

# 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 transitions.  
Supported stimulation methods are TL, CW-OSL, LM-OSL, LM-IRSL, and ITL (ISO-TL).

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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),  
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**Encoding** UTF-8

**VignetteBuilder** R.rsp

**RoxygenNote** 6.1.1

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## Description

A collection of functions to simulate luminescence production in dosimeters using Monte-Carlo methods. Implemented are models for delocalised, localised and tunnelling transitions. Supported stimulation modes are TL, CW-OSL, LM-OSL, LM-IRSL, and ITL (ISO-TL).

## Details

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**Author(s)**

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 Christoph Schmidt, University of Bayreuth (Germany),  
 Ena Rajovic, University of Bayreuth (Germany),  
 Alex Roy Duncan, University of Bayreuth (Germany),  
 Christian Laag, University of Bayreuth (Germany)

**References**

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

plot\_RLumCarlo

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

Visualise 'RLumCarlo' modelling results without extracting the values manually. Typically visualised values are the averaged signal or the number of remaining electrons with a polygon indicating modelling uncertainties.

**Usage**

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

**Arguments**

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

**Details**

For colouring the 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

**Author(s)**

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

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run\_MC\_CW\_IRSL\_LOC

*Monte-Carlo Simulation for CW-IRSL for Localized Transition*


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**Description**

Runs a Monte-Carlo (MC) simulation of constant-wave infrared stimulated luminescence (CW-IRSL) using the generalized one trap (GOT) model. Localized refers to an excited state that is shared by the electron and the recombination centre, so that the conduction band is not involved in the recombination process.

**Usage**

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

**Arguments**

A	<b>numeric (required)</b> : The optical excitation rate from trap to the excited state ( $s^{-1}$ ).
times	<b>numeric (with default)</b> : The sequence of time steps within the simulation (s).
clusters	<b>numeric (with default)</b> : The number of MC runs (unitless).
n_filled	<b>integer (with default)</b> : The number of filled electron traps at the beginning of the simulation (unitless).
r	<b>numeric (with default)</b> : The localized retrapping ratio (unitless).
method	<b>character (with default)</b> : sequential 'seq' or parallel 'par' processing
output	<b>character (with default)</b> : 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:

A := optical excitation rate from trap to the excited state ( $s^{-1}$ )

r := localised retrapping ratio (unitless)

t := time (s)

n := number of filled electron traps

**Value**

This function returns an object of class `RLumCarlo_Model_Output` which is a [list](#) consisting of an [array](#) with dimension `length(times) x length(r) x clusters` and a [numeric](#) time vector.

**Function version**

0.1.0

**Author(s)**

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

**References**

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

**Further reading**

Chen, R., McKeever, S.W.S., 1997. *Theory of Thermoluminescence and Related Phenomena*. WORLD SCIENTIFIC. doi: [10.1142/2781](https://doi.org/10.1142/2781)

**Examples**

```
run_MC_CW_IRSL_LOC(
  A = 0.12,
  times = 0:100,
  clusters = 50,
  n_filled = 1,
  r = 1e-7,
  method = "seq",
  output = "signal"
) %>%
plot_RLumCarlo(legend = TRUE)
```

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<code>run_MC_CW_IRSL_TUN</code>	<i>Run Monte-Carlo Simulation for CW-IRSL for Tunneling Transition</i>
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**Description**

Runs a Monte-Carlo (MC) simulation of constant wave infrared stimulated luminescence (CW-IRSL) using the model for tunneling transition. Tunneling refers to the direct movement of electrons from the excited state of 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	<b>numeric (required)</b> : The optical excitation rate from ground state of trap to excited state of trap ( $s^{-1}$ ).
rho	<b>numeric (required)</b> : The density of recombination centers (defined as rho' in Huntley 2006) (unitless).
times	<b>numeric (with default)</b> : The sequence of time steps within the simulation (s).
clusters	<b>numeric (with default)</b> : The number of MC runs (unitless).
r_c	<b>numeric (with default)</b> : Critical distance (>0) that is to be inserted if the sample has 1 been thermally and/or optically pretreated, so that the electron-hole pairs within r_c have already recombined
delta.r	<b>numeric (with default)</b> : Increments of the unitless distance parameter r
N_e	<b>numeric (with default)</b> : The total number of electron traps available (unitless).
method	<b>character (with default)</b> : sequential 'seq' or parallel processing 'par'
output	<b>character (with default)</b> : output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)
...	further arguments

**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

r' := the unitless tunneling radius

$\rho'$  := rho the unitless density of recombination centres

t := time (s)

n := The Instantaneous number of electrons

**Value**

This function returns an object of class `RLumCarlo_Model_Output` which is a **list** consisting of an **array** with dimension `length(times) x length(r) x clusters` and a **numeric** time vector.

**Function version**

0.2.0

**Author(s)**

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

## References

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

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

## Further reading

Chen, R., McKeever, S.W.S., 1997. *Theory of Thermoluminescence and Related Phenomena*. WORLD SCIENTIFIC. doi: [10.1142/2781](https://doi.org/10.1142/2781)

## Examples

```
run_MC_CW_IRSL_TUN(
  A = 0.8,
  rho = 1e-4,
  times = 0:10,
  r_c = 0.05,
  delta.r = 1e-2,
  method = "seq",
  clusters = 2,
  output = "signal") %>%
plot_RLumCarlo(norm = TRUE, legend = TRUE)
```

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run_MC_CW_OSL_DELOC	<i>Run Monte-Carlo simulation for CW-OSL for delocalized transition</i>
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## Description

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

## Usage

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

## Arguments

A	<b>numeric (required)</b> : The optical excitation rate from trap to conduction band ( $s^{-1}$ ).
times	<b>numeric (with default)</b> : The sequence of temperature steps within the simulation (s)
clusters	<b>numeric (with default)</b> : The number of MC runs (unitless).
N_e	<b>integer (with default)</b> : The total number of electron traps available (unitless).
n_filled	<b>integer (with default)</b> : 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

## Author(s)

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

## References

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

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

## Examples

```
##=====##
## Example 1: Single Plot for Monte-Carlo (MC) simulations for delocalized CW-OSL
##=====##
## Not run:
run_MC_CW_OSL_DELOC(
  A = 0.12,
  R = 0.1,
  times = 0:100
) %>%
  #Plot results of the MC simulation
  plot_RLumCarlo(legend = T)

## End(Not run)
```



```

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

# define your parameters
A <- c(0.1,0.3,0.5,1)
times <- seq(0,60,1)
s <- 1e12
E<- 1
R<-c(1e-7,1e-6,0.01,0.1) # sequence of different R values
clusters <- 1000 # number of Monte Carlo simulations
N_e <- c(200, 500, 700, 400) # number of free electrons
n_filled <- c(200, 500, 100, 70) # number of filled traps
method <- "par"
output <- "signal"
col <- c(1,2,3,4) # different colours for the individual curves
plot_uncertainty <- c(T,F,T,F) # do you want to see the uncertainty?
add_TF <- c(F,rep(T, (length(R)-1)))
for (u in 1:length(R)){
  results <- run_MC_CW_OSL_DELOC(A=A[u], times, clusters =clusters, N_e = N_e[u],
                                n_filled = n_filled[u], R=R[u], method = method, output = output)
  plot_RLumCarlo(results,add=add_TF[u],legend = F, col=col[u], main=" your plot")
}
legend("topright",ncol=4,cex=0.55,title = "parameters" ,legend=c(paste0("A = ", A),
                                                                    paste0("n_filled = ", n_filled),
                                                                    paste0("N_e = ", N_e),
                                                                    paste0("R = ", R)), text.col=col)

## End(Not run)

```

run\_MC\_ISO\_DELOC

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

## Description

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

## Usage

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

## Arguments

**s** **numeric (required)**: The frequency factor of the trap ( $s^{-1}$ ).  
**E** **numeric (required)**: Thermal activation energy of the trap (eV).  
**T** **numeric (with default)**: Constant stimulation temperature (degrees C).

times	<b>numeric</b> ( <i>with default</i> ): the sequence of temperature steps within the simulation (s).
clusters	<b>numeric</b> ( <i>with default</i> ): The number of MC runs (unitless).
N_e	<b>integer</b> ( <i>with default</i> ): The total number of electron traps available (unitless).
n_filled	<b>integer</b> ( <i>with default</i> ): The number of filled electron traps at the beginning of the simulation (unitless).
R	<b>numeric</b> ( <i>with default</i> ): The delocalized retrapping ratio (unitless).
method	<b>character</b> ( <i>with default</i> ): sequential 'seq' or parallel processing 'par'
output	<b>character</b> ( <i>with default</i> ): output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)
...	further arguments

## Details

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

Where in the function:

t := Time

e:= Exponential function

$k_B$  := Boltzmann constant

$T_{ISO} = T$

n := n\_filled

N := N\_e

## Value

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

## Function version

0.0.1

## Author(s)

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

## References

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

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

## Examples

```
##=====##
## Example 1: Single Plot for Monte-Carlo (MC) simulations for delocalized ISO-TL
##=====##
## Not run:
run_MC_ISO_DELOC(
```

```

s = 3.5e12,
E = 1.45,
T = 200,
R = 1,
times = 0:10000
) %>%
#Plot results of the MC simulation
plot_RLumCarlo(legend = T)

## End(Not run)

```

run\_MC\_ISO\_LOC

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

## Description

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

## Usage

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

## Arguments

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

**Details**

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

Where in the function:

t := Time

e := Exponential function

$k_B$  := Boltzmann constant

$T_{ISO}$  = T

n := n\_filled

N := N\_e

**Value**

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

**Function version**

0.0.1

**Author(s)**

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

**References**

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

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run\_MC\_ISO\_TUN

*Monte-Carlo Simulation for Isothermal-TL for Tunneling Transition*

---

**Description**

Runs a Monte-Carlo (MC) simulation of isothermally stimulated luminescence (ISO-TL or ITL) using the tunneling (TUN) model. Tunneling refers to the direct transition of electrons from an excited state directly into the recombination center without involving the conduction band.

**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	<b>numeric (required)</b> : Thermal activation energy of the trap (eV).
s	<b>numeric (required)</b> : Frequency factor of the trap (s <sup>-1</sup> ).
T	<b>numeric (with default)</b> : Constant stimulation temperature (degrees C).
rho	<b>numeric (required)</b> : The density of recombination centres (defined as rho' in Huntley 2006) (unitless).
times	<b>numeric (with default)</b> : The sequence of temperature steps within the simulation (s).
clusters	<b>numeric (with default)</b> : The number of MC runs (unitless).
r_c	<b>numeric (with default)</b> : The radius of tunneling (dimensionless)
delta.r	<b>numeric (with default)</b> : Fractional change of the dimensionless distance of nearest recombination centres (r', which is preset at 2)
N_e	<b>numeric (with default)</b> : The total number of electron traps available (unitless).
method	<b>character (with default)</b> : sequential 'seq' or parallel processing 'par'
output	<b>character (with default)</b> : output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)
...	further arguments

**Details**

**\*\* Model description \*\***

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

$$I_{TUN}(t) = 3 * n * p(t) * (r')^{2 * e^{(-r'^{1/3})}}$$

Where in the function:

p(t) := The experimental stimulation mode

e:= Exponential function

k<sub>B</sub> := Boltzmann constant

r := r

ρ := rho

t := Time

n := The Instantaneous number of electrons

n := n\_filled

t:= times

**Value**

This function returns an object of class `RLumCarlo_Model_Output`

**Function version**

0.1.0

**Author(s)**

Johannes Friedrich, University of Bayreuth (Germany), 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](https://doi.org/10.1016/j.jlumin.2016.09.014)

**Further reading** Aitken, M.J., 1985. Thermoluminescence dating. Academic Press.

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

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

## Examples

```
run_MC_ISO_TUN(
  E = .8,
  s = 1e16,
  T = 50,
  rho = 1e-4,
  times = 0:100,
  clusters = 10,
  N_e = 2,
  r_c = 1e-4,
  delta.r = 0.5,
  method = "seq") %>%
plot_RLumCarlo(legend = TRUE)
```

---

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

---

## Description

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

## Usage

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

## Arguments

A	<b>numeric (required)</b> : The optical excitation rate from trap to conduction band ( $s^{-1}$ ).
times	<b>numeric (with default)</b> : The sequence of temperature steps within the simulation (s).
clusters	<b>numeric (with default)</b> : The number of MC runs (unitless).
N_e	<b>integer (with default)</b> : The total number of electron traps available (unitless).

n_filled	<b>integer</b> (with default): The number of filled electron traps at the beginning of the simulation (unitless).
R	<b>numeric</b> (with default): The delocalized retrapping ratio (unitless).
method	<b>character</b> (with default): sequential 'seq' or parallel processing 'par'
output	<b>character</b> (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

## Author(s)

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

## References

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

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

## Examples

```
##=====##
## Example 1: Single Plot for Monte-Carlo (MC) simulations for delocalized LM-OSL
##=====##
## Not run:
run_MC_LM_OSL_DELOC(
  A = 0.12,
  R = 0.1,
  times = 0:100
) %>%
  #Plot results of the MC simulation
plot_RLumCarlo(legend = T)
```

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

---

```
run_MC_LM_OSL_LOC
```

---



---

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

---

## Description

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

## Usage

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

## Arguments

A	<b>numeric (required)</b> : The optical excitation rate from trap to conduction band ( $s^{-1}$ ).
times	<b>numeric (with default)</b> : The sequence of temperature steps within the simulation (s).
clusters	<b>numeric (with default)</b> : The number of MC runs (unitless).
n_filled	<b>integer (with default)</b> : The number of filled electron traps at the beginning of the simulation (unitless).
r	<b>numeric (with default)</b> : The localized retrapping ratio (unitless)
method	<b>character (with default)</b> : sequential 'seq' or parallel processing 'par'
output	<b>character (with default)</b> : 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



**Author(s)**

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

**References**

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

**Examples**

```
##=====##
## Example 1: Single Plot for Monte-Carlo (MC) simulations for localized LM-OSL
##=====##
## Not run:
run_MC_TL_LOC(
  s = 1e8,
  E = 0.5,
  times = 0:40,
  clusters = 100,
  n_filled = 10,
  r = 1e-7,
  method = "seq",
  output = "signal"
) %>%
  #Plot results of the MC simulation
  plot_RLumCarlo(legend = T)

## End(Not run)
```

---

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

---

**Description**

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

**Usage**

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

**Arguments**

A	<b>numeric (required)</b> : The optical excitation rate from ground state of trap to excited state of trap ( $s^{-1}$ ).
rho	<b>numeric (required)</b> : The density of recombination centers (defined as $\rho'$ in Huntley 2006) (unitless).

times	<b>vector</b> ( <i>with default</i> ): The sequence of temperature steps within the simulation (s).
clusters	<b>numeric</b> ( <i>with default</i> ): The number of clusters.
r_c	<b>numeric</b> ( <i>with default</i> ): The retrapping ratio.
delta.r	<b>numeric</b> ( <i>with default</i> ): Increments of r_c (unitless).
N_e	<b>numeric</b> ( <i>with default</i> ): The total number of electron traps available (unitless).
method	<b>character</b> ( <i>with default</i> ): sequential 'seq' or parallel processing 'par'
output	<b>character</b> ( <i>with default</i> ): output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)
...	further arguments
r	<b>numeric</b> ( <i>with default</i> ): 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

$\rho'$  := rho

n := The instantaneous number of electrons

### Value

This function returns a list.

### Function version

0.1.0

### Author(s)

Johannes Friedrich, University of Bayreuth (Germany)

### References

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

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

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

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

## Examples

```
##=====##
## Example 1: Single Plot for Monte-Carlo (MC) simulations for tunneling LM_OSL
##=====##
## Not run:
run_MC_LM_OSL_TUN(
  A = 1,
  rho = 1e-7,
  times = 0:100,
  clusters = 3,
  N_e = 2,
  r_c = 0.001,
  delta.r = 1e-1,
  method = "par",
  output = "signal"
) %>%
# Plot results of the MC simulation
plot_RLumCarlo(norm = T)

## End(Not run)
```

run\_MC\_TL\_DELOC

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

## Description

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

## Usage

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

## Arguments

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

## Details

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

Where in the function:

t := Time

e:= Exponential function

$k_B$  := Boltzmann constant

T= Temperature

n := The Instantaneous number of electrons

N := N\_e

## Value

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

## Function version

0.0.1

## Author(s)

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

## References

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

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

## Examples

```
#####
## Example 1: Single Plot for Monte-Carlo (MC) simulations for delocalized TL
#######
## Not run:
run_MC_TL_DELOC(
  s = 3.5e12,
  E = 1.45,
  R = 0.1,
  times = 100:450
) %>%
  #Plot results of the MC simulation
  plot_RLumCarlo(legend = T)

## End(Not run)

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

```

## Not run:
# define your parameters
times=seq(100,450,1)
s=rep(3.5e12,4)
E=rep(1.45,4)
R<-c(0.7e-6,1e-6,0.01,0.1)
clusters=1000
N_e =c(400, 500, 700, 400)
n_filled =c(400, 500, 300, 70)
method="par"
output ="signal"
col=c(1,2,3,4) # different colours for the individual curves
plot_uncertainty <- c(TRUE,TRUE,TRUE,TRUE) # do you want to see the uncertainty?
add_TF <- c(FALSE,rep(TRUE, (length(R)-1)))
for (u in 1:length(R)){
  results <-run_MC_TL_DELOC(times=times, s=s[u],E=E[u], clusters =clusters, N_e = N_e[u],
                           n_filled = n_filled[u], R=R[u], method = method, output = output)
  plot_RLumCarlo(results,add=add_TF[u],legend = FALSE, col=col[u], main=" your plot", ylim=c(0,20))
}
legend("topright",ncol=5,cex=0.55,title = "parameters" ,legend=c(paste0("E = ", E),
                           paste0("s = ", s),
                           paste0("n_filled = ", n_filled),
                           paste0("N_e = ", N_e),
                           paste0("R = ", R)), text.col=col)

## End(Not run)

```

run\_MC\_TL\_LOC

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

## Description

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

## Usage

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

## Arguments

s	<b>numeric (required)</b> : The frequency factor of the trap ( $s^{-1}$ ).
E	<b>numeric (required)</b> : Thermal activation energy of the trap (eV).
times	<b>numeric (with default)</b> : The sequence of temperature steps within the simulation (s).
clusters	<b>numeric (with default)</b> : The number of MC run (unitless).
n_filled	<b>integer (with default)</b> : The number of filled electron traps at the beginning of the simulation (unitless).

r	<b>numeric</b> ( <i>with default</i> ): The localized retrapping ratio (unitless).
method	<b>character</b> ( <i>with default</i> ): sequential 'seq' or parallel processing 'par'
output	<b>character</b> ( <i>with default</i> ): output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap)
...	further arguments

### Details

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

Where in the function:

t := Time

e:= Exponential function

$k_B$  := Boltzmann constant

T := Temperature

n := The Instantaneous number of electrons

### Value

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

### Function version

0.1.0

### Author(s)

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

### References

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

### Examples

```
##=====##
## Example 1: Single Plot for Monte-Carlo (MC) simulations for localized TL
##=====##
## Not run:
run_MC_TL_LOC(
  s = 1e14,
  E = 0.9,
  times = 0:180,
  r = 1e4
) %>%
  #Plot results of the MC simulation
  plot_RLumCarlo(legend = T)

## End(Not run)
```

run\_MC\_TL\_TUN

*Run Monte-Carlo simulation for TL for tunnelling transitions***Description**

Runs a Monte-Carlo (MC) simulation of thermo-luminescence (TL) caused by tunnelling (TUN) transitions. Tunneling refers to the direct recombination of electrons from a trap directly from the excited state of the trap, without involvement of the conduction band.

**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	<b>list (required)</b> : The frequency factor of the trap ( $s^{-1}$ ).
E	<b>numeric (required)</b> : Thermal activation energy of the trap (eV).
rho	<b>numeric (required)</b> : The density of recombination centers (defined as $\rho'$ in Huntley 2006) (unitless).
r_c	<b>numeric (with default)</b> : Critical distance ( $>0$ ) that is to be inserted if the sample has been thermally and/or optically pretreated, so that the electron-hole pairs within ' $r_c$ ' have already recombined (unitless).
times	<b>vector (with default)</b> : The sequence of time steps within the simulation (s).
clusters	<b>numeric (with default)</b> : The number of MC runs (unitless).
N_e	<b>numeric (with default)</b> : The total number of electron traps available (unitless).
delta.r	<b>numeric (with default)</b> : The increments of $r_c$ (unitless).
method	<b>character (with default)</b> : sequential 'seq' or parallel processing 'par'.
output	<b>character (with default)</b> : output is either the 'signal' (the default) or 'remaining_e' (the remaining charges, electrons, in the trap).
...	further arguments

**Details**

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

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

Where in the function:

$p(t)$  := The experimental stimulation mode

$k_B$  := Boltzmann constant

T := Temperature

$r'$  := r

$\rho'$  := Density of recombination centers

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

**Author(s)**

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

**References**

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

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

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

**Further reading** Aitken, M.J., 1985. Thermoluminescence dating. Academic Press.

**Examples**

```
##=====##
## Example 1: Single Plot for Monte-Carlo (MC) simulations for tunneling TL
##=====##
## Not run:
run_MC_TL_TUN(
  s = 1e12,
  E = 0.9,
  rho = 1,
  r_c = 1,
  times = 0:180,
  delta.r = 1e-1
) %>%
  #Plot results of the MC simulation
  plot_RLumCarlo(legend = T)

## End(Not run)
```



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