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Title

Phenomenological Studies Towards the Improvement of Methodologies for Thermoluminescence Glow Curve Analysis.

Synopsis

Study of thermoluminescence (TL) involves recording optical glow on heating a previously irradiated TL material. Glow curve analysis (GCA) is a widely used technique to extract important information related to irradiation stage, trap states, charge transfer mechanism etc. For this reason, the TL phenomenon finds applicability in different fields of research like dosimetry, defect studies and dating. However, in an experimental scenario, GCA is quite critical and sometimes may become even misleading due to the lack of ab-intio theoretical background. Hence multiple methods depending on the nature of glow curves are needed to validate the results. For obvious reasons, theoretical analysis of TL is subject to various approximations and grossly depend on various models and methods. Therefore improving the present methodologies on the backdrop of various approximations and developing new methodologies with comparative analysis are in the active interest of researchers. Moreover, analyzing the TL data from a statistical viewpoint and hence to find suitable statistical distribution functions applicable to 'distribution' of intensity over temperature can be a potential approach to develop new methodologies.

This dissertation is organized in six chapters. The outline of the chapters are given below.

Chapter 1

In the 'Introduction' chapter, a brief description of the TL process and its importance in various fields of research is given. An account of the development in this field through different approaches based on various models has been discussed. The basic features of different methodologies of TL glow curve analysis are also included in this chapter. The focus and motivation of the present study on the backdrop of previous developments are discussed.

Chapter 2

The integral of the form $J(T_i, T_f, a) = \int_{T_i}^{T_f} T^a e^{-\frac{E}{kT}} dT$ occurs frequently in the theoretical analysis of various thermally stimulated process. The value of the exponent a may lie within the range $-2 \leq a \leq 2$. However, in traditional TL studies, $a = 0$ is mostly considered. For $a = 0$ the integral is called as 'temperature integral' and for $a \neq 0$, it may be referred to as 'extended temperature integral'. These integrals cannot be evaluated analytically in a closed form and various approximated methods have been reported in literature. In this chapter, we describe a new analytical method to evaluate the temperature integral using converging infinite series. The present method is not subject to any approximation other than truncating the converging infinite series after a suitable number of terms. The evaluation can be computationally realized through a simple computer code. A brief review of some of the previous approaches is also included here. The results of the present method has been compared with other methods for numerical validation of the present approaches.

Chapter 3

In this chapter we have developed two versions of peak shape relations for GCA on the basis of two newly introduced symmetry parameters: (i) average symmetry factor ($< \mu'_g >$) and (ii) skewness (S_k) of TL data. The applicability of both the methods is verified by applying them to simulated and experimental TL peaks. The present methods yield consistent results for all cases except for the highly saturated peaks with heavy retrapping. The reason behind the limitation is also explained by investigating the dependence of S_k and μ'_g and on the ratio of retrapping to recombination probabilities. The results of present peak shape methods are compared with other methods for further establishing their applicability in glow curve analysis.

Chapter 4

Frequency factor related to a trap state slowly varies with temperature. However in TL studies, it is assumed as a temperature independent quantity for experimental intricacies as well as theoretical realization. Such assumption may lead to certain inaccuracy in estimating trapping parameters. In this chapter, an account on the impact of temperature dependence of frequency factor on glow curve analysis is given. The temperature dependence of frequency factor is not known beforehand and hence to simulate the same glow curve for different temperature exponents is quite challenging. An efficient methodology to simulate the same glow peak for temperature dependent frequency factor (TDFF) has been discussed. Impact of TDFF in GCA is investigated by adopting different versions of 'peak shape methods' and 'area methods'. In 'area method' we have emphasized on the newly developed 'Three Point Area' method.

Chapter 5

The challenge in GCA of a complex glow curve is to isolate and analyze its component peaks. Glow curve deconvolution (GCD) is a potential method for this purpose. In this chapter we focus to develop a new GCD function on the basis of statistical distribution of data. At first we adopted the Gaussian distribution as a starting ground to proceed further in this direction. The suitability of Gaussian distribution in GCD have been critically examined, however, for obvious reasons, the results are not quite satisfactory. In the next phase, considering the skewed nature of TL data, we propose a version of skew-normal distribution characterized by five parameters. We investigate the suitability of this new probability function and apply it to a large number of TL glow curves simulated in various models. As a pilot investigation, we have considered the TL curves which are equivalent to first and second order kinetics. The quality of fitting is judged through residue plots as well as through the correlation between the TL data and fitted data. The present analysis shows good possibility of applying the skew-normal distribution for GCD in TL studies.

Chapter 6

We finally conclude all the findings reported in the dissertation in previous chapters. A consolidated account of the present work on developing new methodologies along with the theoretical developments is presented. We also discuss the potential future scopes of these works which will pave the way for further development towards the different fields of research engaging thermoluminescence as well as other thermally stimulated processes.

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