

Package ‘RLumCarlo’

October 10, 2019

Type Package

Title Monte-Carlo Methods for Simulating Luminescence Phenomena

Version 0.1.0.9000-101

Date 2019-10-10

Author Johannes Friedrich [aut, trl] (<<https://orcid.org/0000-0002-0805-9547>>),
Sebastian Kreutzer [aut, trl, cre] (<<https://orcid.org/0000-0002-0734-2199>>),
Vasilis Pagonis [aut] (<<https://orcid.org/0000-0002-4852-9312>>),
Christoph Schmidt [aut] (<<https://orcid.org/0000-0002-2309-3209>>),
Ena Rajovic [ctb],
Alex Roy Duncan [ctb],
Christian Laag [ctb]

Maintainer Sebastian Kreutzer <sebastian.kreutzer@u-bordeaux-montaigne.fr>

Description A collection of functions to simulate luminescence production in minerals using Monte-Carlo methods. Implemented are models for delocalised, localised and tunnelling transition. Supported stimulation methods are TL, CW-OSL, LM-OSL and ITL.

Contact Package Developer Team <sebastian.kreutzer@u-bordeaux-montaigne.fr>

License GPL-3

BugReports <https://github.com/R-Lum/RLumCarlo/issues>

Depends R (>= 3.3.0),
utils,
magrittr

URL <https://CRAN.R-project.org/package=RLumCarlo>

LinkingTo Rcpp (>= 1.0.2),
RcppArmadillo (>= 0.9.700.2.0)

Imports abind (>= 1.4-5),
doParallel (>= 1.0.15),
foreach (>= 1.4.7),
khroma (>= 1.2.0),
parallel,
methods,
Rcpp (>= 1.0.2)

Suggests R.rsp (>= 0.43.1),
testthat (>= 2.0.0)

Encoding UTF-8

VignetteBuilder R.rsp

RoxygenNote 6.1.1

R topics documented:

RLumCarlo-package	2
plot_RLumCarlo	3
run_MC_CW_IRSL_LOC	4
run_MC_CW_IRSL_TUN	6
run_MC_CW_OSL_DELOC	8
run_MC_ISO_DELOC	10
run_MC_ISO_LOC	12
run_MC_ISO_TUN	13
run_MC_LM_OSL_DELOC	15
run_MC_LM_OSL_LOC	17
run_MC_LM_OSL_TUN	19
run_MC_TL_DELOC	21
run_MC_TL_LOC	23
run_MC_TL_TUN	25
Index	27

RLumCarlo-package	<i>Monte-Carlo Methods for Simulating Luminescence Phenomena</i>
-------------------	--

Description

A collection of functions to simulate luminescence production in minerals using Monte-Carlo methods. Implemented are models for delocalised, localised and tunnelling transition. Supported stimulation methods are TL, CW-OSL, LM-OSL and ITL.

Details

Funding

This project benefitted from support by various funding bodies.

- The initial work by Johannes Friedrich, Sebastian Kreutzer and Christoph Schmidt was supported by the DFG (2015–2018, SCHM 3051/4-1, "Modelling quartz luminescence signal dynamics relevant for dating and dosimetry", SCHM 3051/4-1).
- Later financial support was secured through the project "ULTIMO: Unifying Luminescence Models of quartz and feldspar (German Academic Exchange Service) DAAD: Deutscher Akademischer Austauschdienst DAAD PPP USA 2018, ID: 57387041).
- The work of Sebastian Kreutzer as maintainer of the package was supported by LabEx LaS-cArBx (ANR - n. ANR-10-LABX-52).

Author(s)

Johannes Friedrich (University of Bayreuth, Germany),
 Sebastian Kreutzer, IRAMAT-CRP2A, UMR 5060, CNRS-Université Bordeaux Montaigne (France),
 Vasilis Pagonis, McDaniel College Westminster (MD, USA),
 Christoph Schmidt, University of Bayreuth (Germany),
 Ena Rajovic, University of Bayreuth (Germany),
 Alex Roy Duncan, University of Bayreuth (Germany),
 Christian Laag, University of Bayreuth (Germany)

References

Pagonis, V., Friedrich, J., Discher, M., Müller-Kirschbaum, A., Schlosser, V., Kreutzer, S., Chen, R., Schmidt, C., 2019. Excited state luminescence signals from a random distribution of defects_ A new Monte Carlo simulation approach for feldspar. Journal of Luminescence 207, 266–272. doi: [10.1016/j.jlumin.2018.11.024](https://doi.org/10.1016/j.jlumin.2018.11.024)

plot_RLumCarlo

*Plot RLumCarlo Monte-Carlo Simulations Results***Description**

The function allows to visualise 'RLumCarlo' modelling results without extracting the values manually. Typically visualised values are the signal or the number of remaining electrons as averaged values with a polygon indicating modelling uncertainties.

Usage

```
plot_RLumCarlo(object, plot_uncertainty = "range", norm = FALSE,
  add = FALSE, ...)
```

Arguments

object	list of class <code>RLumCarlo_Model_Output</code> (required): input object to be plotted, usually the required input object is generated by one for the functions preceding with <code>run</code> . Alternatively a list of such objects can be provided.
plot_uncertainty	logical (<i>with default</i>): sets the nature of the show uncertainty, allowed values are <code>range</code> , <code>sd</code> (standard deviation), <code>var</code> (variance) and <code>NULL</code> disables the uncertainty visualisation
norm	logical (<i>with default</i>): normalise curve to the highest intensity
add	logical (<i>with default</i>): allows overplotting of results by adding curve to an existing plot
...	further arguments that can be passed to control the plot output. Currently supported are: <code>xlab</code> , <code>xlim</code> , <code>ylim</code> , <code>main</code> , <code>lwd</code> , <code>type</code> , <code>pch</code> , <code>lty,col</code> , <code>grid</code> , <code>legend</code> . The arguments <code>lwd</code> , <code>type</code> , <code>pch</code> , <code>lty</code> , <code>col</code> can be provided as vector if object is a list

Details

The colour curves, the package [khroma::khroma-package](#) is used to provide colours that can be best distinguished, in particular by colour-blind users.

Value

This function returns a graphical output

Function version

0.1.0

How to cite

Friedrich, J., Kreutzer, S., 2019. plot_RLumCarlo(): Plot RLumCarlo Monte-Carlo Simulations Results. Function version 0.1.0. In: Friedrich, J., Kreutzer, S., Pagonis, V., Schmidt, C., 2019. RLumCarlo: Monte-Carlo Methods for Simulating Luminescence PhenomenaR package version 0.1.0.9000-101.

Author(s)

Johannes Friedrich, University of Bayreuth (Germany), Sebastian Kreutzer, IRAMAT-CRP2A, Université Bordeaux Montaigne (France)

run_MC_CW_IRSL_LOC	<i>Run Monte-Carlo simulation for CW-IRSL for localized transition</i>
--------------------	--

Description

Runs a Monte-Carlo (MC) simulation of constant wave infrared stimulated luminescence (CW-IRSL) using the generalized one trap (GOT) model. Localized refers to excitation of an electron before it recombines, but without the involvement of the conduction band.

Usage

```
run_MC_CW_IRSL_LOC(A, times, clusters = 10, n_filled = 100, r,
  method = "par", output = "signal", ...)
```

Arguments

A	numeric (required) : The optical excitation rate from trap to conduction band (s^{-1}).
times	numeric (with default) : The sequence of temperature steps within the simulation (s).
clusters	numeric (with default) : The number of MC runs (unitless).
n_filled	integer (with default) : The number of filled electron traps at the beginning of the simulation (unitless).
r	numeric (with default) : The localized retrapping ratio (unitless).
method	character (with default) : sequential 'seq' or parallel processing 'par'
output	character (with default) : output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)
...	further arguments

Details

$$I_{LOC}(t) = -dn/dt = A * (n^2 / (r + n))$$

Where in the function:

t := Time

n := 'n_filled'

Value

This function returns an [array](#) with dimension length(times) x length(r) x clusters

Function version

0.1.0

How to cite

Kreutzer, S., 2019. run_MC_CW_IRSL_LOC(): Run Monte-Carlo simulation for CW-IRSL for localized transition. Function version 0.1.0. In: Friedrich, J., Kreutzer, S., Pagonis, V., Schmidt, C., 2019. RLumCarlo: Monte-Carlo Methods for Simulating Luminescence Phenomena R package version 0.1.0.9000-101.

Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, UMR 5060, CNRS - Université Bordeaux Montaigne (France)

References

Pagonis, V., Friedrich, J., Discher, M., Müller-Kirschbaum, A., Schlosser, V., Kreutzer, S., Chen, R. and Schmidt, C., 2019. Excited state luminescence signals from a random distribution of defects: A new Monte Carlo simulation approach for feldspar. Journal of Luminescence 207, 266–272. doi: [10.1016/j.jlumin.2018.11.024](https://doi.org/10.1016/j.jlumin.2018.11.024)

Reuven, C. and S. Mckeever, 1997. Theory of thermoluminescence and related phenomena.

Examples

```
##=====##
## Example 1: Single Plot for Monte-Carlo (MC) simulations for localized CW_IRSL
##=====##
## Not run:
run_MC_CW_IRSL_LOC(
  A = 0.12,
  r = 1,
  times = 0:100) %>%
  #Plot results of the MC simulation
  plot_RLumCarlo(legend = T)

## End(Not run)
```

run_MC_CW_IRSL_TUN *Run Monte-Carlo simulation for CW-IRSL*

Description

Runs a Monte-Carlo (MC) simulation of constant wave infrared stimulated luminescence (CW-IRSL) using the model. Tunneling refers to the direct movement of electrons from a trap directly to the recombination center.

Usage

```
run_MC_CW_IRSL_TUN(A, rho, times, clusters = 10, r_c = 0,
    delta.r = 0.1, N_e = 200, method = "seq", output = "signal", ...)
```

Arguments

A	numeric (required) : The optical excitation rate from ground state of trap to excited state of trap (s ⁻¹).
rho	numeric (required) : The density of recombination centers (defined as rho' in Huntley 2006) (unitless).
times	numeric (with default) : The sequence of temperature steps within the simulation (s).
clusters	numeric (with default) : The number of MC runs (unitless).
r_c	numeric (with default) : The retrapping ratio.
delta.r	numeric (with default) :
N_e	numeric (with default) : The total number of electron traps available (unitless).
method	character (with default) : sequential 'seq' or parallel processing 'par'
output	character (with default) : output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)
...	further arguments
r	numeric (with default) : The radius of tunneling (unitless).

Details

$$p(t) = A * e^{(-r'/\rho^{(-1/3)})}$$

$$I_{TUN}(t) = 3 * n * p(t) * (r')^2 * e^{(-r'^3)}$$

Where in the function:

p(t) := The experimental stimulation mode

e:= Exponential function

r' := r

ρ' := rho

t := Time

n := The Instantaneous number of electrons

Value

This function returns a list.

Function version

0.2.0

How to cite

Friedrich, J., Kreutzer, S., 2019. run_MC_CW_IRSL_TUN(): Run Monte-Carlo simulation for CW-IRSL. Function version 0.2.0. In: Friedrich, J., Kreutzer, S., Pagonis, V., Schmidt, C., 2019. RLumCarlo: Monte-Carlo Methods for Simulating Luminescence Phenomena R package version 0.1.0.9000-101.

Author(s)

Johannes Friedrich, University of Bayreuth (Germany), Sebastian Kreutzer, IRAMAT-CRP2A, UMR 5060, Université Bordeaux Montaigne (France)

References

Huntley, D.J., 2006. An explanation of the power-law decay of luminescence. *Journal of Physics: Condensed Matter*, 18(4), 1359. doi: [10.1088/09538984/18/4/020](https://doi.org/10.1088/09538984/18/4/020)

Pagonis, V., Friedrich, J., Discher, M., Müller-Kirschbaum, A., Schlosser, V., Kreutzer, S., Chen, R. and Schmidt, C., 2019. Excited state luminescence signals from a random distribution of defects: A new Monte Carlo simulation approach for feldspar. *Journal of Luminescence* 207, 266–272. doi: [10.1016/j.jlumin.2018.11.024](https://doi.org/10.1016/j.jlumin.2018.11.024)

Reuven, C. and S. McKeever, 1997. Theory of thermoluminescence and related phenomena.

Examples

```
## Not run:

##=====##
## Example 1: Simulate CW-IRSL measurement
##=====##

run_MC_CW_IRSL_TUN(
  A = 1,
  clusters= 500,
  rho = 1e-4,
  N_e = 1E4,
  r_c = 2,
  times = 0:500,
  delta.r = 1e-1,
  method = "seq"
)) %>% plot_RLumCarlo(norm = T, legend = T)

## End(Not run)
```

run_MC_CW_OSL_DELOC *Run Monte-Carlo simulation for CW-OSL for delocalized transition*

Description

Runs a Monte-Carlo (MC) simulation of constant wave optically stimulated luminescence (CW-OSL) using the one trap one recombination center (OTOR) model. Delocalized refers to involvement of the conduction band.

Usage

```
run_MC_CW_OSL_DELOC(A, times, clusters = 10, N_e = 200,
    n_filled = N_e, R, method = "par", output = "signal", ...)
```

Arguments

A	numeric (required) : The optical excitation rate from trap to conduction band (s^{-1}).
times	numeric (with default) : The sequence of temperature steps within the simulation (s)
clusters	numeric (with default) : The number of MC runs (unitless).
N_e	integer (with default) : The total number of electron traps available (unitless).
n_filled	integer (with default) : The number of filled electron traps at the beginning of the simulation (unitless).
R	numeric (with default) : The delocalized retrapping ratio (unitless).
method	character (with default) : sequential 'seq' or parallel processing 'par'
output	character (with default) : output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)
...	further arguments

Details

$$I_{DELOC}(t) = -dn/dt = p(t) * (n^2 / (N * R + n(1 - R)))$$

Where in the function:

t := Time

p(t) := The experimental stimulation mode

n := The Instantaneous number of electrons

N = N_e

Value

This function returns an **array** with dimension length(times) x length(r) x clusters

Function version

0.1.0

How to cite

Kreutzer, S., 2019. run_MC_CW_OSL_DELOC(): Run Monte-Carlo simulation for CW-OSL for delocalized transition. Function version 0.1.0. In: Friedrich, J., Kreutzer, S., Pagonis, V., Schmidt, C., 2019. RLumCarlo: Monte-Carlo Methods for Simulating Luminescence Phenomena R package version 0.1.0.9000-101.

Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, UMR 5060, CNRS - Université Bordeaux Montaigne (France)

References

Pagonis, V., Friedrich, J., Discher, M., Müller-Kirschbaum, A., Schlosser, V., Kreutzer, S., Chen, R. and Schmidt, C., 2019. Excited state luminescence signals from a random distribution of defects: A new Monte Carlo simulation approach for feldspar. Journal of Luminescence 207, 266–272. doi: [10.1016/j.jlumin.2018.11.024](https://doi.org/10.1016/j.jlumin.2018.11.024)

Reuven, C. and S. Mckeever, 1997. Theory of thermoluminescence and related phenomena.

Examples

```
##=====##
## Example 1: Single Plot for Monte-Carlo (MC) simulations for delocalized CW-OSL
##=====##
## Not run:
run_MC_CW_OSL_DELOC(
  A = 0.12,
  R = 1,
  times = 0:100) %>%
  #Plot results of the MC simulation
  plot_RLumCarlo(legend = T)

## End(Not run)

#' @examples
##=====##
## Example 2: Simulate CW-OSL DELOC with several parameter changes
##=====##
## Not run:

# define your parameters
A <- c(0.1,0.3,0.5,1)
times <- seq(0,60,1)
s <- 1e12
E<- 1
R<-c(1e-7,1e-6,0.01,0.1) # sequence of different R values
clusters <- 1000 # number of Monte Carlo simulations
N_e <- c(200, 500, 700, 400) # number of free electrons
n_filled <- c(200, 500, 100, 70) # number of filled traps
method <- "par"
output <- "signal"
col <- c(1,2,3,4) # different colours for the individual curves
plot_uncertainty <- c(T,F,T,F) # do you want to see the uncertainty?
add_TF <- c(F,rep(T, (length(R)-1)))
for (u in 1:length(R)){
```

```

results <-run_MC_CW_OSL_DELOC(A=A[u], times, clusters =clusters, N_e = N_e[u],
                             n_filled = n_filled[u], R=R[u], method = method, output = output)
plot_RLumCarlo(results,add=add_TF[u],legend = F, col=col[u], main=" your plot")
}
legend("topright",ncol=4,cex=0.55,title = "parameters" ,legend=c(paste0("A = ", A),
                                                                    paste0("n_filled = ", n_filled),
                                                                    paste0("N_e = ", N_e),
                                                                    paste0("R = ", R)), text.col=col)

## End(Not run)

```

run_MC_ISO_DELOC

Run Monte-Carlo simulation for ISO-TL for delocalized transition

Description

Runs a Monte-Carlo (MC) simulation of isothermally stimulated luminescence (ISO-TL or ITL) using the one trap one recombination center (OTOR) model. Delocalized refers to involvement of the conduction band.

Usage

```
run_MC_ISO_DELOC(s, E, T = 20, times, clusters = 10, N_e = 200,
                 n_filled = N_e, R, method = "par", output = "signal", ...)
```

Arguments

s	numeric (required) : The frequency factor of the trap (s^{-1}).
E	numeric (required) : Thermal activation energy of the trap (eV).
T	numeric (with default) : Constant stimulation temperature (degrees C).
times	numeric (with default) : the sequence of temperature steps within the simulation (s).
clusters	numeric (with default) : The number of MC runs (unitless).
N_e	integer (with default) : The total number of electron traps available (unitless).
n_filled	integer (with default) : The number of filled electron traps at the beginning of the simulation (unitless).
R	numeric (with default) : The delocalized retrapping ratio (unitless).
method	character (with default) : sequential 'seq' or parallel processing 'par'
output	character (with default) : output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)
...	further arguments

Details

$$I_{DELOC}(t) = -dn/dt = (s * e^{-E/k_b * T_{ISO}}) * (n^2 / (NR + n(1 - R)))$$

Where in the function:

t := Time

e:= Exponential function

k_B := Boltzmann constant

T_{ISO} = T

n := n_filled

N := N_e

Value

This function returns an [array](#) with dimension length(times) x length(r) x clusters

Function version

0.0.1

How to cite

Kreutzer, S., 2019. run_MC_ISO_DELOC(): Run Monte-Carlo simulation for ISO-TL for delocalized transition. Function version 0.0.1. In: Friedrich, J., Kreutzer, S., Pagonis, V., Schmidt, C., 2019. RLumCarlo: Monte-Carlo Methods for Simulating Luminescence PhenomenaR package version 0.1.0.9000-101.

Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, UMR 5060, CNRS - Université Bordeaux Montaigne (France)

References

Pagonis, V., Friedrich, J., Discher, M., Müller-Kirschbaum, A., Schlosser, V., Kreutzer, S., Chen, R. and Schmidt, C., 2019. Excited state luminescence signals from a random distribution of defects: A new Monte Carlo simulation approach for feldspar. Journal of Luminescence 207, 266–272. doi: [10.1016/j.jlumin.2018.11.024](https://doi.org/10.1016/j.jlumin.2018.11.024)

Reuven, C. and S. McKeever, 1997. Theory of thermoluminescence and related phenomena.

Examples

```
##=====##
## Example 1: Single Plot for Monte-Carlo (MC) simulations for delocalized ISO-TL
##=====##
## Not run:
run_MC_ISO_DELOC(
  s = 3.5e12,
  E = 1.45,
  T = 200,
  R = 1,
  times = 0:10000) %>%
#Plot results of the MC simulation
plot_RLumCarlo(legend = T)
```

```
## End(Not run)
```

run_MC_ISO_LOC

Run Monte-Carlo simulation for ISO-TL for localized transition

Description

Runs a Monte-Carlo (MC) simulation of isothermally stimulated luminescence (ISO-TL or ITL) using the generalized one trap (GOT) model. Localized refers to excitation of an electron before it recombines, but without the involvement of the conduction band.

Usage

```
run_MC_ISO_LOC(s, E, T = 20, times, clusters = 10, n_filled = 100, r,
  method = "par", output = "signal", ...)
```

Arguments

s	numeric (required) : The frequency factor of the trap (s^{-1}).
E	numeric (required) : Thermal activation energy of the trap (eV).
T	numeric (with default) : Constant stimulation temperature (degrees C).
times	numeric (with default) : The sequence of temperature steps within the simulation (s).
clusters	numeric (with default) : The number of MC runs (unitless).
n_filled	integer (with default) : The number of filled electron traps at the beginning of the simulation (unitless).
r	numeric (with default) : the localized retrapping ratio (unitless).
method	character (with default) : sequential 'seq' or parallel processing 'par'
output	character (with default) : output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)
...	further arguments

Details

$$I_{LOC}(t) = -dn/dt = (s * e^{-E/k_b * T_{ISO}} * (n^2/(r + n)))$$

Where in the function:

t := Time
e:= Exponential function
 k_B := Boltzmann constant
 $T_{ISO} = T$
n := n_filled
N := N_e

Value

This function returns an [array](#) with dimension length(times) x length(r) x clusters

Function version

0.0.1

How to cite

Kreutzer, S., 2019. run_MC_ISO_LOC(): Run Monte-Carlo simulation for ISO-TL for localized transition. Function version 0.0.1. In: Friedrich, J., Kreutzer, S., Pagonis, V., Schmidt, C., 2019. RLumCarlo: Monte-Carlo Methods for Simulating Luminescence PhenomenaR package version 0.1.0.9000-101.

Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, UMR 5060, CNRS - Université Bordeaux Montaigne (France)

References

Pagonis, V., Friedrich, J., Discher, M., Müller-Kirschbaum, A., Schlosser, V., Kreutzer, S., Chen, R. and Schmidt, C., 2019. Excited state luminescence signals from a random distribution of defects: A new Monte Carlo simulation approach for feldspar. Journal of Luminescence 207, 266–272. doi: [10.1016/j.jlumin.2018.11.024](https://doi.org/10.1016/j.jlumin.2018.11.024)

Examples

```
##=====##
## Example 1: Single Plot for Monte-Carlo (MC) simulations for localized ISO-TL
##=====##
## Not run:
run_MC_ISO_LOC(
  s = 3.5e12,
  E = 1.45,
  T = 200,
  r = 1,
  times = 0:10000) %>%
  #Plot results of the MC simulation
  plot_RLumCarlo(legend = T)

## End(Not run)
```

run_MC_ISO_TUN

Run Monte-Carlo Simulation for ISO-TL for tunneling transition

Description

Runs a Monte-Carlo (MC) simulation of isothermally stimulated luminescence (ISO-TL or ITL) using the tunneling (TUN) model. Tunneling refers to the direct movement of electrons from a trap directly to the recombination center.

Usage

```
run_MC_ISO_TUN(E, s, T = 200, rho, times, clusters = 10, r_c = 0,
  delta.r = 0.1, N_e = 200L, method = "par", output = "signal",
  ...)
```

Arguments

E	numeric (required) : Thermal activation energy of the trap (eV).
s	numeric (required) : Frequency factor of the trap (s^{-1}).
T	numeric (required) : Constant stimulation temperature (degrees C).
rho	numeric (required) : The density of recombination centers (defined as rho' in Huntley 2006) (unitless).
times	numeric (with default) : The sequence of temperature steps within the simulation (s).
clusters	numeric (with default) : The number of MC runs (unitless).
r_c	numeric (with default) : The radius of tunneling (dimensionless)
delta.r	numeric (with default) :
N_e	numeric (with default) : The total number of electron traps available (unitless).
method	character (with default) : sequential 'seq' or parallel processing 'par'
output	character (with default) : output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)
...	further arguments
r	numeric (with default) : The radius of tunneling (unitless).

Details

$$p(t) = s * e^{(-E/k_B * T)} * e^{(-r'/\rho^{1/3})}$$

$$I_{TUN}(t) = 3 * n * p(t) * (r')^{2 * e^{(-r'^3)}}$$

Where in the function:

p(t) := The experimental stimulation mode

e:= Exponential function

k_B := Boltzmann constant

r := r

ρ := rho

t := Time

n := The Instantaneous number of electrons

n := n_filled

t:= times

Value

This function returns a list.

Function version

0.1.0

How to cite

Friedrich, J., Kreutzer, S., 2019. run_MC_ISO_TUN(): Run Monte-Carlo Simulation for ISO-TL for tunneling transition. Function version 0.1.0. In: Friedrich, J., Kreutzer, S., Pagonis, V., Schmidt, C., 2019. RLumCarlo: Monte-Carlo Methods for Simulating Luminescence Phenomena R package version 0.1.0.9000-101.

Author(s)

Johannes Friedrich, University of Bayreuth (Germany), Sebastian Kreutzer, IRAMAT-CRP2A, UMR 5060, CNRS - Université Bordeaux Montaigne (France)

References

Huntley, D.J., 2006. An explanation of the power-law decay of luminescence. Journal of Physics: Condensed Matter, 18(4), 1359. doi: [10.1088/09538984/18/4/020](https://doi.org/10.1088/09538984/18/4/020)

Pagonis, V. and Kulp, C., 2017. Monte Carlo simulations of tunneling phenomena and nearest neighbor hopping mechanism in feldspars. Journal of Luminescence 181, 114–120. doi: [10.1016/j.jlumin.2016.09.014](https://doi.org/10.1016/j.jlumin.2016.09.014)

Pagonis, V., Friedrich, J., Discher, M., Müller-Kirschbaum, A., Schlosser, V., Kreutzer, S., Chen, R. and Schmidt, C., 2019. Excited state luminescence signals from a random distribution of defects: A new Monte Carlo simulation approach for feldspar. Journal of Luminescence 207, 266–272. doi: [10.1016/j.jlumin.2018.11.024](https://doi.org/10.1016/j.jlumin.2018.11.024)

Further reading Aitken, M.J., 1985. Thermoluminescence dating. 276-280. doi: [10.1002/gea.3340020110](https://doi.org/10.1002/gea.3340020110)

Examples

```
## Not run:
##=====##
## Example 1: Simulate isothermal measurement
##=====##
run_MC_ISO_TUN(
  E = 0.5,
  s = 1E8,
  clusters= 100,
  rho = 1e-7,
  N_e = 10,
  r_c = 0.01,
  times = 0:500,
  delta.r = 1e-3,
  method = "seq"
) %>%
  plot_RLumCarlo(legend = TRUE)

## End(Not run)
```

run_MC_LM_OSL_DELOC	<i>Run Monte-Carlo simulation for LM-OSL for delocalized transition</i>
---------------------	---

Description

Runs a Monte-Carlo (MC) simulation of linearly modulated optically stimulated luminescence (LM-OSL) using the one trap one recombination center (OTOR) model. Delocalized refers to involvement of the conduction band.

Usage

```
run_MC_LM_OSL_DELOC(A, times, clusters = 10, N_e = 200,
  n_filled = N_e, R, method = "par", output = "signal", ...)
```

Arguments

A	numeric (required) : The optical excitation rate from trap to conduction band (s^{-1}).
times	numeric (with default) : The sequence of temperature steps within the simulation (s).
clusters	numeric (with default) : The number of MC runs (unitless).
N_e	integer (with default) : The total number of electron traps available (unitless).
n_filled	integer (with default) : The number of filled electron traps at the beginning of the simulation (unitless).
R	numeric (with default) : The delocalized retrapping ratio (unitless).
method	character (with default) : sequential 'seq' or parallel processing 'par'
output	character (with default) : output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)
...	further arguments

Details

$$I_{DELOC}(t) = -dn/dt = p(t) * (n^2 / (N * R + n(1 - R)))$$

Where in the function:

t := Time

p(t) := The experimental stimulation mode

n := The Instantaneous number of electrons

N = N_e

Value

This function returns an **array** with dimension length(times) x length(r) x clusters

Function version

0.1.0

How to cite

Kreutzer, S., 2019. run_MC_LM_OSL_DELOC(): Run Monte-Carlo simulation for LM-OSL for delocalized transition. Function version 0.1.0. In: Friedrich, J., Kreutzer, S., Pagonis, V., Schmidt, C., 2019. RLumCarlo: Monte-Carlo Methods for Simulating Luminescence Phenomena R package version 0.1.0.9000-101.

Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, UMR 5060, CNRS - Université Bordeaux Montaigne (France)

References

- Pagonis, V., Friedrich, J., Discher, M., Müller-Kirschbaum, A., Schlosser, V., Kreutzer, S., Chen, R. and Schmidt, C., 2019. Excited state luminescence signals from a random distribution of defects: A new Monte Carlo simulation approach for feldspar. *Journal of Luminescence* 207, 266–272. doi: [10.1016/j.jlumin.2018.11.024](https://doi.org/10.1016/j.jlumin.2018.11.024)
- Reuven, C. and S. McKeever, 1997. Theory of thermoluminescence and related phenomena.

Examples

```
##=====##
## Example 1: Single Plot for Monte-Carlo (MC) simulations for delocalized LM-OSL
##=====##
## Not run:
run_MC_LM_OSL_DELOC(
  A = 0.12,
  R = 1,
  times = 0:100) %>%
  #Plot results of the MC simulation
  plot_RLumCarlo(legend = T)

## End(Not run)
```

run_MC_LM_OSL_LOC

Run Monte-Carlo simulation for LM-OSL for localized transition

Description

Runs a Monte-Carlo (MC) simulation of linearly modulated optically stimulated luminescence (LM-OSL) using the generalized one trap (GOT) model. Localized refers to excitation of an electron before it recombines, but without the involvement of the conduction band.

Usage

```
run_MC_LM_OSL_LOC(A, times, clusters = 10, n_filled = 100, r,
  method = "par", output = "signal", ...)
```

Arguments

A	numeric (required) : The optical excitation rate from trap to conduction band (s^{-1}).
times	numeric (with default) : The sequence of temperature steps within the simulation (s).
clusters	numeric (with default) : The number of MC runs (unitless).
n_filled	integer (with default) : The number of filled electron traps at the beginning of the simulation (unitless).
r	numeric (with default) : The localized retrapping ratio (unitless)
method	character (with default) : sequential 'seq' or parallel processing 'par'
output	character (with default) : output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)
...	further arguments

Details

$$I_{LOC}(t) = -dn/dt = p(t) * (n^2/(r + n))$$

Where in the function:

t := Time

p(t) := The experimental stimulation mode

n := The Instantaneous number of electrons

Value

This function returns an [array](#) with dimension length(times) x length(r) x clusters

Function version

0.1.0

How to cite

Kreutzer, S., 2019. run_MC_LM_OSL_LOC(): Run Monte-Carlo simulation for LM-OSL for localized transition. Function version 0.1.0. In: Friedrich, J., Kreutzer, S., Pagonis, V., Schmidt, C., 2019. RLumCarlo: Monte-Carlo Methods for Simulating Luminescence PhenomenaR package version 0.1.0.9000-101.

Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, UMR 5060, CNRS - Université Bordeaux Montaigne (France)

References

Pagonis, V., Friedrich, J., Discher, M., Müller-Kirschbaum, A., Schlosser, V., Kreutzer, S., Chen, R. and Schmidt, C., 2019. Excited state luminescence signals from a random distribution of defects: A new Monte Carlo simulation approach for feldspar. Journal of Luminescence 207, 266–272. doi: [10.1016/j.jlumin.2018.11.024](https://doi.org/10.1016/j.jlumin.2018.11.024)

Examples

```
##=====##
## Example 1: Single Plot for Monte-Carlo (MC) simulations for localized LM-OSL
##=====##
## Not run:
run_MC_LM_OSL_LOC(
  A = 0.12,
  r = 1,
  times = 0:100) %>%
  #Plot results of the MC simulation
  plot_RLumCarlo(legend = T)

## End(Not run)
```

run_MC_LM_OSL_TUN	<i>Run Monte-Carlo simulation for LM-OSL for tunneling transition</i>
-------------------	---

Description

Runs a Monte-Carlo (MC) simulation of linearly modulated optically stimulated luminescence (LM-OSL) using the tunneling (TUN) model. Tunneling refers to the direct movement of electrons from a trap directly to the recombination center

Usage

```
run_MC_LM_OSL_TUN(A, rho, times, clusters = 10, r_c = 0,
    delta.r = 0.1, N_e = 200, method = "par", output = "signal", ...)
```

Arguments

A	numeric (required) : The optical excitation rate from ground state of trap to excited state of trap (s ⁻¹).
rho	numeric (required) : The density of recombination centers (defined as rho' in Huntley 2006) (unitless).
times	vector (with default) : The sequence of temperature steps within the simulation (s).
clusters	numeric (with default) : The number of clusters.
r_c	numeric (with default) : The retrapping ratio.
delta.r	numeric (with default) : Increments of r_c (unitless).
N_e	numeric (width default) : The total number of electron traps available (unitless).
method	character (with default) : sequential 'seq' or parallel processing 'par'
output	character (with default) : output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)
...	further arguments
r	numeric (with default) : The radius of tunneling (unitless).

Details

$$p(t) = A * (t/P) * e^{(-r'/\rho'^{(-1/3)})}$$

$$I_{TUN}(t) = 3 * n * p(t) * (r')^2 * e^{(-r'^3)}$$

Where in the function:

p(t) := The experimental stimulation mode

t := Time

P := Maximum stimulation time

e := Exponential function

r' := r

ρ' := rho

n := The instantaneous number of electrons

Value

This function returns a list.

Function version

0.1.0

How to cite

Friedrich, J., 2019. run_MC_LM_OSL_TUN(): Run Monte-Carlo simulation for LM-OSL for tunneling transition. Function version 0.1.0. In: Friedrich, J., Kreutzer, S., Pagonis, V., Schmidt, C., 2019. RLumCarlo: Monte-Carlo Methods for Simulating Luminescence Phenomena R package version 0.1.0.9000-101.

Author(s)

Johannes Friedrich, University of Bayreuth (Germany)

References

Huntley, D.J., 2006. An explanation of the power-law decay of luminescence. Journal of Physics: Condensed Matter, 18(4), 1359. doi: [10.1088/09538984/18/4/020](https://doi.org/10.1088/09538984/18/4/020)

Pagonis, V. and Kulp, C., 2017. Monte Carlo simulations of tunneling phenomena and nearest neighbor hopping mechanism in feldspars. Journal of Luminescence 181, 114–120. doi: [10.1016/j.jlumin.2016.09.014](https://doi.org/10.1016/j.jlumin.2016.09.014)

Pagonis, V., Friedrich, J., Discher, M., Müller-Kirschbaum, A., Schlosser, V., Kreutzer, S., Chen, R. and Schmidt, C., 2019. Excited state luminescence signals from a random distribution of defects: A new Monte Carlo simulation approach for feldspar. Journal of Luminescence 207, 266–272. doi: [10.1016/j.jlumin.2018.11.024](https://doi.org/10.1016/j.jlumin.2018.11.024)

Further reading Aitken, M.J., 1985. Thermoluminescence dating. 276-280. doi: [10.1002/gea.3340020110](https://doi.org/10.1002/gea.3340020110)

Examples

```
## Not run:
```

```
##TODO: Primary example, should be verified
run_MC_LM_OSL_TUN(A = 10000, rho = 0.0001, times = 1:100, clusters = 10, r = NULL,
  delta.r = 0.1,
  N_e = 200, method = "par", output = "signal") %>%
  plot_RLumCarlo(norm = T)
```

```
## End(Not run)
```

run_MC_TL_DELOC

*Run Monte-Carlo simulation for TL for delocalized transition***Description**

Runs a Monte-Carlo (MC) simulation of thermo-luminescence (TL) using the one trap one recombination center (OTOR) model. Delocalized refers to involvement of the conduction band.

Usage

```
run_MC_TL_DELOC(s, E, times, clusters = 10, N_e = 200,
               n_filled = N_e, R, method = "par", output = "signal", ...)
```

Arguments

s	numeric (required) : The frequency factor of the trap (s^{-1}).
E	numeric (required) : Thermal activation energy of the trap (eV).
times	numeric (with default) : The sequence of temperature steps within the simulation (s).
clusters	numeric (with default) : The number of MC runs (unitless).
N_e	integer (with default) : The total number of electron traps available (unitless).
n_filled	integer (with default) : The number of filled electron traps at the beginning of the simulation (unitless).
R	numeric (with default) : The delocalized retrapping ratio (unitless).
method	character (with default) : sequential 'seq' or parallel processing 'par'
output	character (with default) : output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)
...	further arguments

Details

$$I_{DELOC}(t) = -dn/dt = (s * e^{-E/k_b * T}) * (n^2 / (N * R + n(1 - R)))$$

Where in the function:

t := Time

e:= Exponential function

k_B := Boltzmann constant

T= Temperature

n := The Instantaneous number of electrons

N := N_e

Value

This function returns an [array](#) with dimension length(times) x length(r) x clusters

Function version

0.0.1

How to cite

Kreutzer, S., 2019. run_MC_TL_DELOC(): Run Monte-Carlo simulation for TL for delocalized transition. Function version 0.0.1. In: Friedrich, J., Kreutzer, S., Pagonis, V., Schmidt, C., 2019. RLumCarlo: Monte-Carlo Methods for Simulating Luminescence PhenomenaR package version 0.1.0.9000-101.

Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, UMR 5060, CNRS - Université Bordeaux Montaigne (France)

References

Pagonis, V., Friedrich, J., Discher, M., Müller-Kirschbaum, A., Schlosser, V., Kreutzer, S., Chen, R. and Schmidt, C., 2019. Excited state luminescence signals from a random distribution of defects: A new Monte Carlo simulation approach for feldspar. Journal of Luminescence 207, 266–272. doi: [10.1016/j.jlumin.2018.11.024](https://doi.org/10.1016/j.jlumin.2018.11.024)

Reuven, C. and S. McKeever, 1997. Theory of thermoluminescence and related phenomena.

Examples

```
##=====##
## Example 1: Single Plot for Monte-Carlo (MC) simulations for delocalized TL
##=====##
## Not run:
run_MC_TL_DELOC(
  s = 3.5e12,
  E = 1.45,
  R = 1,
  times = 100:450) %>%
#Plot results of the MC simulation
  plot_RLumCarlo(legend = T)

## End(Not run)

#' @examples
##=====##
## Example 2: Plot multiple TL stimulation TL curves in R with varying params
##=====##

## Not run:
# define your parameters
times=seq(100,450,1)
s=rep(3.5e12,4)
E=rep(1.45,4)
R<-c(0.7e-6,1e-6,0.01,0.1)
clusters=1000
N_e =c(400, 500, 700, 400)
n_filled =c(400, 500, 300, 70)
method="par"
output ="signal"
col=c(1,2,3,4) # different colours for the individual curves
plot_uncertainty <- c(TRUE,TRUE,TRUE,TRUE) # do you want to see the uncertainty?
```

```

add_TF <- c(FALSE,rep(TRUE, (length(R)-1)))
for (u in 1:length(R)){
  results <-run_MC_TL_DELOC(times=times, s=s[u],E=E[u], clusters =clusters, N_e = N_e[u],
    n_filled = n_filled[u], R=R[u], method = method, output = output)
  plot_RLumCarlo(results,add=add_TF[u],legend = FALSE, col=col[u], main=" your plot", ylim=c(0,20))
}
legend("topright",ncol=5,cex=0.55,title = "parameters" ,legend=c(paste0("E = ", E),
  paste0("s = ", s),
  paste0("n_filled = ", n_filled),
  paste0("N_e = ", N_e),
  paste0("R = ", R)), text.col=col)

## End(Not run)

```

run_MC_TL_LOC

Run Monte-Carlo simulation for TL for localized transition

Description

Runs a Monte-Carlo (MC) simulation of thermo-luminescence (TL) using the generalized one trap (GOT) model. Localized refers to excitation of an electron before it recombines, but without the involvement of the conduction band.

Usage

```
run_MC_TL_LOC(s, E, times, clusters = 10, n_filled = 100, r,
  method = "par", output = "signal", ...)
```

Arguments

s	numeric (required) : The frequency factor of the trap (s^{-1}).
E	numeric (required) : Thermal activation energy of the trap (eV).
times	numeric (with default) : The sequence of temperature steps within the simulation (s).
clusters	numeric (with default) : The number of MC run (unitless).
n_filled	integer (with default) : The number of filled electron traps at the beginning of the simulation (unitless).
r	numeric (with default) : The localized retrapping ratio (unitless).
method	character (with default) : sequential 'seq' or parallel processing 'par'
output	character (with default) : output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)
...	further arguments

Details

$$I_{LOC}(t) = -dn/dt = (s * e^{-E/k_b * T}) * (n^2 / (r + n))$$

Where in the function:

t := Time

e:= Exponential function

k_B := Boltzmann constant

T := Temperature

n := The Instantaneous number of electrons

Value

This function returns an [array](#) with dimension length(times) x length(r) x clusters

Function version

0.1.0

How to cite

Kreutzer, S., 2019. run_MC_TL_LOC(): Run Monte-Carlo simulation for TL for localized transition. Function version 0.1.0. In: Friedrich, J., Kreutzer, S., Pagonis, V., Schmidt, C., 2019. RLumCarlo: Monte-Carlo Methods for Simulating Luminescence Phenomena R package version 0.1.0.9000-101.

Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, UMR 5060, CNRS - Université Bordeaux Montaigne (France)

References

Pagonis, V., Friedrich, J., Discher, M., Müller-Kirschbaum, A., Schlosser, V., Kreutzer, S., Chen, R. and Schmidt, C., 2019. Excited state luminescence signals from a random distribution of defects: A new Monte Carlo simulation approach for feldspar. Journal of Luminescence 207, 266–272. doi: [10.1016/j.jlumin.2018.11.024](https://doi.org/10.1016/j.jlumin.2018.11.024)

Examples

```
##=====##
## Example 1: Single Plot for Monte-Carlo (MC) simulations for localized TL
##=====##
## Not run:
run_MC_TL_LOC(
  s = 1e8,
  E = 0.5,
  times = 0:100,
  clusters = 1e1,
  n_filled = 1,
  r = 1e-7) %>%
  #Plot results of the MC simulation
  plot_RLumCarlo(legend = T)

## End(Not run)
```


run_MC_TL_TUN

*Run Monte-Carlo Simulation for TL for tunnelling transition***Description**

Runs a Monte-Carlo (MC) simulation of thermo-luminescence (TL) using the tunneling (TUN) model. Tunneling refers to the direct movement of electrons from a trap directly to the recombination center

Usage

```
run_MC_TL_TUN(s, E, rho, r_c = 0, times, clusters = 10, N_e = 200,
              delta.r = 0.1, method = "par", output = "signal", ...)
```

Arguments

s	list (required) : The frequency factor of the trap (s^{-1}).
E	numeric (required) : Thermal activation energy of the trap (eV).
rho	numeric (required) : The density of recombination centers (defined as rho' in Huntley 2006) (unitless).
r_c	numeric (with default) : Distance parameter (radius of tunneling) (unitless).
times	vector (with default) : The sequence of temperature steps within the simulation (s).
clusters	numeric (with default) : The number of MC runs (unitless).
N_e	numeric (with default) : The total number of electron traps available (unitless).
delta.r	numeric (with default) : The increments of r_c (unitless).
method	character (with default) : sequential 'seq' or parallel processing 'par'
output	character (with default) : output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)
...	further arguments
r	numeric (with default) : The radius of tunneling (unitless).

Details

$$p(t) = s * e^{(-E/k_B * T)} * e^{(-r'/\rho^{1/3})}$$

$$I_{TUN}(t) = 3 * n * p(t) * (r')^2 * e^{-(r')^3}$$

Where in the function:

p(t) := The experimental stimulation mode

e:= Exponential function

k_B := Boltzmann constant

T := Temperature

r' := r

ρ := rho

t := Time

n := The Instantaneous number of electrons

Value

This function returns an [array](#) with dimension length(times) x length(r) x clusters

Function version

0.1.0

How to cite

Friedrich, J., Kreutzer, S., 2019. run_MC_TL_TUN(): Run Monte-Carlo Simulation for TL for tunnelling transition. Function version 0.1.0. In: Friedrich, J., Kreutzer, S., Pagonis, V., Schmidt, C., 2019. RLumCarlo: Monte-Carlo Methods for Simulating Luminescence PhenomenaR package version 0.1.0.9000-101.

Author(s)

Johannes Friedrich, University of Bayreuth (Germany), Sebastian Kreutzer, IRAMAT-CRP2A, UMR 5060, Université Bordeaux Montaigne (France)

References

Huntley, D.J., 2006. An explanation of the power-law decay of luminescence. Journal of Physics: Condensed Matter, 18(4), 1359.doi: [10.1088/09538984/18/4/020](#)

Pagonis, V. and Kulp, C., 2017. Monte Carlo simulations of tunneling phenomena and nearest neighbor hopping mechanism in feldspars. Journal of Luminescence 181, 114–120. doi: [10.1016/j.jlumin.2016.09.014](#)

Pagonis, V., Friedrich, J., Discher, M., Müller-Kirschbaum, A., Schlosser, V., Kreutzer, S., Chen, R. and Schmidt, C., 2019. Excited state luminescence signals from a random distribution of defects: A new Monte Carlo simulation approach for feldspar. Journal of Luminescence 207, 266–272. doi: [10.1016/j.jlumin.2018.11.024](#)

Further reading Aitken, M.J., 1985. Thermoluminescence dating. 276-280. doi: [10.1002/gea.3340020110](#)

Examples

```
## Not run:
##=====##
## Example 1: Simulate TL measurement
##=====##
run_MC_TL_TUN(
  s = 1e8,
  E = 0.5,
  rho = 1e-7,
  r_c = 0.1,
  times = seq(0,700,10),
  clusters = 100,
  N_e = 20,
  delta.r = 1e-3
) %>%
  plot_RLumCarlo(legend = T)

## End(Not run)
```

Index

* **package**

RLumCarlo-package, [2](#)

array, [5](#), [8](#), [11](#), [13](#), [16](#), [18](#), [21](#), [24](#), [26](#)

character, [4](#), [6](#), [8](#), [10](#), [12](#), [14](#), [16](#), [17](#), [19](#), [21](#),
[23](#), [25](#)

integer, [4](#), [8](#), [10](#), [12](#), [16](#), [17](#), [21](#), [23](#)

khroma::khroma-package, [3](#)

list, [3](#), [25](#)

logical, [3](#)

numeric, [4](#), [6](#), [8](#), [10](#), [12](#), [14](#), [16](#), [17](#), [19](#), [21](#), [23](#),
[25](#)

plot_RLumCarlo, [3](#)

RLumCarlo (RLumCarlo-package), [2](#)

RLumCarlo-package, [2](#)

run_MC_CW_IRSL_LOC, [4](#)

run_MC_CW_IRSL_TUN, [6](#)

run_MC_CW_OSL_DELOC, [8](#)

run_MC_ISO_DELOC, [10](#)

run_MC_ISO_LOC, [12](#)

run_MC_ISO_TUN, [13](#)

run_MC_LM_OSL_DELOC, [15](#)

run_MC_LM_OSL_LOC, [17](#)

run_MC_LM_OSL_TUN, [19](#)

run_MC_TL_DELOC, [21](#)

run_MC_TL_LOC, [23](#)

run_MC_TL_TUN, [25](#)

vector, [19](#), [25](#)