Package 'RLumCarlo'

October 9, 2019

```
Type Package
Title Monte-Carlo Methods for Simulating Luminescence Phenomena
Version 0.1.0.9000-73
Date 2019-10-09
Author Johannes Friedrich [aut, trl] (<a href="https://orcid.org/0000-0002-0805-9547">https://orcid.org/0000-0002-0805-9547</a>),
       Sebastian Kreutzer [aut, trl, cre] (<a href="https://orcid.org/0000-0002-0734-2199">https://orcid.org/0000-0002-0734-2199</a>),
       Vasilis Pagonis [aut] (<a href="https://orcid.org/0000-0002-4852-9312">https://orcid.org/0000-0002-4852-9312</a>),
      Christoph Schmidt [aut] (<a href="https://orcid.org/0000-0002-2309-3209">https://orcid.org/0000-0002-2309-3209</a>),
      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.
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),
      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
```

2 plot_RLumCarlo

R topics documented:

Index		22
	run_MC_TL_TUN	20
	run_MC_TL_LOC	
	run_MC_TL_DELOC	
	run_MC_LM_OSL_TUN	15
	run_MC_LM_OSL_LOC	14
	run_MC_LM_OSL_DELOC	12
	run_MC_ISO_TUN	11
	run_MC_ISO_LOC	9
	run_MC_ISO_DELOC	8
	run_MC_CW_OSL_DELOC	6
	run_MC_CW_IRSL_TUN	4
	run_MC_CW_IRSL_LOC	3
	plot_RLumCarlo	

plot_RLumCarlo

Plot results from Monte-Carlo simulations with RLumCarlo

Description

Plot results from Monte-Carlo simulations with RLumCarlo

Usage

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

Arguments

object data.frame (required)

times numeric (optinal): Optional vector for the x-axis

plot_uncertainty

logical (with default): Enable/disable uncertainty polygon plot

norm logical (with default): Normalise curve to the highest intensity

add logical (with default): allow overplotting of results

. further arguments that can be passed to control the plot output. Currently sup-

ported are: xlab, xlim, ylim, main, lwd, type, pch, lty,col, grid, legend

Value

This function returns a graphical output

Function version

0.1.0

How to cite

Friedrich, J., Kreutzer, S., 2019. plot_RLumCarlo(): Plot results from Monte-Carlo simulations with RLumCarlo. 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 0.1.0.9000-73.

Author(s)

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

run_MC_CW_IRSL_LOC

Run Monte-Carlo simulation for CW-IRSL for localised transition

Description

Runs a Monte-Carlo (MC) simulation of constant wave infrared stimulated luminesence (CW-IRSL) using the generalized one trap (GOT) model.

Usage

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

Arguments

Α	numeric (required): The transition probability (cm ³ /s).
times	numeric (with default): The number of MC runs.
clusters	numeric (with default): The number of clusters.
n_filled	integer (with default): The number of electron traps that are filled at the beginning of the simulation.
r	numeric (with default): The retrapping ratio.
method	character (with default): sequential 'seq' or parallel processing 'par'
output	<pre>character (with default): output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)</pre>
	further arguments

Details

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

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 localised 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 0.1.0.9000-73.

Author(s)

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

References

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.

Examples

run_MC_CW_IRSL_TUN

Run Monte-Carlo simulation for CW-IRSL

Description

Runs a Monte-Carlo (MC) simulation of constant wave infrared stimulated luminesence (CW-IRSL) using the model.

Usage

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

Arguments

```
A numeric (required): The transition probability (cm^3/s).

rho numeric (required): The calculated dimesionless Charge density (normally written Rho').

times numeric (with default): The number of MC runs.

clusters numeric (with default): The number of clusters.
```

```
r numeric (with default): The retrapping ratio.

N_e numeric (with default): The number of electrons

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

####equation here please####

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 PhenomenaR package version 0.1.0.9000-73.

Author(s)

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

References

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

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 infrared stimulated luminesence (CW-OSL) using the one trap one recombination center (OTOR) model.

Usage

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

Arguments

Α	numeric (required): The transition probability (cm ³ /s).
times	numeric (with default): The number of MC runs.
clusters	numeric (with default): The number of clusters.
N_e	integer (with default): The number of electrons.
n_filled	integer (with default): The number of electron traps that are filled at the beginning of the simulation.
R	numeric (with default): The retrapping ratio.
method	character (with default): sequential 'seq' or parallel processing 'par'
output	<pre>character (with default): output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)</pre>
	further arguments

Details

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

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 PhenomenaR package version 0.1.0.9000-73.

Author(s)

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

End(Not run)

References

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

```
## Example 1: Simulate CW-OSL
## Not run:
run_MC_CW_OSL_DELOC(
A = 0.12,
R = 1,
times = 0:100) %>%
  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) # ifferent colours for the individual curves
plot_uncertainty <- c(T,F,T,F) # do you want to see the uncertainty?
add_{TF} \leftarrow 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)
```

run_MC_ISO_DELOC

Run Monte-Carlo simulation for ISO for delocalized transition

Description

Runs a Monte-Carlo (MC) simulation of isothermally stimulated luminesence (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): Escape frequency of the trap (s^-1).
E	numeric (required): Thermal activation energy of the trap (eV).
T	numeric (with default): Temperature (deg. C).
times	numeric (with default): The number of MC runs.
clusters	numeric (with default): The number of clusters.
N_e	integer (with default): The number of electrons.
n_filled	integer (with default): The number of electron traps that are filled at the beginning of the simulation.
R	numeric (with default): The retrapping ratio.
method	character (with default): sequential 'seq' or parallel processing 'par'
output	<pre>character (with default): output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)</pre>
• • •	further arguments

Details

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

Where in the function $n := n_filled := N := N_e$

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 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 0.1.0.9000-73.

run_MC_ISO_LOC 9

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

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

Examples

```
##=========##
## Example 1: Simulate ITL
##==========##
## Not run:
run_MC_ISO_DELOC(
    s = 3.5e12,
    E = 1.45,
    T = 200,
    R = 1,
    times = 0:10000) %>%
        plot_RLumCarlo(legend = T)
## End(Not run)
```

run_MC_ISO_LOC

Run Monte-Carlo simulation for ITL for localised transition

Description

Runs a Monte-Carlo (MC) simulation of isothermally stimulated luminesence (ISO-TL or ITL) using the genralized one trap (GOT) model. Localized refers to the lack of 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): Escape frequency of the trap (s^-1).

E numeric (required): Thermal activation energy of the trap (eV).

T numeric (with default): Temperature (deg. C).

times numeric (with default): The number of MC runs.

clusters numeric (with default): The number of clusters.
```

10 run_MC_ISO_LOC

n_filled	integer (with default): The number of electron traps that are filled at the beginning of the simulation.
r	numeric (with default): The retrapping ratio.
method	character (with default): sequential 'seq' or parallel processing 'par'
output	<pre>character (with default): output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)</pre>
	further arguments

Details

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

Where in the function $n := n_filled := N := N_e$

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 ITL for localised 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 0.1.0.9000-73.

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

 $run_MC_ISO_TUN$ 11

End(Not run)

run_MC_ISO_TUN

Run Monte-Carlo Simulation for Isothermal Measurements for Tunneling Transition

Description

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

Usage

```
run_MC_ISO_TUN(E, s, T = 200, rho, times, clusters = 10, r = NULL, N_e = 200, method = "par", output = "signal", ...)
```

Arguments

Е	numeric (required): Thermal activation energy of the trap (eV).
S	numeric (required): Escape frequency of the trap (s^-1).
T	numeric (required): Temperature (deg. C).
rho	numeric (required): The calculated dimesionless Charge density (normally written Rho').
times	numeric (with default): The number of MC runs.
clusters	numeric (with default): The number of clusters.
r	numeric (with default): The retrapping ratio.
N_e	numeric (with default): The number of electrons.
method	character (with default): sequential 'seq' or parallel processing 'par'
output	<pre>character (with default): output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)</pre>
	further arguments

Details

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

Where in the function $n := n_filled := N := N_e := rho := rho'$:= \code{r_c} := \code{rho'_c}

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 Isothermal Measurements 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 PhenomenaR package version 0.1.0.9000-73.

Author(s)

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

References

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

for a discussion of tunneling see: Aitken, M.J., 1985. Thermoluminescence dating. 276-280. doi: 10.1002/gea.3340020110

Examples

run_MC_LM_OSL_DELOC

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

Description

Runs a Monte-Carlo (MC) simulation of linearly modulated optically stimulated luminesence (LM-OSL) using the one trap one recombination center (OTOR) model.

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 transition probability (cm ³ /s).
times	numeric (with default): The number of MC runs.
clusters	numeric (with default): The number of clusters.
N_e	integer (with default): The number of electrons.
n_filled	integer (with default): The number of electron traps that are filled at the beginning of the simulation.
R	numeric (with default): The retrapping ratio.
method	character (with default): sequential 'seq' or parallel processing 'par'
output	<pre>character (with default): output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)</pre>
	further arguments

Details

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

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 PhenomenaR package version 0.1.0.9000-73.

Author(s)

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

References

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

```
times = 0:100) %>%
  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 luminesence (LM-OSL) using the generalized one trap (GOT) model.

Usage

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

Arguments

Α	numeric (required): The transition probability (cm ³ /s).
times	numeric (with default): The number of MC runs.
clusters	numeric (with default): The number of clusters.
n_filled	integer (with default): The number of electron traps that are filled at the beginning of the simulation.
r	numeric (with default):
method	character (with default): sequential 'seq' or parallel processing 'par'
output	<pre>character (with default): output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)</pre>
	further arguments

Details

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

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_LM_OSL_LOC(): Run Monte-Carlo simulation for LM-OSL 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 0.1.0.9000-73.

Author(s)

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

References

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

Examples

run_MC_LM_OSL_TUN

Run Monte-Carlo simulation for LM-OSL

Description

Run Monte-Carlo simulation for LM-OSL

Usage

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

Arguments

```
Α
                   numeric (required): The transition probaility (cm<sup>3</sup>/s).
rho
                   numeric (required): The calculated dimesionless Charge density (normally writ-
                   ten Rho').
times
                   vector (with default): The number of MC runs.
                   numeric (with default): The number of clusters.
clusters
                   numeric (with default): The retrapping ratio.
delta.r
                   numeric (with default):
                   numeric (with default): The number of electrons.
N_e
                   character (with default): sequential 'seq' or parallel processing 'par'
method
                   character (with default): output is either the 'signal' (the default) or 'remaining_e'
output
                   (the remaining charges, electrons, in the trap)
                   further arguments
. . .
```

run_MC_TL_DELOC

Details

ADD EQUATION

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. 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 0.1.0.9000-73.

Author(s)

Johannes Friedrich, University of Bayreuth (Germany)

References

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

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-luminesence (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", ...)
```

run_MC_TL_DELOC 17

Arguments

numeric (**required**): Escape frequency of the trap (s^-1). Ε numeric (required): Thermal activation energy of the trap (eV). times numeric (with default): the number of MC runs. clusters numeric (with default): the number of clusters. integer (with default): The number of electrons. Νe n_filled integer (with default): The number of electron traps that are filled at the beginning of the simulation. R numeric (with default): The retrapping ratio. character (with default): sequential 'seq' or parallel processing 'par' method character (with default): output is either the 'signal' (the default) or 'remaining_e' output (the remaining charges, electrons, in the trap)

Details

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

where in the function $N := N_e := n := n_filled$

further arguments

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 0.1.0.9000-73.

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

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

run_MC_TL_LOC

Examples

```
## Example 1: Simulate TL
## Not run:
run_MC_TL_DELOC(
 s = 3.5e12,
E = 1.45,
R = 1,
 times = 100:450) %>%
   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 \leftarrow c(TRUE, TRUE, TRUE, TRUE) \# do you want to see the uncertainty?
add_TF <- c(FALSE,rep(TRUE, (length(R)-1)))</pre>
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 localised transition

Description

Runs a Monte-Carlo (MC) simulation of thermo-luminesence (LM-OSL) using the generalized one trap (GOT) model. Localized refers to the lack of involvement of the conduction band.

run_MC_TL_LOC 19

Usage

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

Arguments

s numeric (**required**): Escape frequency of the trap (s^{-1}).

E numeric (**required**): Thermal activation energy of the trap (eV).

times numeric (with default): The number of Mc runs.
clusters numeric (with default): The number of clusters.

n_filled integer (with default): The number of electron traps that are filled at the begin-

ning of the simulation.

r numeric (with default): The retrapping ratio.

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 $n := n_filled$

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_TL_LOC(): Run Monte-Carlo simulation for TL for localised 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 0.1.0.9000-73.

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

20 run_MC_TL_TUN

Examples

run_MC_TL_TUN

Run Monte-Carlo Simulation for TL using Tunnelling Transition

Description

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

Usage

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

Arguments

```
list (required): Escape frequency of the trap (s^-1).
s
Ε
                   numeric (required): Thermal activation energy of the trap (eV).
rho
                   numeric (required): The calculated dimesionless Charge density.
                   numeric (with default): The dimensionless minimal critical radius.
r_c
times
                   vector (with default): The number of MC runs.
                   numeric (with default): The number of clusters.
clusters
N_e
                   numeric (with default): The number of electrons
delta.r
                   numeric (with default): The approriate distance interval along the r axis (dimen-
                   sionless).
                   character (with default): sequential 'seq' or parallel processing 'par'
method
output
                   character (with default): output is either the 'signal' (the default) or 'remaining_e'
                   (the remaining charges, electrons, in the trap)
                   further arguments
. . .
```

 $run_MC_TL_TUN$ 21

Details

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

where in the function $N := N_e := rho' \} := \code{r_c} := \code{rho'_c}$

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 using 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 0.1.0.9000-73.

Author(s)

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

References

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

Index

```
array, 3, 6, 8, 10, 13, 14, 17, 19, 21
character, 3, 5, 6, 8, 10, 11, 13-15, 17, 19, 20
data.frame, 2
integer, 3, 6, 8, 10, 13, 14, 17, 19
list, 20
logical, 2
numeric, 2-6, 8-11, 13-15, 17, 19, 20
plot_RLumCarlo, 2
run_MC_CW_IRSL_LOC, 3
run_MC_CW_IRSL_TUN, 4
run_MC_CW_OSL_DELOC, 6
run_MC_ISO_DELOC, 8
run_MC_ISO_LOC, 9
\verb"run_MC_ISO_TUN, 11"
run_MC_LM_OSL_DELOC, 12
run_MC_LM_OSL_LOC, 14
run_MC_LM_OSL_TUN, 15
\texttt{run\_MC\_TL\_DELOC}, \textcolor{red}{16}
run_MC_TL_LOC, 18
run_MC_TL_TUN, 20
vector, 15, 20
```