Deconvolution of Thermoluminescence glow curves due to kinetic consideration: TL Simulation of natural quartz and feldspar

*Alvaro Josue Amaya[1], Nobuo Hirano[1], Noriyoshi Tsuchiya[1]

1. Tohoku University. Graduate School of Environmental Studies

Thermoluminescence is a property of some minerals to emit light when they are heated (McKeever, 1985); the TL concept is explained by physics atomic science and it is possible in natural minerals due to defects in the crystal lattices, provides the possibility that excited electrons (from natural or artificial irradiation source) can be trapped and recombined at specific activation of energy levels when they are heated, that’s why TL is used in radiation measurement science, but its applications in earth science are also being increased each time, g.e TL has been widely used for geological dating materials that were annealed with heat in an undetermined but specific time event through additive paleodose experiments for mineral analysis, also used for young thermochronology geomaterials since the middle of 20th century. Also, TL is used in Natural geothermal systems since Tsuchiya (2000) thermoluminescence of quartz has been used as natural heat sensor for prospection uses. The accuracy of mathematical expression that simulates experiments can affect geochronology or datation analysis, therefore in this research analytic exact expressions of glow curve deconvolution equations and its demonstration were developed for all thermoluminescence application that needs kinetic parameters extraction or simulation by using the widely known Randal and Wilkins (1945) thermoluminescence model, but this time considering a new mathematical way to get solutions through the establishment of an explicit reference point for experimental initial temperature and time in linear heating rated TL processes. A validation with Kitis (1998) expressions shows the accuracy in between them, considering that this method proposes an exact solution of the equation system the figure of merits FOM shows higher differences for first order of kinetics for artificial traps when peak temperatures increases and activation energy decreases, (e.g. FOM 6.29%, at Tm=600K and E=0.7eV). This new equation set was used to simulate natural quartz and feldspar from geothermal areas in Japan, providing a kinetic parameter analysis useful for other applications developments as for instance, geothermometers or new datation methodologies. The functionality of this new set of equations is emphasized since thermoluminescence is a phenomenon where the probability of thermal excitation of a carrier is assumed to be given by a Boltzmann factor [s=so.exp(-E/KT)] that contains the kinetic variables necessary for mathematical modeling from each trap center, therefore the exponential treatment for integration or derivation necessary for getting solutions of the differential system of equations, finally imposes some restrictions or approximations for the classic approaching that this new solution has improved in analytical or explicit way. This research and functions resultants are useful for materials which are wanted to be evaluated for any application of TL by parametric analysis, some of the parameters gotten are: maximum peak intensity or initial concentration of holes trap, activation energy, peak temperature, the probability of electron escape. This model uses the 2 levels system for one trap and one recombination level but expressions resultants are autoconvoluted, it means that can be used also for materials or minerals with multitrap centers by a simple addition of the expression in an analytical way. The functions presented are for a first, second and general order of kinetics and set of analytical expressions can be chosen for classic parameters or those ones which prefer maximum peak conditions for easy and quick fitting. Also set of equations are presented for both independent variable possible temperature and time. The simulation of quartz and feldspar give us some important properties for future application of them in different earth scientific application.

Keywords: Thermoluminescence, GLow curve deconvolution equations, TL Kinetic of natural quartz and feldspar, Thermochronology

