Optical band gap determination issues for amorphous and crystalline metal-oxide thin films

Ilze Aulika, Martins Zubkins, Jelena Butikova, Juris Purans
Institute of Solid State Physis, University of Latvia, Kengaraga 8, LV-1063, Riga, Latvia

The Tauc's method [1] is a much-preferred optical band gap (OBG) evaluate method for amorphous (or glassy) materials. However, regardless its clear and simple purpose, it has been routinely and incorrectly applied to study crystalline semiconductors and dielectrics.

In Tauc relation the density of electron states is close to the VB and CB extrema and it is proportional to the square root of the photon energy E. Thus, the Tauc's bandgap E_{Tauc} of any amorphous semiconductor can be determined by extrapolating the linear least squares fit of absorption α curve $(\alpha \cdot E)^{1/2}$ to zero "$(\alpha \cdot E)^{1/2}$ *versus* E" plot. Assuming a constant dipole transition matrix element, another possibility to determine OBG is to apply the Cody relation [2], in which the Cody's bandgap E_{Cody} arises from the extrapolation of the linear least squares fit of $(\alpha/E)^{1/2}$ to zero "$(\alpha/E)^{1/2}$ *versus* E" plot.

In spite of the method chosen to determine the OBG of either crystalline or amorphous materials, all of them are influenced by the $\alpha(E)$ spectrum and its following data analysis [3].

Recently very nice revision on OBG was published by A. R. Zanatta [3] proposing a unified methodology to its determination for semiconductors by applying the sigmoid-Boltzmann function to fit $\alpha(E)$ spectra and obtain OBG, which works well in case the $\alpha(E)$ spectra is measured at high enough photon energies.

In this work we propose an alternative by using the Johs-Herzinger generalized critical point model [4] or Herzinger-Jobs parameterized semiconductor (HJPS) oscillator function [5] to directly fit the $\alpha(E)$ spectra. The results are discussed for amorphous and crystalline ZnO, ZnO_2 and YHO [6] thin films by applying Tauc, Cody, sigmoid-Boltzmann function and HJPS.

ACKNOWLEDGMENTS
This research is supported by the Horizon 2020 Project CAMART² under grant agreement No 739508, ERAF national project "Smart metal-oxide nanocoating and HIPIMS technologies" No 1.1.1.1/18/A/073, and national project "Thin films of rare-earth oxy-hydrides for photochromic applications" FLPP No LZP-2020/2-0291.

References

[1] Tauc, J., Grigorovici, R. & Vancu, A. Optical properties and electronic structure of amorphous germanium. phys. stat. sol. (1966) 15(2), 627–637, https://doi.org/10.1002/pssb.19660150224
[2] Cody, G. D., Brooks, B. G. & Abeles, B. Optical absorption above the optical gap of amorphous silicon hydride. *Solar Energy Mater.* (1982) 8(1–3), 231–240, https://doi.org/10.1016/0165-1633(82)90065-X
[3] A. R. Zanatta, Revisiting the optical bandgap of semiconductors and the proposal of a unified methodology to its determination, Scientific Reports (2019) 9:11225, https://doi.org/10.1038/s41598-019-47670-y
[4] P. Petrik, Parameterization of the dielectric function of semiconductor nanocrystals, Physica B: Condensed Matter (2014) V453, 2-7, https://doi.org/10.1016/j.physb.2014.03.065
[5] Craig M. Herzinger; Blaine D. Johs., DIELECTRIC FUNCTION PARAMETRIC MODEL, AND METHOD OF USE, Patent Number: 5796983
[6] M. Zubkins et al., Amorphous ultra-wide bandgap ZnOx thin films deposited at cryogenic temperatures, J. Appl. Phys. 128, 215303 (2020), https://doi.org/10.1063/5.0028901