# 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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**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:



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`RLumCarlo-package` *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.

## Details

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- 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 LaSciArBx (ANR - n. ANR-10-LABX-52).

## Author(s)

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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

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`plot_RLumCarlo` *Plot RLumCarlo Monte-Carlo Simulations Results*

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## 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 0.1.0.9000-90.

## Author(s)

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

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# 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 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

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

## 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 0.1.0.9000-90.

## 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 trap to conduction band (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 `n` := `n_filled`:= `t` := `times`

## 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 0.1.0.9000-90.

### Author(s)

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

```
## 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 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

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

## 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 0.1.0.9000-90.

## 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*): 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 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

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

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-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 0.1.0.9000-90.

### 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*): 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 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

$$ISOI_{LOC}(t) = -dn/dt = (s * e^{-}E/kT_{I}TL/ISO) * (n^{2}/(r+n)))$$

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 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 0.1.0.9000-90.

## 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**): 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

$$p(t) = s * e^(-E/kB * T) * e^(-r/rho^1/3)$$

$$I_{TUN}(t) = 3 * n * p(t) * r^2 * e^(-r^3)$$

Where in the function `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 0.1.0.9000-90.

## 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

**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 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

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

## 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 0.1.0.9000-90.

## 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 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

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

## 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_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 0.1.0.9000-90.

## 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 trap to conduction band (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 `n` := `n_filled`:= `t` := `times`

## 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 0.1.0.9000-90.

### 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 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 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

$$TLI_{DELOC}(t) = -dn/dt = (s * e^{-}E/kT) * (n^2/(NR + n(1 - R))))$$

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

## 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 0.1.0.9000-90.

## 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 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

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

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 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 0.1.0.9000-90.

## 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

$$p(t) = s * e^(-E/kB * T) * e^(-r/rho^1/3)$$

$$I_{TUN}(t) = 3 * n * p(t) * r^2 * e^(-r^3)$$

Where in the function n := n_filled := t:= times:= $\rho$ := $\rho'$ := r_c := $\rho'_c$

## 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 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 0.1.0.9000-90.

## 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

## 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)
```

# Index