Nuclear Inst. and Methods in Physics Research B 436 (2018) 249–256

Contents lists available at ScienceDirect

Nuclear Inst. and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

Thermoluminescence glow curves in preheated feldspar: A Monte Carlo study

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ARTICLE INFO

Keywords:
Thermoluminescence in feldspars
Monte Carlo kinetic analysis
Tunneling

ABSTRACT

Thermoluminescence (TL) glow curves from feldspars have been the subject of numerous experimental and modeling studies, because of their importance in dosimetry and luminescence dating. Recently there also has been increased interest in using these signals for temperature sensing and for thermochronometry studies. It is now generally accepted that these materials exhibit anomalous fading phenomena due to quantum mechanical tunneling, and that several of their luminescence signals can be described by localized energy transitions taking place in a randomly distributed system of trapped electrons and recombination centers. Our recent modeling work showed that the TL signals of freshly irradiated feldspar samples can also be described from a completely microscopic point of view, by using Monte Carlo methods. This paper extends this recent work, and shows how the Monte Carlo method can also describe TL signals from thermally pretreated feldspars. Specifically, the simulations show that the Monte Carlo method can describe several types of TL experiments for irradiated samples that underwent partial thermal cleaning, and for samples that underwent more complex multistage isothermal procedures. The results from the Monte Carlo simulations are compared quantitatively with experimental data from several types of feldspars, which were preheated at temperatures above 200–300 °C. Common experimental characteristics are pointed out for these preheated feldspars, and the experimental data suggest the possibility of a universal description of the thermal behavior of TL glow curves in feldspars. Specifically, it is found that the shape and width of the experimental TL glow curves do not change significantly for different preheat temperatures, and also do not change when different preheat times are used at a fixed preheat temperature. The relevance of these results for dosimetric and thermochronometry studies is discussed.

1. Introduction

Thermoluminescence (TL) signals from feldspars have been studied extensively both experimentally and by modelling, due to their importance in dosimetry and luminescence dating. During the past few years, there has also been increased interest in using TL glow curves in feldspars as the basis of temperature sensing and in thermochronometry studies (Brown et al. [1]; Yukihara et al. [2]; Biswas et al. [3]; and references therein). These studies have been based on changes taking place on the properties of TL glow curves when samples have been exposed to different thermal or optical treatments, for both naturally and laboratory irradiated samples.

It is now generally accepted that luminescence signals in feldspars originate from a random distribution of trapped electrons and acceptors in these materials, and that the luminescence process involves localized transitions (Jain et al. [4]).

From a modeling point of view, two different approaches have been developed which are based on a *macroscopic* versus a *microscopic* description of the luminescence process.

In the *macroscopic* point of view based on differential equations, it is assumed that the number of trapped electrons is much smaller than the number of acceptors, and therefore the system can be described by a constant number density of acceptors . Based on this assumption and on the quasi-equilibrium conditions, Kitis and Pagonis [5] obtained analytical solutions of the system of differential equations in the model by Jain et al. [4], and these equations have been used to analyze a wide variety of luminescence signals in feldspars and other dosimetric materials ([6–8], and references therein).

In the alternative *microscopic* point of view, a Monte Carlo approach has been used to describe the luminescence process based on quantum tunneling interactions of a small number of defects in a nanometer-sized volume [9–13]. In this second approach, it is not necessary to assume that the number density of acceptors is constant, and the results of the simulations depend on the relative concentrations of electrons

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https://doi.org/10.1016/j.nimb.2018.09.036
Received 14 September 2018; Received in revised form 25 September 2018; Accepted 25 September 2018

and acceptors. A significant advantage of the Monte Carlo method is that it can easily be extended to include additional phenomena of interest to the luminescence dosimetry and dating community. Specifically, the Monte Carlo method can also be used to study irradiation phenomena, the presence of multiple types of traps, and retrapping phenomena [10–12].

In a typical TL experiment, one measures two different types of signals. In the first type of measurement, a freshly irradiated sample is immediately heated with a linear heating rate, and one measures the *prompt* TL signal. In the second type of measurement, the freshly irradiated sample undergoes a thermal or optical treatment, before measurement of the *remnant* TL signal.

The recent modeling work by Pagonis and Truong [13] showed that *prompt* TL signals of freshly irradiated feldspar samples can be described from a completely *microscopic* point of view, by using Monte Carlo methods. By using the alternative *macroscopic* differential equation approach, Polymeris et al. [7] showed that it is possible to simulate complex experimental protocols in feldspars, which involve multiple stages required to measure the *remnant* TL signal.

The general purpose of this paper is to extend the work of Polymeris et al. [7] and Pagonis and Truong [13], by using the alternative Monte Carlo method to describe TL glow curves in preheated feldspar samples.

The specific goals of the simulations in this paper are:

- To simulate the well-known fractional glow method of analyzing TL glow curves in feldspars, by using a Monte Carlo technique.
- To investigate by simulation the effect of varying the preheat temperature and preheat time on the TL glow curves, and to compare with experimental data in a quantitative manner.
- To examine in detail the changes occurring in the shape and position of the TL glow curves, and to look for universal behaviors in both the simulated glow curves, and in available experimental data.

2. Experimental

Two sets of experimental data in this paper are analyzed in this paper, and these were previously described by Pagonis et al. [8,14] and by Polymeris et al. [7]. What is new in this paper is the analysis of these previously published data using Monte Carlo methods, based on the microscopic description of tunneling phenomena.

The first set of experimental data shown in Fig. 1a, concerns a museum specimen of feldspar (laboratory code FL3), which was placed in the plagioclase feldspar series by the detailed analysis presented in Morthekai et al. [15]. The analysis included elemental concentrations using ICP-MS measurements and X-ray Diffraction analysis. The 90–150 μm size fraction of the samples were used without any further chemical treatment, and a Risø TL/OSL Reader DA-20 was used for all measurements. The luminescence emission was detected using a photomultiplier tube (EMI 9235QB; 30% QE at ~395 nm) with a combination of optical filters BG-39 (2 mm) and Corning 7–59 (4 mm), transmitting in the wavelength region (395 ± 50) nm. The heating rate was 1.8 °C/s in a nitrogen atmosphere. The TL glow curves of the feldspar samples shown in Fig. 1a are obtained using a T_{MAX}–T_{STOP} thermal cleaning procedure, as follows. A single aliquot of the material is irradiated with a beta dose of 21.3 Gy, then subsequently heated up to a temperature T_{STOP}, and cooled to room temperature. Immediately after, the aliquot is heated all the way to a high temperature of 450 °C and the *remnant* TL glow curve is obtained. The process is then repeated several times by irradiating with the same dose and heating the same aliquot to a slightly higher temperature T_{STOP} each time, in steps of 10 °C for the complete interval T_{STOP} = 210–400 °C.

Fig. 1b shows the same results as in Fig. 1a, with the TL glow curves shifted along the temperature axis, and scaled to the maximum intensity of the first TL glow curve. After this scaling and temperature-shifting procedure, the twenty remnant TL glow curves coincide with each other within experimental error, indicating that *the preheating procedure did not significantly change the TL glow curve*. This is a rather remarkable experimental result, which to the best of our knowledge has not been pointed out previously for feldspars, and which is discussed further later in this paper.

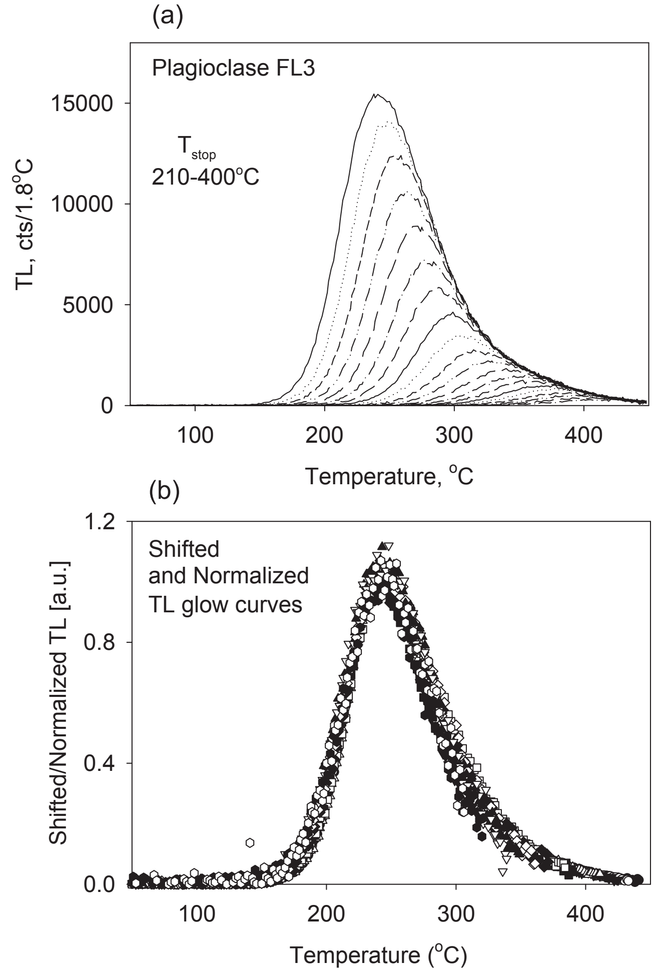

Fig. 1. (a) Remnant TL glow curves of a plagioclase feldspar sample FL3, obtained using a T_{MAX}–T_{STOP} thermal cleaning procedure. This sample was previously studied in Refs. [14,15]. (b) The same data as in (a), after the TL glow curves are shifted along the temperature axis, and scaled to the maximum intensity of the first TL glow curve. This scaling and temperature-shifting procedure shows that the preheating procedure did not significantly change the shape of the TL glow curve.

The second set of experimental data analyzed in his paper concerns a set of K-feldspar samples shown in Fig. 2a and 3a of this paper, and previously studied by Pagonis et al. [8], and Polymeris et al. [7,16]. These previous experimental studies demonstrated the possibility of using TL for structural characterization of ten K-feldspar samples consisting of 3 sanidine, 4 orthoclase and 3 microcline feldspars. A good correlation was shown between TL sensitivity and individual K-feldspar structure, and it was suggested that these samples are ideal for investigating various basic luminescence signals in feldspars. Data from five of the ten samples described in Polymeris et al. [16] are analyzed in this paper, namely microcline samples KST4 and LED1, sanidine sample SAM3, orthoclase sample VRS3 and sanidine sample BAL21. The luminescence measurements were carried out using a Risø TL/OSL reader (model TL/OSL-DA-15), equipped with a $^{90}Sr/^{90}Y$ beta particle source, delivering a nominal dose rate of 0.075 Gy/s. A 9635QA photomultiplier tube was used with a 7.5 mm Hoya U-340 filter (~340 nm, FWHM ~80 nm). A combination of Pilkington HA-3 heat absorbing and Corning 7–59 (320–440 nm) blue filter were used for light detection,