Package 'RLumCarlo'

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Type Package

Title Monte-Carlo Methods for Simulating Luminescence Phenomena

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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.

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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` *Monte-Carlo Methods for Simulating Luminescence Phenomena*

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

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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

`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 `RLumCarlo_Model_Output` (**required**): input object to be plotted, usually the required input object is generated by one for the functions preceeding with `run`. Alternatively a list of such objects can be provided.
`plot_uncertainty`	logical (*with default*): sets the nature of the show uncertainty, allowed values are `range`, `sd` (standard deviation), `var` (variance) and `NULL` disables the uncertaintiy visualisation
`norm`	logical (*with default*): normalise curve to the highest intensity
`add`	logical (*with default*): 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: `xlab`, `xlim`, `ylim`, `main`, `lwd`, `type`, `pch`, `lty`,`col`, `grid`, `legend`. The arguments `lwd`, `type`, `pch`, `lty`, `col` 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 0.1.0.9000-98.

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 localized transition*

Description

Runs a Monte-Carlo (MC) simulation of constant wave infrared stimulated luminesence (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 PhenomenaR package version 0.1.0.9000-98.

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 CW-IRSL
##============================================================================##
## Not run:
run_MC_CW_IRSL_LOC(
 A = 0.12,
 r = 1,
 times = 0:100) %>%
   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 luminesence (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 (*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

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

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

Where in the function:
`p(t)` := The experimental stimulation mode
`e`:= Exponentional 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 PhenomenaR package version 0.1.0.9000-98.

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., 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

```
## Not run:

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

run_MC_CW_IRS_TUNL(A = 0.12, rho = 0.003, times = 0:1000) %>%
    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 luminesence (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 PhenomenaR package version 0.1.0.9000-98.

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 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 <- 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 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**): 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:= Exponentional 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 0.1.0.9000-98.

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 ISO-TL for localized 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 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

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

Where in the function:
`t` := `Time`
e:= `Exponentional 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 0.1.0.9000-98.

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

Examples

```
##============================================================================##
## Example 1: Simulate ITL
##============================================================================##




    ## Not run:
run_MC_ISO_LOC(
 s = 3.5e12,
 E = 1.45,
 T = 200,
 r = 1,
 times = 0:10000) %>%
   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 luminesence (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 (*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

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

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

Where in the function:
`p(t)` := The experimental stimulation mode
`e`:= Exponentional 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 PhenomenaR package version 0.1.0.9000-98.

Author(s)

Johannes Friedrich, University of Bayreuth (Germany), Sebastian Kreutzer, IRAMAT-CRP2A, UMR 5060, CNRS - Univerité 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 isothermal measurement
##============================================================================##
run_MC_ISO_TUN(
 E = 1.2,
 s = 1e10,
 T = 200,
 rho = 0.007,
 times = 0:5000) %>%
  plot_RLumCarlo(legend = TRUE)

## End(Not run)
```

`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. 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 PhenomenaR package version 0.1.0.9000-98.

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 LM-OSL
##============================================================================##
## Not run:
run_MC_LM_OSL_DELOC(
```

```
  A = 0.12,
  R = 1,
  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. 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 0.1.0.9000-98.

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

Examples

```
##============================================================================##
## Example 1: Simulate LM-OSL
##============================================================================##
## Not run:
run_MC_LM_OSL_LOC(
 A = 0.12,
 r = 1,
 times = 0:100) %>%
   plot_RLumCarlo(legend = T)


## End(Not run)
```

---

run_MC_LM_OSL_TUN *Run Monte-Carlo simulation for LM-OSL for tunneling transition*

Description

Runs a Monte-Carlo (MC) simulation of linearly modulated optically stimulated luminesence (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 PhenomenaR package version 0.1.0.9000-98.

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

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:

##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", ...)
```

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:= Exponentional 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 0.1.0.9000-98.

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 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 <- 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-luminesence (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`:= Exponentional 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 PhenomenaR package version 0.1.0.9000-98.

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

Examples

```
##============================================================================##
## Example 1: Simulate TL
##============================================================================##


## Not run:
run_MC_TL_LOC(
 s = 3.5e12,
 E = 1.45,
 r = 1,
 times = 100:450) %>%
   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-luminesence (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`:= Exponentional 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 0.1.0.9000-98.

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 = 3.5e12,
          E = 1.45,
          rho = 0.015,
          r_c = 0.85,
          times = 200:500) %>%
    plot_RLumCarlo(legend = T)

## End(Not run)
```

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