Package ‘tgcd’

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Title   Thermoluminescence Glow Curve Deconvolution
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Author  Jun Peng [aut, cre],
        John Burkardt [ctb],
        Jorge More [ctb],
        Burton Garbow [ctb],
        Kenneth Hillstrom [ctb],
        Linda R. Petzold [ctb],
        Alan C. Hindmarsh [ctb],
        R. Woodrow Setzer [ctb],
        Andrew Horchler [ctb],
        William Cody [ctb],
        Cleve Moler [ctb],
        Jack Dongarra [ctb]
Maintainer Jun Peng <pengjun10@mails.ucas.ac.cn>
Description Deconvolving thermoluminescence glow curves according to various
kinetic models (first-order, second-order, general-order, and mixed-order) using
a modified Levenberg-Marquardt algorithm (More, 1978) <DOI:10.1007/BFb0067700>. It
provides the possibility of setting constraints or fixing any of parameters. It
offers an interactive way to initialize parameters by clicking with a mouse on
a plot at positions where peak maxima should be located. The optimal estimate is
obtained by “trial-and-error”. It also provides routines for simulating first-order,
second-order, and general-order glow peaks.
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tgcd-package

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tgcd-package  
tgcd: An R package for analyzing thermoluminescence glow curves

Description

Package for thermoluminescence glow curve deconvolution (tgcd) and glow peak simulation.

Details

Package: tgcd
Type: Package
Version: 2.7
Date: 2023-09-08
License: GPL-2 | GPL-3

Author(s)

Jun Peng    Hunan University of Science and Technology, Xiangtan, China

Package maintainer

Jun Peng <pengjun10@mails.ucas.ac.cn>

Related package projects

R program KMS https://github.com/pengjunUCAS/KMS
R package numOSL https://CRAN.R-project.org/package=numOSL

References


Kitis: Thermoluminescence glow curves provided by George Kitis

Description
A total of 22 thermoluminescence glow curves measured from various materials provided by George Kitis.

Usage
data(Kitis)

Format
A list that contains 22 thermoluminescence glow curves.

Details
This object contains 22 thermoluminescence glow curves (x001 to x022) provided by George Kitis. x001 (Al2O3:C), x002 (CaF2:Dy), x003 (LBO), x004 (Background), x005 (MgO), x006 (BeO), x007 (CaF2:Tm), x008 (Salt), x009 (CaF2:Dy), x010 to x016 (quartz irradiated with dose of 1, 2, 4, 8, 16, 32, and 64 Gy), x017 and x018 (BeO), x019 and x020 (Salt), x021 and x022 (MgO).

Examples
# Load package "tgcd".
require(tgcd)
data(Kitis)
names(Kitis)

Refglow: Reference glow curves

Description
Synthetic and measured thermoluminescence glow curves from the GLOCANIN project.

Usage
data(Refglow)

Format
A list that contains 10 thermoluminescence glow curves.
Details

This object contains 10 thermoluminescence glow curves (x001 to x010) from the GLOCANIN project (Bos et al., 1993, 1994).

References


Examples

```r
# Load package "tgcd".
require(tgcd)
data(Refglow)
names(Refglow)

savgol # Apply a Savitzky-Golay algorithm to smooth thermoluminescence glow curves
```

Description

Smooth thermoluminescence glow curves with a Savitzky-Golay smoothing filter and calculate derivatives.

Usage

`savgol(y, drv, hwd = 3 * (drv + 2), pod = 4)`

Arguments

- `y` numeric(required): the data to be filtered
- `drv` integer(required): the order of the derivative to be calculated
- `hwd` integer(with default): half width of the segment used for filter
- `pod` integer(with default): order of the polynomial used for filter

Details

The Savitzky-Golay smoothing algorithm is particularly good at preserving lineshape while removing high frequency squiggles (Press et al., 1986). The procedure can be used to calculate derivatives of thermoluminescence data to identify the location of glow peaks.
**simPeak**

**Value**

The filtered signal, which has the same length as \( y \).

**References**


**See Also**

tgcd

**Examples**

```r
library(tgcd)
data(Refglow)

x <- Refglow$x009[,1]
y <- Refglow$x009[,2]
y0 <- savgol(y, drv=0)
dy <- savgol(y, drv=1)

plot(x, y, type="p", pch=21, bg="black")
points(x, y0, type="l", col="blue", lwd=2)
plot(x, dy, type="l", col="blue", lwd=2)
abline(h=0, lty="dashed", col="red", lwd=2)
```

---

**simPeak**

*Thermoluminescence glow peak simulation*

**Description**

Simulating first-order, second-order, or general-order glow peaks.

**Usage**

```r
simPeak(temps, n0, Nn = NULL, bv = NULL, ff, ae, hr, typ = c("f", "s", "g"), outfile = NULL, plot = TRUE)
```

**Arguments**

- `temps` **vector(required):** temperature values (K) where the values of the thermoluminescence intensity will be computed. It needs to be sorted increasingly. A vector of temperature values may be generated using the internal function `seq`
- `n0` **numeric(required):** initial concentration of trapped electrons (1/cm^3)
**simPeak**

- **Nn**: numeric (required): total concentration of the traps in the crystal (1/cm^3)
- **bv**: numeric (required): order number for the general order glow peak
- **ff**: numeric (required): the frequency factor (1/s)
- **ae**: numeric (required): the activation energy (eV)
- **hr**: numeric (with default): the linear heating rate (K/s)
- **typ**: character (with default): the type of a glow peak, typ="f" means first-order, typ="s" means second-order, typ="g" means general-order, default typ="f"
- **outfile**: character (optional): if specified, simulated intensities of glow peaks will be written to a file named "outfile" in CSV format and saved to the current work directory
- **plot**: logical (with default): draw a plot according to the simulated glow peak or not

**Details**

Function `simPeak` simulates glow peaks of various orders. The first-, second-, and general-order glow peak can be simulated using the following three ordinary equations, respectively (Pagonis et al., 2006):

\[
\frac{dn}{dT} = -nS \exp\left(-\frac{E}{RT}\right)
\]

\[
\frac{dn}{dT} = -n^2 S \exp\left(-\frac{E}{RT}\right)
\]

\[
\frac{dn}{dT} = -n^b S \exp\left(-\frac{E}{RT}\right)
\]

where \( n \) is the concentration of trapped electrons, \( \frac{dn}{dT} \) the rate of change of the concentration of trapped electrons, \( S \) the frequency factor, \( E \) the activation energy, \( T \) the absolute temperature, \( k \) the Boltzmann constant, \( N_n \) the total concentration of the traps in the crystal, \( b \) the b value (kinetic order), and \( \beta \) the linear heating rate.

The ordinary equation is solved by the Fortran 77 subroutine `lsoda` (original version written by Linda R. Petzold and Alan C. Hindmarsh available at Netlib: [https://www.netlib.org/odepack/](https://www.netlib.org/odepack/), modified version by R. Woodrow Setzer from the R package `deSolve` (Soetaert et al., 2010) available at CRAN: [https://CRAN.R-project.org/package=deSolve](https://CRAN.R-project.org/package=deSolve).

**Value**

Return an invisible list containing the following elements:

- **temps**: a vector of temperature values
- **tl**: values of the thermoluminescence intensity
- **n**: variation of concentration of trapped electrons with temperature
- **sp**: parameters used for describing the shape of a glow peak (Pagonis et al., 2006):
  - the temperature corresponding to half intensity on the left side of the peak (T1);
  - the temperature corresponding to half intensity on the right side of the peak (T2);
  - the temperature corresponding to maximum intensity (Tm);
  - the half-width at the left side of the peak (d1=Tm-T1);
  - the half-width at the right side of the peak (d2=T2-Tm);
  - the total half-width (thw=d1+d2);
  - the symmetry factor (sf=d2/thw)
References


See Also
tgcd; simqOTOR

Examples

```r
# Simulate second-order glow peaks with various
# initial electron trap concentration (n0).
temps <- seq(400, 600, by=0.5)
peak1 <- simPeak(temps, n0=0.2e10, Nn=1e10,
ffa=2.0, hr=1, typ="s")
peak2 <- simPeak(temps, n0=0.4e10, Nn=1e10,
ffa=2.0, hr=1, typ="s")
peak3 <- simPeak(temps, n0=0.6e10, Nn=1e10,
ffa=2.0, hr=1, typ="s")
peak4 <- simPeak(temps, n0=0.8e10, Nn=1e10,
ffa=2.0, hr=1, typ="s")
peak5 <- simPeak(temps, n0=1.0e10, Nn=1e10,
ffa=2.0, hr=1, typ="s")
peaks <- cbind(peak1$tl, peak2$tl, peak3$tl, peak4$tl, peak5$tl)
matplot(temps, peaks, type="l", lwd=2, lty="solid",
xlab="Temperature (K)", ylab="TL intensity (counts)"
)
```

simqOTOR

Thermoluminescence glow peak simulation

Description

Simulating glow peaks according to the one trap-one recombination center (OTOR) model using the quasi-equilibrium approximation.

Usage

```r
simqOTOR(temps, n0, Nn, Ah, An, ff, ae,
hr, outfile = NULL, plot = TRUE)
```
Arguments

- **temps** (vector(required)): temperature values (K) where the values of the thermoluminescence intensity will be computed, it needs to be sorted increasingly
- **n0** (numeric(required)): initial concentration of trapped electrons (1/cm^3)
- **Nn** (numeric(required)): total concentration of the traps in the crystal (1/cm^3)
- **Ah** (numeric(optional)): probability coefficient of electron recombining with holes in the recombination center (cm^3/s)
- **An** (numeric(optional)): probability coefficient of electron retrapping in the traps (cm^3/s)
- **ff** (numeric(required)): the frequency factor (1/s)
- **ae** (numeric(required)): the activation energy (eV)
- **hr** (numeric(with default)): the linear heating rate (K/s)
- **outfile** (character(optional)): if specified, simulated intensities of glow peaks will be written to a file named "outfile" in CSV format and saved to the current work directory
- **plot** (logical(with default)): draw a plot according to the simulated glow peak or not

Details

Function `simqOTOR` simulates a synthetic glow peak according to the OTOR model using the quasi-equilibrium approximation. This function may be used to simulating glow peaks of first-, second-, and general-order, depending on the given kinetic parameters. The approximate equation of the OTOR model derived using the quasi-equilibrium approximation can be described by (Pagonis et al., 2006):

\[
\frac{dn}{dT} = \frac{-A_h n^2 S \exp(-\frac{E}{kT})}{n A_h + (N_n - n) A_n \beta}
\]

where \( n \) is the concentration of trapped electrons, \( \frac{dn}{dT} \) the rate of change of the concentration of trapped electrons, \( S \) the frequency factor, \( E \) the activation energy, \( T \) the absolute temperature, \( k \) the Boltzmann constant, \( N_n \) the total concentration of the traps in the crystal, \( A_h \) the probability coefficient of electron recombining with holes in the recombination center, \( A_n \) the probability coefficient of electron retrapping in the traps, and \( \beta \) the linear heating rate.

The ordinary equation is solved by the Fortran 77 subroutine `lsoda` (original version written by Linda R. Petzold and Alan C. Hindmarsh available at Netlib: https://www.netlib.org/odepack/, modified version by R. Woodrow Setzer from the R package `deSolve` (Soetaert et al., 2010) available at CRAN: https://CRAN.R-project.org/package=deSolve).

Value

Return an invisible list containing the following elements:

- **temps**: a vector of temperature values
- **tl**: values of the thermoluminescence intensity
- **n**: variation of concentration of trapped electrons with temperature
- **sp**: parameters used for describing the shape of a glow peak, see function `simPeak` for details
tgcd

Thermoluminescence glow curve deconvolution (tgcd)

Description

Thermoluminescence glow curve deconvolution according to various first-order, second-order, general-
order, and mixed-order empirical expressions.

Usage

```r
tgcd(Sigdata, npeak, model = "g1", subBG = FALSE, pickp = "d2",
pickb = "d0", nstart = 60, kkf = 0.03, mdt = NULL, mwt = NULL,
mr = NULL, edit.inis = TRUE, inisPAR = NULL, inisBG = NULL,
hr = NULL, hwd = NULL, pod = NULL, plot = TRUE, outfile = NULL)
```

Examples

```r
# Synthesizing a glow curve consisting of five glow peaks.
tems <- seq(330, 730, by=0.5)
peak1 <- simqOTOR(temps, n0=0.7e10, Nn=1e10, Ah=1e-3, An=1e-7,
  ff=1e14, ae=1.5, hr=1, outfile = NULL, plot = TRUE)
peak2 <- simqOTOR(temps, n0=0.5e10, Nn=1e10, Ah=1e-7, An=1e-7,
  ff=1e17, ae=1.9, hr=1, outfile = NULL, plot = TRUE)
peak3 <- simqOTOR(temps, n0=0.2e10, Nn=1e10, Ah=1e-5, An=1e-7,
  ff=1e15, ae=1.45, hr=1, outfile = NULL, plot = TRUE)
peak4 <- simqOTOR(temps, n0=0.2e10, Nn=1e10, Ah=1e-5, An=1e-7,
  ff=1e9, ae=0.85, hr=1, outfile = NULL, plot = TRUE)
peak5 <- simqOTOR(temps, n0=0.3e10, Nn=1e10, Ah=1e-7, An=1e-7,
  ff=1e11, ae=1.4, hr=1, outfile = NULL, plot = TRUE)
peaks <- cbind(peak1$tl, peak2$tl, peak3$tl, peak4$tl, peak5$tl,
  peak1$tl+peak2$tl+peak3$tl+peak4$tl+peak5$tl)
matplot(temps, y=peaks, type="l", lwd=2, lty="solid",
xlab="Temperature (K)", ylab="TL intensity (counts)")
```
Arguments

**Sigdata**

matrix**(required)**: a 2-column matrix, temperature values (in unit K) and thermoluminescence signal values are stored in the first and second column, respectively

**npeak**

integer**(required)**: number of glow peaks, the allowed maximum number of glow peaks is set equal to 13

**model**

character**(with default)**: model used for glow curve deconvolution, "f1", "f2", and "f3" for first-order models, "s1", "s2" for second-order models, "g1", "g2", "g3" for general-order models, "wo" and "lw" for the Wright Omega and the Lambert W functions, "m1", "m2", and "m3" for the mixed-order models (see Details)

**subBG**

logical**(with default)**: whether the user want to subtract the background during the deconvolution

**pickp**

character**(with default)**: mode used for initialization of kinetic parameters if `inisPAR=NULL`, "d0" and "d01" prompt the user to click with a mouse on the original and log-scale glow curves respectively to locate each glow peak, "d1", "d2", "d3", and "d4" prompt the user to click with a mouse on the first-, second-, third-, and fourth-derivative of the glow curve respectively to locate each glow peak

**pickb**

character**(with default)**: mode used for initialization of background parameters if `inisBG=NULL`, "d0" and "d01" prompt the user to click with a mouse on the original and log-scale glow curves respectively to initialize the background parameters

**nstart**

integer**(with default)**: number of trials performed in a "trial-and-error" protocol, the upper limit is set equal to 10000

**kkf**

numeric**(with default)**: factor controlling the range of values from which random starting parameters will be generated during the "trial-and-error" protocol, 0<kkf<1. For example, if kkf=0.03 then kinetic parameters will be generated uniformly between (1.0-kkf)*inisPAR and (1.0+kkf)*inisPAR and background parameters will be generated uniformly between (1.0-kkf)*inisBG and (1.0+kkf)*inisBG

**mdt**

numeric**(optional)**: allowed minimum distance between Tm values of glow peaks. A larger mdt prevents the appearance of strongly overlapping peaks

**mwt**

numeric**(optional)**: allowed maximum total half-width of deconvoluted glow peaks. A smaller mwt prevents the appearance of glow peaks with large total half-width

**mr**

numeric**(optional)**: allowed minimum resolution of glow peaks. A larger mr prevents the appearance of strongly overlapping peaks

**edit.inis**

logical**(with default)**: whether the user want to further modify, constrain, or fix the initialized kinetic (and/or background) parameters through an automatically generated **Dialog Table**

**inisPAR**

matrix**(optional)**: a matrix (3 or 4 columns) used for storing initial kinetic parameters Im, E, Tm, b (or R, a) (see Examples)

**inisBG**

vector**(optional)**: a 3-element vector containing initial background parameters A, B, and C used for background subtraction (see Examples)
tgcd

hr numeric(optional): linear heating rate used for calculating the frequency factor

hwd integer(with default): half width (length) of the segment used for Savitzky-Golay smoothing

pod integer(with default): order of the polynomial used for Savitzky-Golay smoothing

plot logical(with default): draw a plot according to the fitting result or not

outfile character(optional): if specified, fitted signal values for each glow peak will be written to a file named "outfile" in CSV format and saved to the current work directory

Details

Function tgcd is used for deconvolving thermoluminescence glow curves according to various kinetic models. In the text below, \( I(T) \) is the thermoluminescence intensity as function of temperature \( T \), \( E \) the activation energy in eV, \( k \) the Boltzmann constant in eV/k, \( T \) the temperature in K with constant heating rate \( K/s \), \( T_m \) the temperature at maximum thermoluminescence intensity in K, \( I_m \) the maximum intensity, \( b \) is an extra parameter (the kinetic order) in application of a general-order model, \( R \) is an extra parameter in application of the Lambert W (Wright Omega) function, and \( \alpha \) is an extra parameter in application of the mixed-order models.

First-order glow peaks appear if the recombination probability \( (A_m) \) is greater than that of re-trapping \( (A_n) \) during excitation. The three parameters describing a glow peak are: \( I_m, E, \) and \( T_m \).

Three empirical expressions describing first-order glow peaks are available in function tgcd:

<1> The first type of first-order empirical expression (model="f1") is (Bos et al., 1993a)

\[
I(T) = I_m \exp\left(\frac{E}{kT_m} - \frac{E}{kT}\right) \exp\left(\frac{E}{kT_m} \alpha\left(\frac{E}{kT_m}\right) - \left(\frac{T}{T_m}\right) \alpha\left(\frac{E}{kT_m}\right) \exp\left(\frac{E}{kT_m} - \frac{E}{kT}\right)\right)
\]

where \( \alpha(x) \) is a quotient of 4th-order polynomials of the form

\[
\alpha(x) = \frac{a_0 + a_1 x + a_2 x^2 + a_3 x^3 + x^4}{b_0 + b_1 x + b_2 x^2 + b_3 x^3 + x^4}
\]

\( a_0 = 0.267773734, a_1 = 8.6347608925, a_2 = 8.059016973, a_3 = 8.5733287401, b_0 = 3.9584969228, b_1 = 21.0996530827, b_2 = 25.6329561486, b_3 = 9.5733223454 \)

<2> The second type of first-order empirical expression (model="f2") is (Kitis et al., 1998)

\[
I(T) = I_m \exp\left[1 + \frac{E}{kT} \frac{T_m - T}{T_m} - \frac{3}{kT} \exp\left(\frac{E}{kT} \frac{T_m - T}{T_m}\right)\right] \left(1 - \frac{2kT}{E}\right) - \frac{2kT_m}{E}
\]

<3> The third type of first-order function fits a weibull function (model="f3") (Pagonis et al., 2001)

\[
I(T) = 2.713 I_m \left(\frac{T_m - T}{b}\right)^{0.996} \exp\left[-\left(\frac{T_m - T}{b}\right)^{0.996}\right]
\]

where \( b = \sqrt{\frac{242.036 T_m^3 k^3}{(E + T_m k)^{0.996} T_m k}} \)

Second-order glow peaks appear if the re-trapping probability is comparable with or greater than that of recombination during excitation. The three parameters describing a glow peak are the same
as those of first-orders. Two empirical expressions describing second-order glow peaks are available in function \texttt{tgcd}:

\begin{equation}
I(T) = 4I_m\exp(\frac{E}{kT} - \frac{T_m}{T_m})\left[\frac{T^2}{T_m^2}(1 - \frac{2kT}{E})\exp(\frac{E}{kT} - \frac{T_m}{T_m}) + 1 + \frac{2kTm}{E}\right]^{-2}
\end{equation}

\textbf{General-order} glow peaks are produced in intermediate cases (neither of first-order, nor of second-order). The four parameters describing a glow peak are: \(I_m, E, T_m\), and \(b\). Three empirical expressions describing general-order glow peaks are available in function \texttt{tgcd}:

\begin{equation}
I(T) = 5.2973I_m[1 + \exp(-\frac{(T_Tm) + 0.38542)}{-2.4702\exp[-\frac{(T_Tm) + 0.38542]}]}
\end{equation}

where \(a_2 = \sqrt{\frac{1.189T^4k^2}{E^2+4ET_mk}}\)

\textbf{One trap-one recombination (OTOR) model} based semi-analytical expressions have also been applied to fit glow peaks, by using either the Lambert W function (Kitis and Vlachos, 2013; Sadik et al., 2015; Kitis et al., 2016) or the Wright Omega function (Singh and Gartia, 2013; 2014; 2015). The four parameters describing a glow peak are: \(I_m, E, T_m\), and \(R = \frac{A_n}{A_m}\) (where \(A_n\) and \(A_m\) represent the retrapping and recombination probabilities, respectively). Two analytical expressions describing the OTOR model are available in function \texttt{tgcd}:

\begin{equation}
I(T) = I_m\exp(-\frac{E}{kT}(T - T_m))[\frac{1}{b} + \frac{b-1}{b}\exp(-\frac{E}{kTm}(T - T_m))]^{-\frac{1}{b-1}}
\end{equation}

\begin{equation}
I(T) = I_m\exp(-\frac{E}{kTm}(T - T_m))\left[\frac{\omega(Z_m) + |\omega(Z_m)|^2}{\omega(Z) + |\omega(Z)|^2}\right]
\end{equation}
where $Z_m = \frac{R}{1-R} - \log(\frac{1-R}{R}) + \frac{E \exp\left(\frac{E}{kT_m}\right)}{kT_m(1-1.05R^{1.05})} F(T_m, E)$, and $Z = \frac{R}{1-R} - \log(\frac{1-R}{R}) + \frac{E \exp\left(\frac{E}{kT_m}\right)}{kT_m(1-1.05R^{1.05})} F(T, E)$.

**<10.1>** The semi-analytical expression derived using the Lambert W function for $R = \frac{A_n}{A_m} < 1$

$$I(T) = I_m \exp\left(-\frac{E}{kT_m} T_{m-T} T_m\right) \frac{W(\exp(Z_m)) + [W(\exp(Z_m))]^2}{W(\exp(Z)) + [W(\exp(Z))]^2}$$

where $Z_m = \frac{R}{1-R} - \log(\frac{1-R}{R}) + \frac{E \exp\left(\frac{E}{kT_m}\right)}{kT_m(1-1.05R^{1.05})} F(T_m, E)$, and $Z = \frac{R}{1-R} - \log(\frac{1-R}{R}) + \frac{E \exp\left(\frac{E}{kT_m}\right)}{kT_m(1-1.05R^{1.05})} F(T, E)$.

**<10.2>** The semi-analytical expression derived using the Lambert W function for $R = \frac{A_n}{A_m} > 1$

$$I(T) = I_m \exp\left(-\frac{E}{kT_m} T_{m-T} T_m\right) \frac{W(-1, -\exp(-Z_m)) + [W(-1, -\exp(-Z_m))]^2}{W(-1, -\exp(-Z)) + [W(-1, -\exp(-Z))]^2}$$

where $Z_m = |\frac{R}{1-R}| + \log(\frac{1-R}{R}) + \frac{E \exp\left(\frac{E}{kT_m}\right)}{kT_m(2.963-3.24R^{1.05})} F(T_m, E)$, and $Z = |\frac{R}{1-R}| + \log(\frac{1-R}{R}) + \frac{E \exp\left(\frac{E}{kT_m}\right)}{kT_m(2.963-3.24R^{1.05})} F(T, E)$

$F(T_m, E)$ and $F(T, E)$ are described as follows.

$$F(T_m, E) = T_m \exp\left(-\frac{E}{kT_m}\right) + \frac{E}{k} E i\left(-\frac{E}{kT_m}\right)$$

$$F(T, E) = T \exp\left(-\frac{E}{kT}\right) + \frac{E}{k} E i\left(-\frac{E}{kT}\right)$$

where $\omega(x)$ and $E i(x)$ are the Wright Omega function and the exponential integral function for variable $x$, respectively. $W(x)$ and $W(-1, x)$ are the principal and the second branches of the Lambert W function, respectively. The Fortran 90 subroutine used for evaluating the Wright Omega function is transformed from the Matlab code provided by Andrew Horchler (https://github.com/horchler/wrightOmega). The Fortran 90 subroutine (original Fortran 77 version by William Cody) used for evaluating the Lambert W function written by John Burkardt is available at https://people.sc.fsu.edu/~jburkardt/f_src/toms743/toms743.f90. The Fortran 90 subroutine used for evaluating the exponential integral function is written by John Burkardt (original Fortran 77 version by William Cody) (https://people.sc.fsu.edu/~jburkardt/f_src/toms715/toms715.f90).

**Mixed-order** kinetic models introduce an extra parameter $\alpha = \frac{n_0}{n_0 + M}$ where $n_0$ is the initial filled concentration of the active traps and $M$ is the trap concentration of the thermally disconnected deep traps (Sunta et al., 2002). The four parameters describing a glow peak are: $I_m$, $E$, $T_m$, and $\alpha$. Three empirical expressions describing mixed-order glow peaks are available in function `tgcd`.

**<11>** The first type of mixed-order empirical expression (model="m1") is (Kitis and Gomez-Ros, 2000)
\[
I(T) = \frac{I_m [\exp(\frac{2kT_m}{R_m})] - \alpha^2 \exp(\frac{E}{R_m} T - \frac{T_m}{R_m}) \exp(\frac{T^2}{T_m R_m} \exp(\frac{E}{R_m} T - \frac{T_m}{R_m})(1 - \frac{2kT}{E}))]}{\exp(\frac{1 - \frac{2kT_m}{R_m}}{R_m}) \exp(\frac{T^2}{T_m R_m} \exp(\frac{E}{R_m} T - \frac{T_m}{R_m})(1 - \frac{2kT}{E})) - \alpha^2}
\]

where \( R_m = \frac{A_m}{m} + \frac{a}{m} \) and \( A_m = \exp(\frac{A_m}{m} + \frac{a}{m} (1 - \frac{2kT_m}{E})) \)

The second type of mixed-order empirical expression (model="m2") is (Gomez-Ros and Kitis, 2002)

\[
I(T) = \frac{4I_m R_m^2 \exp(\frac{E}{R_m} T) \exp(R_m \frac{E}{R_m} T) \exp(\frac{T^2}{T_m R_m} \exp(\frac{E}{R_m} T - \frac{T_m}{R_m}) F(\frac{E}{R_m} T) - F(\frac{E}{R_m} T)))}{1 + R_m \exp(\frac{R_m E}{R_m} T) \exp(\frac{T^2}{T_m R_m} \exp(\frac{E}{R_m} T - \frac{T_m}{R_m}) F(\frac{E}{R_m} T) - F(\frac{E}{R_m} T))) - (1 - R_m)^2}
\]

where \( R_m = (1 - \alpha)(1 + 0.2922\alpha - 0.2783\alpha^2) \)

\[
F(x) = 1 - \frac{a_0 + a_1 x + a_2 x^2}{b_0 + b_1 x + b_2 x^2}
\]

\( a_0 = 0.250621, a_1 = 2.334733, b_0 = 1.681534, b_1 = 3.330657 \)

The third type of mixed-order empirical expression (model="m3") is (Vejnovic et al., 2008)

\[
I(T) = \frac{I_m (2-l)^2 \exp(\frac{T^2}{T_m} (\frac{1}{T} - l) \exp(\frac{E}{R_m} T - \frac{T_m}{R_m}) (1 - \frac{2kT}{E})) \exp(\frac{E}{R_m} T - \frac{T_m}{R_m}) \exp(\frac{T^2}{T_m R_m} \exp(\frac{E}{R_m} T - \frac{T_m}{R_m}) (1 - \frac{2kT}{E})) - \alpha^2}}{(l-1) \exp(\frac{T^2}{T_m} (\frac{1}{T} - l) \exp(\frac{E}{R_m} T - \frac{T_m}{R_m}) (1 - \frac{2kT}{E})) - \alpha^2}
\]

where \( \alpha = (1 - 1) \exp(\frac{2-l}{l} (1 - \frac{2kT_m}{E})) \)

The background will be subtracted using the following expression if subBG=TRUE (Horowitz and Yossian, 1995; Kitis et al., 2012)

\[
I(T) = A + B \exp(\frac{T}{C})
\]

where \( A, B, \) and \( C \) are positive parameters to be optimized.

The procedure minimizes the objective: \( fcn = \sum_{i=1}^{n} |y_o^i - y_f^i|, i = 1, \ldots, n \) where \( y_o^i \) and \( y_f^i \) denote the \( i \)-th observed and fitted signal value, respectively, and \( n \) indicates the number of data points.

The Levenberg-Marquardt algorithm (More, 1978) \( \text{minpack: } \) https://netlib.org/minpack/, original Fortran 77 version by Jorge More, Burton Garbow, Kenneth Hillstrom. Fortran 90 version by John Burkardt https://people.sc.fsu.edu/~jburkardt/f_src/minpack/minpack.f90 was modified so as to supports constraints and fixes of parameters. A "trial-and-error" protocol with starting values generated uniformly around the given starting parameters inisPAR and inisBG is performed repeatedly to search the optimal parameters that give a minimum Figure Of Merit (FOM) value (Balian and Eddy, 1977).

Kinetic parameters can be initialized by the user through argument inisPAR or by clicking with a mouse on the plot of the thermoluminescence glow curve showing peak maxima if inisPAR=NULL. Background parameters can be initialized by the user through argument inisBG or by clicking with a mouse on the plot of the thermoluminescence glow curve to select 4 data points if inisBG=NULL.
Parameters can be interactively constrained and fixed by modifying the following elements in a automatically generated Dialog Table if edit.inis=TRUE:

1. **INTENS\[min,max,ini,fix\]**: lower and upper bounds, starting and fixing values of $I_m$
2. **ENERGY\[min,max,ini,fix\]**: lower and upper bounds, starting and fixing values of $E$
3. **TEMPER\[min,max,ini,fix\]**: lower and upper bounds, starting and fixing values of $T_m$
4. **bValue\[min,max,ini,fix\]**: lower and upper bounds, starting and fixing values of $b$ in the general-order model
5. **rValue\[min,max,ini,fix\]**: lower and upper bounds, starting and fixing values of $R$ in the OTOR model
6. **aValue\[min,max,ini,fix\]**: lower and upper bounds, starting and fixing values of $\alpha$ in the mixed-order model
7. **BG\[min,max,ini,fix\]**: lower and upper bounds, starting and fixing values of background parameters $A$, $B$, and $C$

**Value**

Return an invisible list containing the following elements:

- `comp.sig` calculated signal values for each glow peak
- `residuals` calculated residual values
- `pars` optimized parameters stored in a matrix
- `BGpars` optimized background parameters, it returns NULL if subBG=FALSE
- `ff` calculated frequency factors, it returns NULL if hr=NULL
- `sp` parameters used for describing the shape of a glow peak, see function `simPeak` for details
- `resolution` resolutions of optimized glow peaks calculated after Kitis and Pagonis (2019), it returns NULL if npeak=1
- `SSR` Squared Sum of Residuals
- `RCS` Reduced Chi-Square value
- `R2` squared "pearson" correlation between observed and fitted signals
- `FOM` Figure Of Merit value calculated after Balian and Eddy (1977)

**Note**

Function `tgcd` analyzes only thermoluminescence glow curves recorded with linear heating function (LHF) profile. The model to be optimized should not be underdetermined. This means that the number of data points ($n_d$) should exceed the number of parameters ($n_2$).

If it is not NULL the argument `inisPAR`, the procedure used for initializing kinetic parameters by clicking with a mouse will not be triggered. Similarly, if it is not NULL the argument `inisBG`, the procedure used for initializing background parameters by clicking with a mouse will not be triggered.

The user is advocated to use `mwt`, `mdt`, and `mr` to specify the allowed maximum total half-width, the allowed minimum distance, and the allowed minimum resolution respectively to resolve seriously.

Note
overlapped glow peaks during the trial-and-error protocol.

Adrie J.J. Bos is appreciated for providing the reference glow curves of the GLOCANIN project to test this routine.

Amr M. Sadek is thanked for providing the Matlab code implementing the Lambert W (Wright Omega) function for reference.

George Kitis is appreciated for giving some useful suggestions to improve the program and providing many experimentally measured thermoluminescence glow curves to check the routine.

References


Further reading


Horowitz YS, Moscovitch M. 2012. Highlights and pitfalls of 20 years of application of computerised glow curve analysis to thermoluminescence research and dosimetry. Radiation Protection Dosimetry, 1-22.


See Also

simPeak; simqOTOR; savgol

Examples

# Load the data.
data(Refglow)
data(Kitis)

# (1) Deconvolution of a glow curve using 4 peaks (no background subtraction) with
# the Wright Omega function using specified initial kinetic parameters.

knPars <-
cbind(c(400, 550, 850, 1600), # Im
c(1.4, 1.5, 1.6, 2), # E
c(420, 460, 480, 510), # Tm
c(0.1, 0.1, 0.1, 0.1)) # R

dd1 <- tgcd(Refglow$x002, npeak=4, model="wo",
inisPAR=knPars, nstart=10, edit.inis=FALSE)

head(dd1$comp.sig)
dd1$pars
dd1$sp
dd1$FOM

# (2) Deconvolution of a glow curve using 5 peaks (with background subtraction) with
# a mixed-order model using user-supplied intial kinetic and background parameters.

knPars <-
cbind(c(46829.06, 187942.43, 121876.22, 110390.55, 67978.33), # Im
      c(1.17, 1.14, 1.57, 0.77, 1.31), # E
      c(369.86, 400.69, 428.51, 482.41, 537.28), # Tm
      c(0.75, 0.81, 0.92, 0.001, 0.29)) # a
bgPars <- c(1, 10, 100) # A, B, C.

dd2 <- tgcdf(Kitis$x009, npeak=5, model="m1", subBG=TRUE,
             inisPAR=knPars, inisBG=bgPars, nstart=10, edit.inis=FALSE)

dd2$residual
dd2$SSR
dd2$R2
dd2$BGpars
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