Considerations about the determination of the band gap from diffuse reflectance spectroscopy

Salmon Landi Jr.[a,*], Iran Rocha Segundo[b,**], Elisabete Freitas[b], Mikhail Vasilevskiy[c], Carlos José Tavares[c], Joaquim Carneiro[c]

[a]Federal Institute Goiano, Rio Verde, Goiás, 75901-970, Brazil

[b]Civil Engineering Department, University of Minho, Azurém Campus, Guimarães, 4800-058, Portugal

[c]Centre of Physics of the Universities of Minho and Porto, Gualtar Campus, Braga, 4710-057, Portugal

[*]salmon.landi@ifgoiano.edu.br

[**]iran_gomes@hotmail.com

The determination of the band gap energy of semiconductors is important for the understanding of the production of the electron/hole pairs under the light irradiation, which, in the case of photocatalytic materials, are related to their properties and efficiency. The photoexcited electrons and holes are good reductant and powerful oxidant species, respectively. As consequence the free radicals formed can to degrade, after a sequence of redox reactions, various pollutants present in water or air. Diffuse Reflectance Spectroscopy (DRS) is a technique frequently employed to study the optical properties of solids. In this context, the Kubelka-Munk model (K-M model) [1] has been extensively applied to investigate the light scattered diffusely from the surface of semiconductor materials in the form of powders including composite materials. However, in some papers published recently, including some in prestigious journals in the field of Materials Science, it is possible to perceive some inconsistency when the subject matter is the K-M model. Specifically, these problems consist in interpreting the Kubelka-Munk function, $F(R)$, as the absorption coefficient [2,3], assigning an arbitrary unit for the dimensionless $F(R)$ [4–6] or even confuse the K-M function with the equation that frequently is used to estimate the band gap energy [7–9]. These oversimplified or even incorrect interpretations may confuse the readers concerning the applicability and validity of the K-M model. Therefore, the main objective of this work is to explain all the necessary steps to obtain and interpret $F(R)$, as well as to apply it for the determination of the band gap from DRS data of a polycrystalline powder of the wide-gap semiconductor TiO_2. Thus, with this work it is expected to help researchers who are starting their studies involving the determination of the band gap from DRS data and to clarify the procedure to those who could be confused due to the various drawbacks previously identified.

[1] P. Kubelka and F. Munk, Zeitschrift Fur Tech. Phys. **12**, 593 (1931).

[2] D.M. Tobaldi, R.C. Pullar, A.F. Gualtieri, G. Otero-Irurueta, M.K. Singh, M.P. Seabra, J.A. Labrincha, J. Solid State Chem. 231 (2015) 87–100.

[3] B. Dai, M. Xuan, Y. Lv, C. Jin, S. Ran, Mater. Res. 22 (2019).

[4] Y. Zhang, C. Pan, J. Mater. Sci. 46 (2011) 2622–2626.