Available online at www.sciencedirect.com
ScienceDirect
SoftwareX 5 (2016) 112–120
SoftwareX
www.elsevier.com/locate/softx

tgcd: An R package for analyzing thermoluminescence glow curves

Jun Peng[a,*], ZhiBao Dong[a], FengQing Han[b]

[a] Cold and Arid Regions Environmental and Engineering Research Institute, Chinese Academy of Sciences, 320 Donggang West Road, Lanzhou, China
[b] Qinghai Institute of Salt Lakes, Chinese Academy of Sciences, 18 Xinning Road, Xining, China

Received 21 September 2015; received in revised form 1 June 2016; accepted 3 June 2016

Abstract

Thermoluminescence (TL) glow curves are widely used in dosimetric studies. Many commercial and free-distributed programs are used to deconvolute TL glow curves. This study introduces an open-source R package tgcd to conduct TL glow curve analysis, such as kinetic parameter estimation, glow peak simulation, and peak shape analysis. TL glow curves can be deconvoluted according to the general-order empirical expression or the semi-analytical expression derived from the one trap-one recombination center (OTOR) model based on the Lambert *W* function by using a modified Levenberg–Marquardt algorithm from which any of the parameters can be constrained or fixed. The package provides an interactive environment to initialize parameters and offers an automated "trial-and-error" protocol to obtain optimal fit results. First-order, second-order, and general-order glow peaks (curves) are simulated according to a number of simple kinetic models. The package was developed using a combination of Fortran and R programming languages to improve efficiency and flexibility.

Keywords: TL glow curve; Deconvolution; Simulation; R package

Code metadata

Current code version	v1.9
Permanent link to code/repository used of this code version	https://github.com/ElsevierSoftwareX/SOFTX-D-15-00066
Legal Code License	GPL-2 or GPL-3
Code versioning system used	None
Software code languages, tools, and services used	Fortran 77, Fortran 90, and R
Compilation requirements, operating environments & dependences	R software
If available Link to developer documentation/manual	https://github.com/ElsevierSoftwareX/SOFTX-D-15-00066/blob/master/README.pdf
Support email for questions	pengjun10@mails.ucas.ac.cn

1. Motivation and significance

Thermoluminescence (TL) is the light emitted by a material when heated, which results from emissions of absorbed energy. Most semiconductors or insulators display a TL glow curve that consists of one or more peaks when charge carriers are released. The goal of TL glow curve analysis is to estimate parameters that can then be used to describe TL processes that take place in the material [1]. A number of computer procedures have been developed to fit TL glow curves. Many use commercial software as running platforms. Using Mathematica software, Pagonis et al. [1] presented comprehensive examples of TL data analysis for glow curves following first-order, second-order, and general-order kinetics. Harvey et al. [2] and El-Hafez et al. [3] used MATLAB software to fit first-order TL glow curves. Afouxenidis et al. [4] employed a spreadsheet program to fit general-order TL glow curves. Kiisk [5] used the Mathcad program to fit a few common analytical approximations of first-order TL glow curves. Some studies have also used the PEAKFIT and MINUIT software programs to fit TL glow

* Corresponding author.
E-mail address: pengjun10@mails.ucas.ac.cn (J. Peng).

http://dx.doi.org/10.1016/j.softx.2016.06.001

curves [6,7]. Two self-contained and freely accessible packages for TL glow curve deconvolution are TLanal [8], which fits first-order, second-order, and general-order kinetics, and Glowfit [9], which fits first-order kinetics. Given that many researchers do not have access to commercial software, the use of commercial software as running platforms largely results in the restrictive redistribution of a program. Moreover, some popular programs (such as TLanal and Glowfit) are designed to only work under Microsoft Windows operating systems and are therefore black boxes to non-software engineers. Alternatively, R is a free software environment for statistical computing and graphics [10]. Furthermore, R runs on a wide variety of operating systems (Linux, Windows, and MacOS). It is also considered as a well-developed, simple, and effective programming language. R can easily communicate with external programming languages such as Fortran, C++, and C. Acceptable running speeds can be achieved by writing the time-consuming part of a program in Fortran or C++ and linking it to R using an interface [11].

It has been previously reported that TL glow curve deconvolution can yield unreliable fit results while being mathematically correct [9]. The analysis of TL glow curves relies on using carefully measured data sets, given that any errors in measurements can lead to incorrect results in computerized programs [1]. Curve fitting methods based on a particular theoretical model should be applied with the utmost care, and extreme caution should be taken when drawing conclusions [12]. Furthermore, the deconvolution of complex glow curves may not converge to unique results unless sufficiently stringent constraints are imposed [5]. Complex glow curves consisting of strongly overlapping peaks or having very poor statistics can be resolved by setting constraints or by fixing particular parameters [9]. In the R package tgcd, the Levenberg–Marquardt algorithm, implemented using the Fortran subroutine MINPACK [13], was modified to allow the fixing or constraining of any parameter in order to enable the user to obtain meaningful fit results from complex glow curves. Fixed parameters remain unchanged during the fitting process.

May and Partridge [14] first proposed a general-order kinetic equation with the kinetic order b, ranging from 1 to 2 for intermediate cases between first-order and second-order kinetics. For over two decades, general-order kinetics have most commonly been applied to analyze TL glow curves. Recently, Kitis and Vlachos [15] developed new semi-analytical expressions for TL glow peaks based on the one trap-one recombination center (OTOR) model using the Lambert W function. Sadek et al. [16,17] found that the developed OTOR TL expressions can accurately describe TL glow peaks even in cases where other TL expressions have failed. Sadek et al. [18] suggested that OTOR TL expressions are the most suitable expressions to use in deconvolution of experimental glow curves given that the peak fitting method applying these expressions can provide accurate values for activation energy of glow peaks whether re-trapping or recombination is dominated. In the R package tgcd, glow curves can be deconvoluted according to the general-order empirical expression provided by Kitis et al. [19] or the semi-analytical expression derived from the OTOR model using the Lambert W function outlined by Sadek et al. [20] and Kitis et al. [21]. Fitting equations of the two different types of models are presented in detail in the User Manual of the R package (for the permanent link, see row 7 of the Code Metadata Table) and therefore will not be repeated here. The quality of fit is measured by the figure-of-merit (FOM) [22].

Mathematically speaking, fitting TL glow curves is an ill-conditioned problem, and fit results are very sensitive to the choice of initial parameters. To obtain reasonable fit results, it is essential to rerun procedures with various initial parameters. In the MATLAB program developed by Harvey et al. [2], for example, parameters were repeatedly optimized using previously gathered knowledge related to peak positions and activation energies taken from literature as starting points until the best possible fits were obtained. A differential evolution algorithm was also suggested to automatically initialize starting parameters of an optically stimulated luminescence (OSL) decay curve [23]. This algorithm has been successfully implemented in R package numOSL [24]. For fitting TL glow curves, however, stochastic algorithms of this kind are impracticable as the number of unknown parameters is very large compared to those in OSL decay curves. Accordingly, user-provided initial parameters are generally required by most existing programs. The glow curve analysis (GCA) program [25] provides an algorithm to automatically search glow peak positions, but some peaks initialized by this method may require manual adjustment before running the program [9].

It demonstrates that quality of fit is much more dependent on the position of glow peaks than on other parameters [26]. Both TLanal [8] and Glowfit [9] software offers a convenient and intuitive way to initialize parameters by using a mouse to click on glow curves at positions where peak maxima should be located. The R package tgcd offers a similar way to locate peak temperature (T_m) and peak intensity (I_m) for each glow peak with the aid of a mouse. On execution, a graph of the original glow curve data is automatically drawn to prompt the user to locate the coordinate ($x = T_m$, $y = I_m$) of each glow peak. The R package also offers an alternative to initialize parameters by using a matrix to store initial parameter guess values [5]. However, this method is only feasible if the peak position and activation energy of each glow peak have been well determined for the type of TL dosimeter being analyzed [2]. For complex glow curves that consist of a number of glow peaks, this parameter initialization method can be tedious.

To enable the user to obtain an optimal fit result, the R package provides an automated "trial-and-error" protocol using random parameters generated around starting values to repeatedly fit the glow curve at certain times (the allowed maximum number of random trials *nstart* is specified by the user). Given that the procedure was programmed using the Fortran language, the "trial-and-error" protocol is very efficient. Fitting parameters that yield the lowest FOM values will be treated as optimal fit results. However, "optimal" parameters with very low FOM values that are minimized using the automated "trial-and-error" protocol may be characterized by glow peaks with large total half-widths

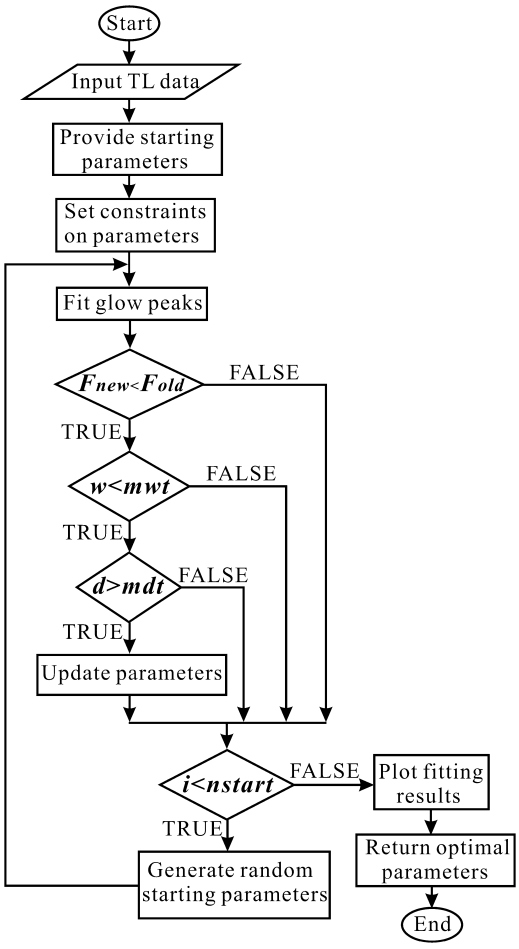


Fig. 1. Flow chart of TL glow curve deconvolution using the automated "trail-and-error" protocol. F_{new} and F_{old} denote FOM values that are minimized from current and prior random trials, respectively. w denotes the calculated maximum total half-width of the optimized glow peaks, *mwt* represents a threshold of allowed maximum total half-width of glow peaks specified by the user, d denotes the calculated minimum distance between peak temperatures, *mdt* represents a threshold of allowed minimum distance between peak temperatures specified by the user, i denotes the current number of random trials, and *nstart* represents the allowed total number of random trials specified by the user.

or by severely overlapping glow peaks with undistinguishable peak temperatures. In such cases, the parameters obtained may be meaningless from a physical point of view. In the R package tgcd, the appearance of glow peaks with large total half-widths is avoided by setting the threshold *mwt* that denotes the allowed maximum total half-width for glow peaks, and the appearance of glow peaks with undistinguishable peak temperatures is avoided by setting the threshold *mdt* that denotes the allowed minimum distance between peak temperatures. In these ways, the program will be prompted to accept fit results for which glow peaks have smaller total half-widths and more distinguishable peak temperatures. A flow chart using the automated "trial-and-error" protocol to obtain meaningful fit results for complex glow curves is provided in Fig. 1.

Kinetic models can improve our basic understanding of the physical processes being studied [27]. For example, they can be used to investigate the effects of kinetic parameters on characteristic properties of glow peaks [1,28]. However, most of the existing programs designed for TL glow curve deconvolution do not provide routines to simulate TL glow peaks or to analyze the shape of a glow peak. TL processes for first-order, second-order, and general-order glow peaks can be simulated using the Randall–Wilkins, Garlick–Gibson, and May–Partridge kinetic models, respectively [1]. Sunta [28] provided a detailed description of these conventional models. Under certain conditions, the OTOR model may also lead to first-order, second-order, and intermediate kinetic order glow peaks [29]. Pagonis et al. [1] used these kinetic models to simulate TL glow peaks of various kinetic orders using Mathmatica. The R package tgcd offers numeric routines to simulate glow peaks according to these kinetic models. Ordinary differential equations were solved using a robust Fortran subroutine called DLSODA [30,31] in which temperature values, where TL intensities will be computed, are supplied by the user as a vector. The procedure can also be used to simulate glow curves consisting of a number of glow peaks via summating.

To conclude, the aim of the development of the R package tgcd was to: (1) achieve an openly accessible and easy-to-use numeric package that is portable across a wide range of computers and operating systems; (2) realize flexible and efficient optimization tactics that make it easy to obtain optimal fit results in TL glow curve deconvolution; (3) offer handy numeric routines to simulate TL glow peaks (curves) according to several simple kinetic models; and (4) provide convenient data import/export and high-quality graphical outputs.

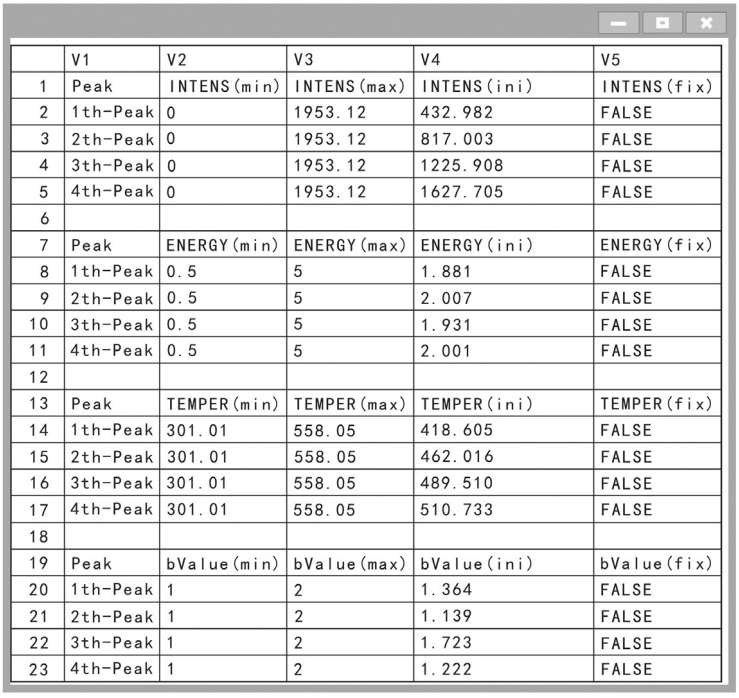
2. Software description

The R package tgcd is self-contained and does not depend on any other external R package. Programs were developed using Fortran and were wrapped by R using an interface. A data set containing two reference glow curves (Refglow002 and Refglow009) from the GLOCANIN project [32,33] were bundled into this package. A summary of data sets and functions available from this package is provided in Table 1. The package was assessed using a variety of running platforms, and its latest version (version 1.9), including the User Manual, is downloadable from the Comprehensive R Archive Network (CRAN) (http://CRAN.R-project.org/package=tgcd). The package can be downloaded and installed into R software by following the two subsequent steps: (1) download and install the package from CRAN via inputting the command *install.packages("tgcd")* into the R console; (2) load the package using the command *library(tgcd)* or *require(tgcd)*.

To simulate a glow peak, the user needs to supply parameters, such as the initial concentration of trapped electrons (n_0), the frequency factor (*ff*), the activation energy (*ae*), the heating rate (*hr*), etc. For glow curve deconvolution, the user must supply temperature and TL signal values stored in a two-column data frame (or matrix). The data set can be loaded into the R console using the internal R function *read.table()*. Additional arguments that need to be specified

Table 1
A summary of data sets and functions available from the latest version of the R package tgcd (version 1.9).

Function/data set	Description
Refglow	Reference glow curves Refglow002 and Refglow009 from the GLOCANIN project
simPeak()	To simulate first-order, second-order, and general-order glow peaks
simqOTOR()	To simulate glow peaks according to the OTOR model using quasi-equilibrium approximation
tgcd()	To deconvolute TL glow curves according to the general-order empirical expression or the semi-analytical expression based on the Lambert *W* function



	V1	V2	V3	V4	V5
1	Peak	INTENS(min)	INTENS(max)	INTENS(ini)	INTENS(fix)
2	1th-Peak	0	1953.12	432.982	FALSE
3	2th-Peak	0	1953.12	817.003	FALSE
4	3th-Peak	0	1953.12	1225.908	FALSE
5	4th-Peak	0	1953.12	1627.705	FALSE
6					
7	Peak	ENERGY(min)	ENERGY(max)	ENERGY(ini)	ENERGY(fix)
8	1th-Peak	0.5	5	1.881	FALSE
9	2th-Peak	0.5	5	2.007	FALSE
10	3th-Peak	0.5	5	1.931	FALSE
11	4th-Peak	0.5	5	2.001	FALSE
12					
13	Peak	TEMPER(min)	TEMPER(max)	TEMPER(ini)	TEMPER(fix)
14	1th-Peak	301.01	558.05	418.605	FALSE
15	2th-Peak	301.01	558.05	462.016	FALSE
16	3th-Peak	301.01	558.05	489.510	FALSE
17	4th-Peak	301.01	558.05	510.733	FALSE
18					
19	Peak	bValue(min)	bValue(max)	bValue(ini)	bValue(fix)
20	1th-Peak	1	2	1.364	FALSE
21	2th-Peak	1	2	1.139	FALSE
22	3th-Peak	1	2	1.723	FALSE
23	4th-Peak	1	2	1.222	FALSE

Fig. 2. Dialog table used to initialize, constrain, and fix parameters. Values in the table are modifiable. It is the responsibility of the user to ensure that all initial parameters fall within their respective bounds.

for glow curve fitting include the number of glow peaks to be deconvoluted (*npeak*), the allowed maximum number of random trials (*nstart*), the allowed maximum total half-width of glow peaks (*mwt*), the allowed minimum distance between peak temperatures (*mdt*), etc. A plot showing simulated or deconvoluted glow peaks can be automatically produced once the calculation is terminated. The user can also specify a file to save the fit data for further usage.

3. Illustrative examples

A number of examples are provided in this section. The first two examples are for glow curve deconvolution using the general-order empirical expression and the semi-analytical expression based on the Lambert *W* function; the third example is for glow peak simulation; and the final example is for multi-peak glow curve simulation.

3.1. Glow curve deconvolution

For the first example, the synthetic glow curve Refglow002 of the GLOCANIN project [32] was deconvoluted into four glow peaks using the general-order empirical expression. This artificial glow curve is the sum of four glow peaks simulated according to the Randall–Wilkins model. After all peak maxima are selected from the glow curve by clicking on the mouse, a dialog table will be automatically generated (as shown in Fig. 2). Values in the table can be modified to constrain or fix parameters. *INTENSE* (*min*, *max*, *ini*), *ENERGY* (*min*, *max*, *ini*), *TEMPER* (*min*, *max*, *ini*), and *bValue* (*min*, *max*, *ini*) denote the lower and upper limits and initial values for peak intensity, activation energy, peak temperature, and kinetic order of a glow peak, respectively. The last column made up of logical values (TRUE or FALSE) is also modifiable if the user wants to fix any parameter during optimization. Fit results for reference glow curve Refglow002 are automatically produced (as shown in Fig. 3) once the optimization process has terminated. The upper and lower parts of Fig. 3 show fitted glow peaks and residuals, respectively. Fig. 3 shows that the program fits well with the Refglow002 synthetic glow curve.

Estimated parameters (peak intensity *INTENS*, activation energy *ENERGY*, peak temperature *TEMPER*, kinetic order *bValue*, and frequency factor *ff*) and shape parameters (tem-

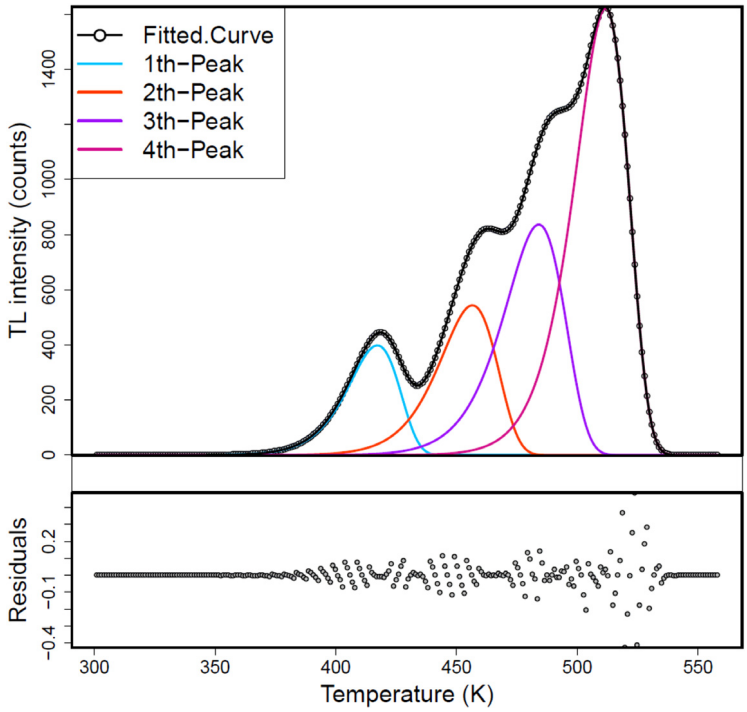


Fig. 3. Four deconvoluted glow peaks for the Refglow002 synthetic glow curve using the general-order empirical expression.

peratures that correspond to half intensities on the left and right sides of the peak ($T1$ and $T2$), the half-widths at the left and right sides of the peak ($d1$ and $d2$), the total half-width *thw*, and the symmetry factor *sf*) for glow peaks are outputted into the R console. Readers are advised to consult the textbook by Pagonis et al. [1] for a detailed introduction on peak shape analysis. The minimized FOM value (0.0086%) was consistent with that reported in previous studies [5,9,32]. Fitted signal values for each glow peak can be written to a file in CSV format (Fig. 4) and saved to the current work directory. The file can be opened and operated using widely-available spreadsheet programs.

For a more realistic example, we deconvoluted the experimental TL glow curve Refglow009 of the GLOCANIN project [33] into nine glow peaks using the OTOR TL expression based on the Lambert W function (with the assumption of $rValue = A_n/A_m < 1$, where A_n and A_m are the re-trapping and recombination probability coefficients, respectively). The reference glow curve Refglow009 measured for TLD-700 (LiF:Mg, Ti) that irradiated with a dose of 600 Gy showed a complexity in high temperature peaks, and it is one of the most interesting glow curves to analyze due to its complexity. These overlapping peaks complicate the fitting process, and previous studies reported that fit results for this glow curve were not unique [5,9,33]. Fit results between different programs differ not only in the number of resolved glow peaks but also in their position and shape [33]. It takes less than 20 s to run 10 random trails ($nstart = 10$) for this complex glow curve. Fit results are provided in Fig. 5. The minimized FOM value of 0.75% was significantly smaller than that reported by Mathcad (FOM = 1.12%) [5], GlowFit (FOM = 1.35%) [9], and program B used in the GLOCANIN project (FOM = 1.7%) [33]. Better fit results can be obtained only by employing more glow peaks [4,33].

3.2. Glow peak (curve) simulation

For the third example, first-order and second-order glow peaks were simulated using the Randall–Wilkins and Garlick–Gibson model, respectively. Simulation results of a first-order glow peak are provided in Fig. 6(A). The upper and lower parts of the plot showed variation in TL intensity and concentrations of trapped electrons with temperature, respectively. The peak shape of a glow peak is automatically evaluated once the simulation has terminated. Simulated glow peaks can also be saved to a file in CSV format (the same as Fig. 4). Fig. 6(B) and (C) show the effects of initial electron trap concentration on the shape of first-order and second-order glow peaks, respectively, as investigated by Pagonis et al. [1]. With regard to first-order glow peaks, changes in initial electron trap occupancies do not affect the position of peak temperatures. However, in the case of second-order glow peaks, the position of the peak temperature decreased with an increase in the initial electron trap concentration.

Pagonis et al. [1] obtained first-order and second-order glow peaks by changing the ratio of the probability coefficient of electron re-trapping in the traps (An) to the probability coefficient of electron recombining with holes in the recombination center (Am) in the OTOR model. A similar method was used by Sadek [34] to simulate first-order and second-order glow curves to test the accuracy of the computerized glow curve deconvolution algorithm. For the final example, five glow peaks were simulated according to the

```
$pars
              INTENS   ENERGY   TEMPER   bValue
1th-Peak  398.2452 1.383473 417.1689 1.000730
2th-Peak  543.6544 1.483410 456.5080 1.000712
3th-Peak  836.6947 1.584328 484.0083 1.001309
4th-Peak 1622.9313 2.004553 511.6640 1.000729

$ff
    1th-Peak     2th-Peak     3th-Peak     4th-Peak
4.006247e+16 1.651101e+16 2.069488e+16 4.142189e+19

$sp
               T1       T2     Tm       d1       d2      thw       sf
1th-Peak 402.2128 427.8543 416.93 14.71724 10.92427 25.64151 0.4260384
2th-Peak 439.8265 468.4429 456.24 16.41346 12.20291 28.61636 0.4264311
3th-Peak 466.4406 496.5764 484.46 18.01939 12.11644 30.13583 0.4020609
4th-Peak 496.0010 522.7496 511.68 15.67898 11.06955 26.74853 0.4138377

$FOM
[1] 0.00858612
```

	A	B	C	D	E	F	G	H
1		Temperature	Obs.Signal	Fit.Signal	Comp.1	Comp.2	Comp.3	Comp.4
2	1	301.01	0.000368	0.00037175	0.0003666	4.91E-06	2.06E-07	6.67E-11
3	2	302.02	0.00044	0.00044439	0.0004382	5.94E-06	2.53E-07	8.64E-11
4	3	303.02	0.000525	0.00052967	0.0005222	7.17E-06	3.09E-07	1.11E-10
5	4	304.03	0.000626	0.00063168	0.0006226	8.66E-06	3.78E-07	1.44E-10
6	5	305.04	0.000746	0.00075247	0.0007416	1.04E-05	4.62E-07	1.85E-10
7	6	306.05	0.000887	0.00089531	0.0008822	1.26E-05	5.63E-07	2.38E-10
8	7	307.06	0.001055	0.00106406	0.0010482	1.51E-05	6.86E-07	3.05E-10
9	8	308.06	0.001252	0.00126105	0.0012421	1.82E-05	8.33E-07	3.90E-10
10	9	309.07	0.001484	0.00149538	0.0014726	2.18E-05	1.01E-06	4.99E-10
11	10	310.08	0.001758	0.00177129	0.0017439	2.61E-05	1.23E-06	6.38E-10
12	11	311.09	0.00208	0.00209581	0.002063	3.13E-05	1.49E-06	8.14E-10
13	12	312.1	0.002458	0.0024771	0.0024379	3.74E-05	1.80E-06	1.04E-09
14	13	313.1	0.002901	0.00291981	0.002873	4.46E-05	2.18E-06	1.31E-09
15	14	314.11	0.003421	0.00344366	0.0033878	5.32E-05	2.63E-06	1.67E-09
16	15	315.12	0.00403	0.00405721	0.0039906	6.35E-05	3.17E-06	2.11E-09
17	16	316.13	0.004743	0.00477508	0.0046957	7.56E-05	3.82E-06	2.68E-09
18	17	317.14	0.005575	0.00561415	0.0055197	8.99E-05	4.59E-06	3.38E-09
19	18	318.14	0.006547	0.00658344	0.0064714	0.0001066	5.51E-06	4.26E-09
20	19	319.15	0.00768	0.00772457	0.0075915	0.0001265	6.62E-06	5.37E-09
21	20	320.16	0.009001	0.00905438	0.0088965	0.0001499	7.93E-06	6.75E-09

Fig. 4. Fit results saved in CSV format. Column B, C, and D show temperature values, observed TL signal values, and fitted TL signal values, respectively. Column E–H show fitted signal values of the four glow peaks.

OTOR model using quasi-equilibrium approximation. For the first three glow peaks the ratios of *An* to *Am* were significantly smaller than 1 (i.e., the recombination probability was greater than that of re-trapping), and the peaks were of first-order kinetics. In the last two glow peaks the ratios of *An* to *Am* were set to be equal to 1, and the peaks were of second-order kinetics. Finally, the five glow peaks simulated using the same sequence of temperature values were summated to produce a multi-peak glow curve, as indicated by the black line in Fig. 6(D).

4. Impact and conclusions

As mentioned above, TL glow curve deconvolution is an ill-conditioned problem. The model may converge to various local minima when different initial parameters are undertaken. Consequently, for complex glow curves consisting of overlapping glow peaks (such as reference glow curve Refglow009), the user may need to manually rerun the program a certain number of times to obtain a reasonable fit result. Generally, the process is tedious and time-consuming. Compared to existing programs, the R package tgcd adopts an automated "trial-and-error" protocol in which the program is repeatedly called using randomly generated initial parameters to derive the optimal fit result in TL glow curve deconvolution. The program also offers options to specify the allowed maximum total half-width for glow peaks and minimum distance between peak temperatures in order to obtain meaningful fitting parameters for complex glow curves. In theory, the probability of obtaining an optimal fit result increases with the increase in the number of random trials. The resultant fit of reference glow curve Refglow009 provided in Fig. 5 demonstrates that the automated "trial-and-error" protocol is very efficient and appears to be very useful for deriving high-quality fit results. Minimized FOM was significantly smaller than that reported in previous studies.

Moreover, the traditional method used for parameter initialization (i.e., manually initializing parameters one after another) becomes increasingly impracticable with the increase in the dimension of the problem under consideration. The R package tgcd offers an interactive environment to make it easy for the user to initialize the model, to impose constraints on parameters, and to fix any parameters. Functions in this package also support convenient data import/export and high-quality graphical outputs.

In addition, semi-analytical expressions derived from the OTOR model using the Lambert *W* function are based on

```
$pars
             INTENS   ENERGY   TEMPER       rValue
1th-Peak  9855.768 1.225681 387.5201 2.142983e-02
2th-Peak 21554.421 1.370533 428.8617 2.011305e-01
3th-Peak 24719.536 2.285317 462.6737 8.251181e-01
4th-Peak 54945.499 2.314386 488.3172 5.790214e-02
5th-Peak  5261.516 1.106069 494.5081 8.828895e-03
6th-Peak  3758.059 1.436794 523.9569 7.012545e-02
7th-Peak  7353.395 1.678277 555.0372 3.662934e-04
8th-Peak  2109.270 2.619323 583.3247 2.225439e-07
9th-Peak  2298.912 1.879263 603.2252 4.821910e-01

$ff
    1th-Peak     2th-Peak     3th-Peak     4th-Peak     5th-Peak
8.097164e+14 1.011137e+15 9.351044e+23 8.304493e+22 9.746454e+09
    6th-Peak     7th-Peak     8th-Peak     9th-Peak
3.820569e+12 1.095153e+14 3.811940e+21 2.705034e+14

$sp
              T1       T2     Tm       d1        d2      thw        sf
1th-Peak 372.8793 397.9503 387.05 14.17072 10.900273 25.07099 0.4347763
2th-Peak 412.2858 442.3678 429.15 16.86420 13.217813 30.08202 0.4393926
3th-Peak 449.1462 475.5654 461.75 12.60377 13.815437 26.41921 0.5229316
4th-Peak 475.6541 497.3953 487.85 12.19590  9.545314 21.74122 0.4390423
5th-Peak 468.7745 513.1690 493.75 24.97552 19.419038 44.39456 0.4374193
6th-Peak 501.0738 540.8808 523.05 21.97617 17.830810 39.80698 0.4479317
7th-Peak 533.2778 570.5446 554.95 21.67217 15.594621 37.26679 0.4184589
8th-Peak 567.6144 594.3224 583.75 16.13555 10.572438 26.70799 0.3958530
9th-Peak 578.4889 627.0950 604.15 25.66105 22.945003 48.60605 0.4720606

$FOM
[1] 0.7538409
```

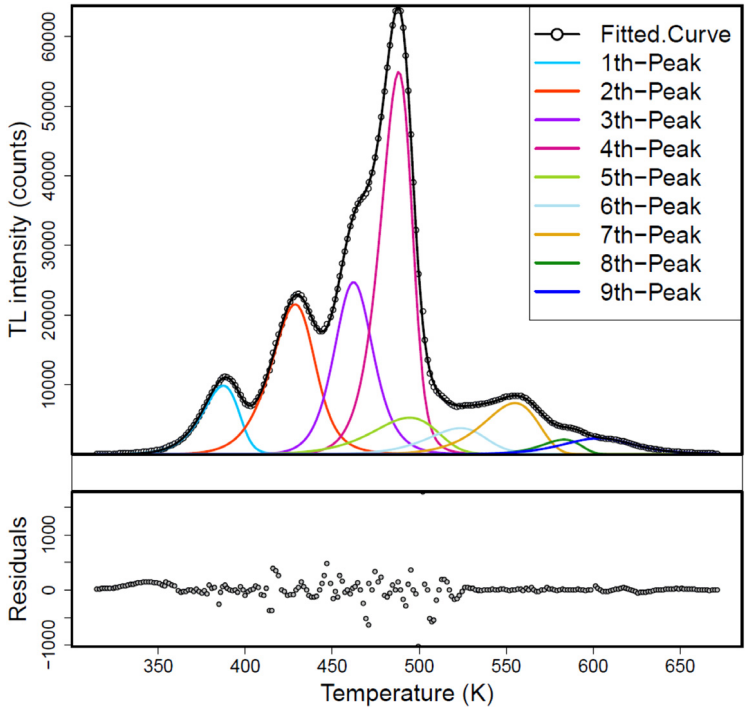


Fig. 5. Nine deconvoluted glow peaks for the measured glow curve Refglow009 using the OTOR TL expression based on the Lambert *W* function.

a physical model and can accurately fit experimental glow peaks, even in cases of saturation. However, to the best of our knowledge, there is no openly accessible program that can be employed to deconvolute TL glow curves using these recently developed OTOR TL expressions. We therefore incorporated these new expressions into the latest version of the R package and made the program openly accessible to all users.

Finally, R allows for the creation of complex and flexible data processing routines that are not available in existing programs. Most programs designed to analyze TL glow curves focus on glow curve deconvolution. In contrast, the R package presented here also provides routines for simulating TL glow peaks (curves) using several simple kinetic models and analyzing the shape of a glow peak. These kinetic models provided in the package may prove useful in understanding the TL process governing a glow peak and the characteristic properties of glow peaks of various kinetic orders. In this respect, the package offers a comprehensive numerical tool for analyzing TL glow curves. We invite users to use the program or adapt the program to their own specific TL glow curve analysis requirements.

Acknowledgments

We would like to thank A.J.J. Bos for providing reference glow curves of the GLOCANIN project to test our program. This work was funded by the Major State Basic Research Development Program of China (Grant No. 2013CB956000 and 2012CB426501).

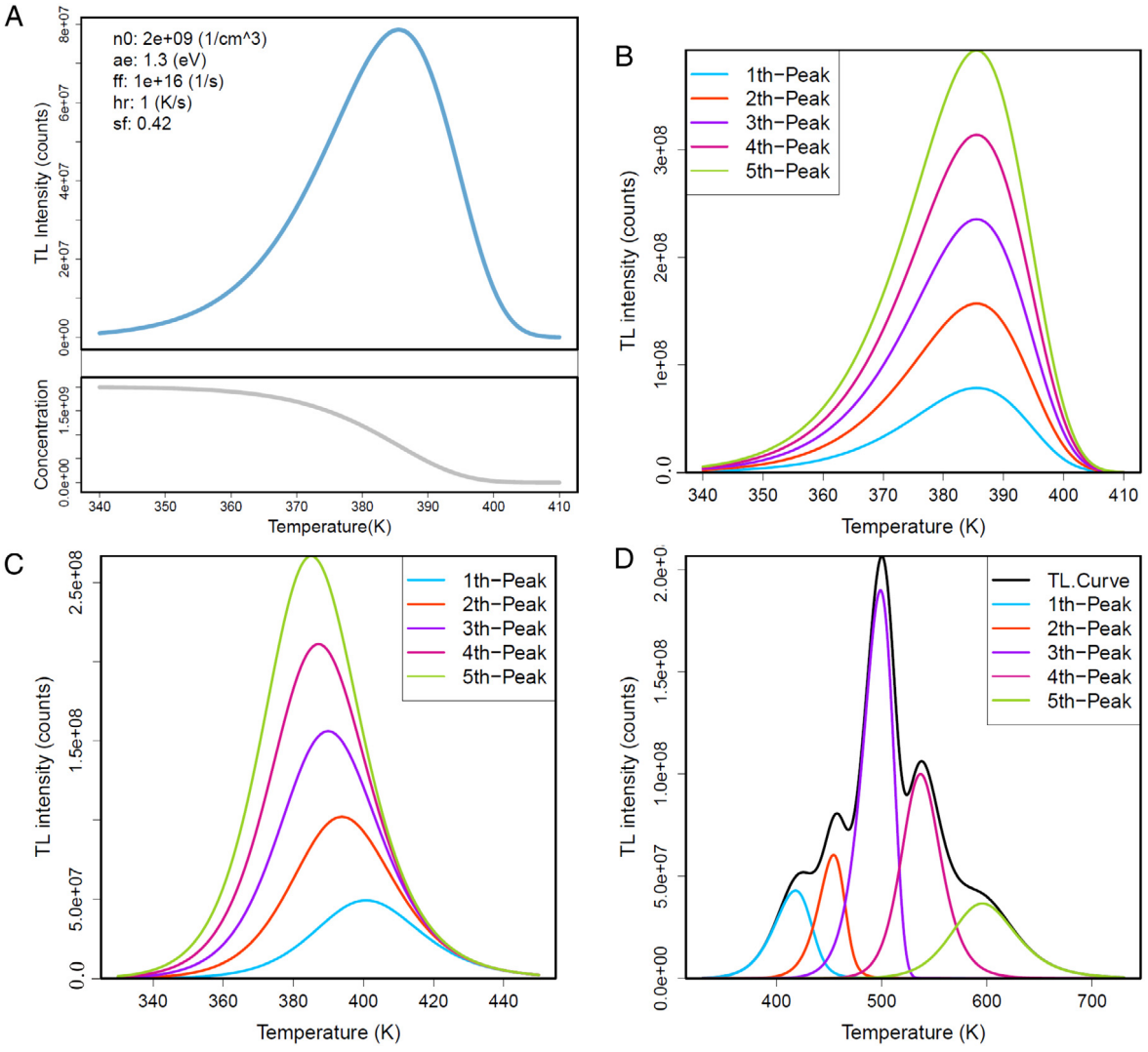


Fig. 6. (A) A first-order glow peak simulated using the Randall–Wilkins model. (B) Five first-order glow peaks simulated with different initial electron trap concentrations. (C) Five second-order glow peaks simulated with different initial electron trap concentrations. (D) A glow curve consisting of five glow peaks simulated according to the OTOR model using quasi-equilibrium approximation.

References

[1] Pagonis V, Kitis G, Furetta C. Numerical and practical exercises in thermoluminescence. New York: Springer Science and Business Media; 2006.

[2] Harvey JA, Rodrigues ML, Kearfott KJ. A computerized glow curve analysis (GCA) method for WinREMS thermoluminescent dosimeter data using MATLAB. Appl Radiat Isot 2011;69(9):1282–6.

[3] El-Hafez AI, Yasin MM, Sadek AM. GCAFIT-A new tool for glow curve analysis in thermoluminescence nanodosimetry. Nucl Instrum Methods Phys Res A 2011;637(1):58–163.

[4] Afouxenidis D, Polymeris GS, Tsirliganis NC, Kitis G. Computerised curve deconvolution of TL/OSL curves using a popular spreadsheet program. Radiat Prot Dosim 2012;149(4):363–70.

[5] Kiisk V. Deconvolution and simulation of thermoluminescence glow curves with Mathcad. Radiat Prot Dosim 2013;156(3):261–7.

[6] Pagonis V, Mian SM, Kitis G. Fit of first order thermoluminescence glow peaks using the Weibull distribution function. Radiat Prot Dosim 2001; 93(1):11–7.

[7] Pagonis V, Kitis G. On the possibility of using commercial software packages for thermoluminescence glow curve deconvolution analysis. Radiat Prot Dosim 2002;101(1–4):93–8.

[8] Chung KS, Choe HS, Lee JI, Kim JL, Chang SY. A computer program for the deconvolution of thermoluminescence glow curves. Radiat Prot Dosim 2005;115(1–4):345–9.

[9] Puchalska M, Bilski P. GlowFit–a new tool for thermoluminescence glow-curve deconvolution. Radiat Meas 2006;41(6):659–64.

[10] R Core Team. R: A Language and Environment for Statistical Computing. R Foundation for Statistical Computing, 2014. URL http://www.R-project.org/.

[11] Matloff N. The art of R programming: A tour of statistical software design. San Francisco: No Starch Press; 2011.

[12] Chen R, McKeever SWS. Theory of thermoluminescence and related phenomena. Singapore: World Scientific; 1997.

[13] More JJ. The Levenberg–Marquardt algorithm: implementation and theory. In: Lecture notes in mathematics: numerical analysis. Berlin: Springer-Verlag; 1978.

[14] May CE, Partridge JA. TL kinetics of alpha-irradiated alkali halides. J Chem Phys 1964;40(5):1401–9.

[15] Kitis G, Vlachos ND. General semi-analytical expressions for TL, OSL and other luminescence stimulation modes derived from the OTOR model using the Lambert W-function. Radiat Meas 2013;48:47–54.

[16] Sadek AM, Eissa HM, Basha AM, Kitis G. Resolving the limitation of the peak fitting and peak shape methods in the determination of the activation energy of thermoluminescence glow peaks. J Lumin 2014;146:418–23.

[17] Sadek AM, Eissa HM, Basha AM, Kitis G. Development of the peak fitting and peak shape methods to analyze the thermoluminescence glow-curves generated with exponential heating function. Nucl Instrum Methods Phys Res B 2014;330:103–7.

[18] Sadek AM, Eissa HM, Basha AM, Kitis G. Properties of the thermoluminescence glow peaks simulated by the interactive multiple-trap system (IMTS) model. Phys Status Solidi B 2014;252(4):721–729.
[19] Kitis G, Gómez Ros JM, Tuyn JWN. Thermoluminescence glow curve deconvolution functions for first, second and general orders of kinetics. J Phys D Appl Phys 1998;31(19):2636–41.
[20] Sadek AM, Eissa HM, Basha AM, Carinou E, Askounis P, Kitis G. The deconvolution of thermoluminescence glow-curves using general expressions derived from the one trap-one recombination (OTOR) level model. Appl Radiat Isot 2015;95:214–21.
[21] Kitis G, Polymeris GS, Sfampa IK, Prokic M, Meriç N, Pagonis V. Prompt isothermal decay of thermoluminescence in MgB_4O_7:Dy, Na and LiB_4O_7:Cu, In dosimeters. Radiat Meas 2016;84:15–25.
[22] Balian HG, Eddy NW. Figure-of-merit (FOM), an improved criterion over the normalized chi-squared test for assessing goodness-of-fit of gamma-ray spectral peaks. Nucl Instrum Methods 1977;145(2):389–95.
[23] Bluszcz A, Adamiec G. Application of differential evolution to fitting OSL decay curves. Radiat Meas 2006;41(7–8):886–91.
[24] Peng J, Dong ZB, Han FQ, Long H, Liu XJ. R package numOSL: numeric routines for optically stimulated luminescence dating. Anc TL 2013;31(2):41–8. URL http://CRAN.R-project.org/package=numOSL.
[25] Delgado A, Gómez Ros JM. Computerised glow curve analysis: a tool for routine thermoluminescence dosimetry. Radiat Prot Dosim 2001;96(1–3):127–32.
[26] Gómez Ros JM, Kitis G. Computerised glow curve deconvolution using general and mixed order kinetics. Radiat Prot Dosim 2002;101(1–4):47–52.
[27] Chen R, Pagonis V. Thermally and optically stimulated luminescence: a simulation approach. Chichester: John Wiley and Sons; 2011.
[28] Sunta CM. Unraveling Thermoluminescence. New Delhi: Springer India; 2015.
[29] Chen R, Pagonis V, Lawless JL. A new look at the linear-modulated optically stimulated luminescence (LM-OSL) as a tool for dating and dosimetry. Radiat Meas 2009;44(4):344–50.
[30] Petzold LR. Automatic selection of methods for solving stiff and nonstiff systems of ordinary differential equations. Siam J Sci Stat Comput 1983;4(1):136–48.
[31] Soetaert K, Petzoldt T, Setzer RW. Solving differential equations in R: Package deSolve. J Stat Softw 2010;33(9):1–25. URL http://CRAN.R-project.org/package=deSolve.
[32] Bos AJJ, Piters TM, Gómez Ros JM, Delgado A. An intercomparison of glow curve analysis computer programs: I. Synthetic glow curves. Radiat Prot Dosim 1993;47(1–4):473–7.
[33] Bos AJJ, Piters TM, Gómez Ros JM, Delgado A. An intercomparison of glow curve analysis computer programs: II. Measured glow curves. Radiat Prot Dosim 1994;51(4):257–64.
[34] Sadek AM. Test of the accuracy of the computerized glow curve deconvolution algorithm for the analysis of thermoluminescence glow curves. Nucl Instrum Methods Phys Res A 2013;712:56–61.