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Colloidal synthesis of pure $CuInTe_2$ crystallites based on the HSAB theory

Nthabiseng Ntholeng[1], Benny Mojela[1], Siziwe Gqoba[1], Mildred Airo[1], Stefan Govindraju[1,2], Makwena J. Moloto[3], Juanita van Wyk[1], Nosipho Moloto[1,2*]

[1]Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Private Bag X3, Johannesburg, South Africa, 2050

[2]Materials for Energy Research Group, University of the Witwatersrand, Private Bag 3, Wits, 2050, Republic of South Africa

[3]Department of Chemistry, Vaal University of Technology, Private Bag X021, Vanderbijlpark, 1900, Republic of South Africa

*Corresponding Author: N. Moloto

Email: Nosipho.Moloto@wits.ac.za

Tel: +27117176774

Fax: +27865228349

Optical measurement calculations

The UV-Vis absorption spectroscopy is frequently used to characterize semiconductors thin films.[1] Due to low scattering in solid films, it is easy to extract the E_g values from their absorption spectra knowing their thickness.[1] However, it is possible to obtain the powdered samples instead of thin films or colloids and their UV-Vis absorption measurements is frequently carried out by dispersing samples in liquid media.[2] Dispersing the powdered materials in liquid media can result in contamination or consumption of the material which will make the absorption spectrum challenging to interpret.[2] If the absorption peak is not well resolved, it may be difficult to estimate the E_g thus leading to inaccurate conclusion. On the hand the use of DRS (Diffuse Reflectance Spectroscopy) is more convenient as it takes advantage of the enhanced light scattering in powdered materials.[2] However, it is possible to determine the band gap from diffuse reflectance spectrum using the Tauc plot. The following relational expression proposed by Tauc, Davis, and Mott is used.

$$(h\nu\alpha)^{1/n} = A(h\nu - Eg) \qquad (1)$$

Where, h: Planck's constant, ν: frequency of vibration, α: absorption coefficient, Eg: band gap, A: proportional constant. The value of the exponent n denotes the nature of the sample transition.

For direct allowed transition, n = 1/2

For direct forbidden transition, n = 3/2

For indirect allowed transition, n = 2

For indirect forbidden transition, n = 3

Since the direct allowed sample transition is used in this experiment, n = 1/2 is used for these samples. The acquired diffuse reflectance spectrum is converted to Kubelka-Munk function.

Thus, the vertical axis is converted to quantity F(R∞), which is proportional to the absorption coefficient. The α in the Tauc equation is substituted with F(R∞). Thus, in the actual experiment, the relational expression becomes:

$$(h\nu F(R\infty))^2 = A(h\nu - Eg) \qquad (2)$$

Using the Kubelka-Munk function, the $(h\nu F(R\infty))^2$ was plotted against the hν. The curve that plots the value of $(h\nu - (h\nu F(R\infty))^2)$ on the horizontal axis hν and vertical axis (hνF(R∞))2 is drawn. Here, the unit for hν is eV (electron volts), and its relationship to the wavelength λ (nm) becomes hν= 1239.7/λ. A line is drawn tangent to the point of inflection on the curve of step (3), and the hν value at the point of intersection of the tangent line and the horizontal axis is the band gap E_g value.

References

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