part of the dielectric function can be expressed in the form

$$\epsilon_1(E) = \epsilon_{1,\infty} + \epsilon_{1,TL}(E) + \epsilon_{1,UT}(E), \tag{5}$$

where the Tauc-Lorentz part (interval from E_c to infinity) is in the form

$$\begin{aligned} \epsilon_{1,TL}(E) = &-AE_0C\frac{E^2 + E_g^2}{\pi\zeta_4 E}\ln\frac{|E_c - E|}{E_c + E} + \\ &+ \frac{2AE_0CE_g}{\pi\zeta_4}\ln\frac{|E_c - E|(E_c + E)}{\sqrt{(E_0^2 - E_c^2)^2 + C^2E_c^2}} + \\ &+ \frac{ACa_L}{2\pi\zeta_4\alpha E_0}\ln\frac{E_0^2 + E_c^2 + \alpha E_c}{E_0^2 + E_c^2 - \alpha E_c} - \\ &- \frac{Aa_A}{\pi\zeta_4 E_0}\left[\pi - \arctan\frac{2E_c + \alpha}{C} - \arctan\frac{2E_c - \alpha}{C}\right] + \\ &+ 4AE_0E_g\frac{E^2 - \gamma^2}{\pi\zeta_4\alpha}\left[\frac{\pi}{2} - \arctan\frac{2(E_c^2 - \gamma^2)}{\alpha C}\right], \end{aligned} \tag{6}$$

where

$$\begin{aligned}
a_L &= (E_g^2 - E_0^2)E^2 + E_g^2C^2 - E_0^2(E_0^2 + 3E_g^2), \\
a_A &= (E^2 - E_0^2)(E_0^2 + E_g^2) + E_g^2C^2, \\
\gamma &= \sqrt{E_0^2 - \frac{C^2}{2}}, \\
\alpha &= \sqrt{4E_0^2 - C^2}, \\
\zeta_4 &= (E^2 - E_0^2)^2 + C^2E^2,
\end{aligned} \tag{7}$$

and the Urbach tail part (interval from 0 to E_c) leads using sequence evaluation to

$$\begin{aligned}
\epsilon_{1,UT}(E) = \frac{A_u}{E\pi} \sum_{n=1}^{\infty} \frac{1}{{E_u}^n \cdot n \cdot n!} \Bigg\{ & \exp\left(-\frac{E}{E_u}\right) [E^n - (E+E_c)^n] + \\
& + \exp\left(\frac{E}{E_u}\right) [(E_c - E)^n - (-E)^n] \Bigg\} + \\
& + \frac{A_u}{E\pi} \exp\left(-\frac{E}{E_u}\right) [\ln|E| - \ln|E+E_c|] + \\
& + \frac{A_u}{E\pi} \exp\left(\frac{E}{E_u}\right) [\ln|E_c - E| - \ln|E|]
\end{aligned} \tag{8}$$

or using exponential integrals to

$$\begin{aligned}
\epsilon_{1,UT}(E) = \frac{A_u}{E\pi} \Bigg\{ & \exp\left(-\frac{E}{E_u}\right) \left[Ei\left(\frac{E}{E_u}\right) - Ei\left(\frac{E_c+E}{E_u}\right) \right] + \\
& + \exp\left(\frac{E}{E_u}\right) \left[Ei\left(\frac{E_c - E}{E_u}\right) - Ei\left(-\frac{E}{E_u}\right) \right] \Bigg\},
\end{aligned} \tag{9}$$

where the generalized exponential integral is defined by

$$Ei(x) = (C.P.) \int_{-\infty}^{x} \frac{\exp(t)}{t} \, \mathrm{d}t. \tag{10}$$

3 RESULTS AND DISCUSSIONS

Model presented in previous section can be applied to obtain optical material properties from ellipsometric, reflectivity and transmission measurements. For determination of TL function we need to find five parameters (A, E_0, C, E_g, $\epsilon_{1,\infty}$) and only one more parameter is added for Urbach tail extension (E_c). In some cases one can set $\epsilon_{1,\infty} = 1$.

We applied presented model to hydrogenated amorphous silicon Amorphous silicon data were obtained from Palik handbook [7]. Figure 1a shows the models compared with the data. The Tauc-Lorentz model (dashed line) fits well whole spectral range. However the range near (below) edge is improved by inclusion of the Urbach tail (Tauc-Lorentz-Urbach model presented in this paper - solid line). Figure 1b shows detail of the Urbach region. Figure 2 shows the plot of the absorption coefficient in logarithmic scale. Necessity of Urbach tail inclusion is evident.

4 CONCLUSIONS

This paper presents the extension of the Tauc-Lorentz model by inclusion of the Urbach tail. Fitting of tabulated amorphous silicon values shows necessity of using TLU model for modeling dielectric function of amorphous material. Urbach tail extension makes modeled function much closer to measured data, especially at part of the spectra below absorption edge.

Fast evaluation of dielectric function is necessary for many optimization problems, especially for using of this function for in-situ measurement. Presented expressions using sum of elementary functions or exponential integrals (rapidly evaluated by using continuous fractions [8]) are well suited for this objective.

5 ACKNOWLEDGMENTS

The work was partially supported by the projects GA 202/01/0077, GA 202/03/0776 from Grant Agency of Czech Republic and by the projects KONTAKT ME 507, ME 508 from Ministry of Education, Youth and Sport of the Czech Republic.

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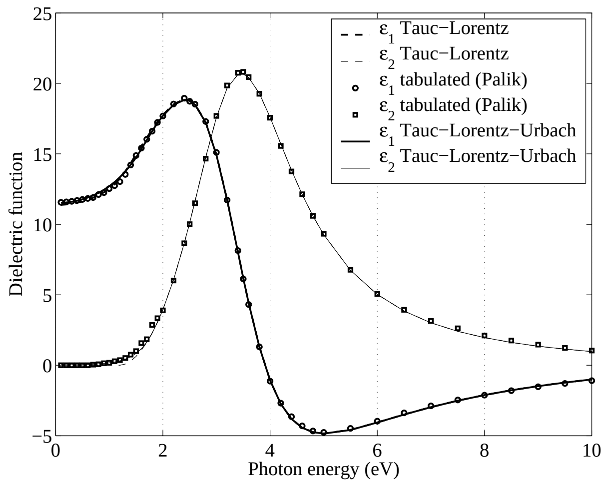
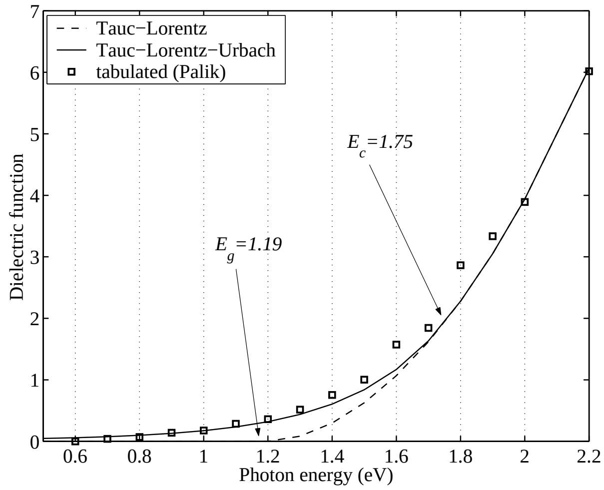


(a)



(b)

Fig. 1. (a) The real and imaginary part of the dielectric function of amorphous silicon as a function of energy,
(b) detail of the imaginary part near the absorption edge.

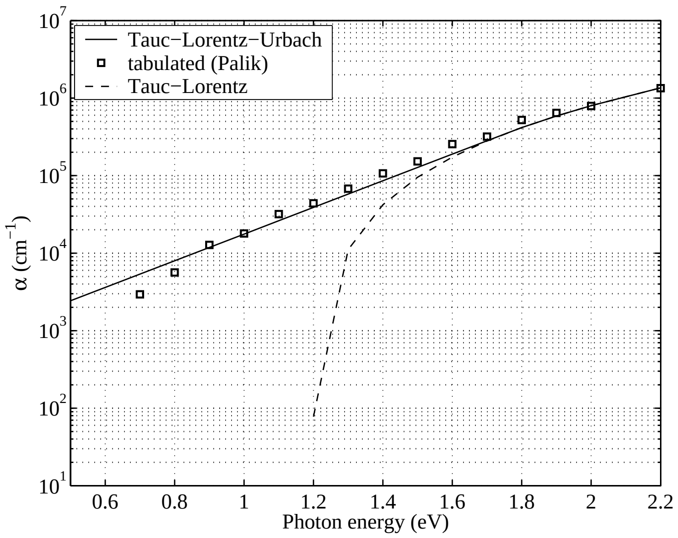


Fig. 2. Detail of absorption coefficient for TL and TLU model in logarithmic scale.