# Package 'Luminescence'

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```
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Description A collection of various R functions for the purpose of Luminescence
      dating data analysis. This includes, amongst others, data import, export,
      application of age models, curve deconvolution, sequence analysis and
      plotting of equivalent dose distributions.
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      'CW2pPMi.R' 'Luminescence-package.R' 'RLum-class.R'
      'structure RLum.R' 'set RLum.R' 'length RLum.R' 'get RLum.R'
      'RLum.Analysis-class.R' 'RLum.Data-class.R'
      'RLum.Data.Curve-class.R' 'RLum.Data.Image-class.R'
      'RLum.Data.Spectrum-class.R' 'merge_RLum.R'
      'RLum.Results-class.R' 'RcppExports.R'
      'Risoe.BINfileData2RLum.Analysis.R'
      'Risoe.BINfileData2RLum.Data.Curve.R' 'set_Risoe.BINfileData.R'
```

2 R topics documented:

'get Risoe.BINfileData.R' 'RisoeBINfileData-class.R' 'Second2Gray.R' 'analyse IRSAR.RF.R' 'analyse SAR.CWOSL.R' 'analyse\_SAR.TL.R' 'analyse\_pIRIRSequence.R' 'apply\_CosmicRayRemoval.R' 'apply\_EfficiencyCorrection.R' 'calc\_AliquotSize.R' 'calc\_CentralDose.R' 'calc\_CommonDose.R' 'calc\_CosmicDoseRate.R' 'calc\_FadingCorr.R' 'calc\_FiniteMixture.R' 'calc\_FuchsLang2001.R' 'calc\_HomogeneityTest.R' 'calc\_IEU.R' 'calc\_MaxDose.R' 'calc\_MinDose.R' 'calc\_OSLLxTxRatio.R' 'calc\_SourceDoseRate.R' 'calc\_Statistics.R' 'calc\_TLLxTxRatio.R' 'calc\_gSGC.R' 'extract\_IrradiationTimes.R' 'fit\_CWCurve.R' 'fit\_LMCurve.R' 'get\_Layout.R' 'get\_Quote.R' 'merge\_RLum.Analysis.R' 'merge RLum.Data.Curve.R' 'merge Risoe.BINfileData.R' 'methods DRAC.R' 'plot AbanicoPlot.R' 'plot DRTResults.R' 'plot\_GrowthCurve.R' 'plot\_Histogram.R' 'plot\_KDE.R' 'plot\_NRt.R' 'plot\_RLum.Analysis.R' 'plot\_RLum.Data.Curve.R' 'plot\_RLum.Data.Image.R' 'plot\_RLum.Data.Spectrum.R' 'plot\_RLum.R' 'plot\_RLum.Results.R' 'plot\_RadialPlot.R' 'plot\_Risoe.BINfileData.R' 'read\_BIN2R.R' 'read\_Daybreak2R.R' 'read\_SPE2R.R' 'read\_XSYG2R.R' 'template\_DRAC.R' 'use\_DRAC.R' 'write R2BIN.R' 'zzz.R'

# **NeedsCompilation** yes

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Luminescence-package Comprehensive Luminescence Dating Data Analysis

# **Description**

A collection of various R functions for the purpose of Luminescence dating data analysis. This includes, amongst others, data import, export, application of age models, curve deconvolution, sequence analysis and plotting of equivalent dose distributions.

### **Details**

Package: Luminescence Type: Package Version: 0.5.0

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# **Project source code repository**

https://github.com/R-Lum/Luminescence

# Related package projects

http://cran.r-project.org/package=RLumShiny
http://shiny.r-luminescence.de

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# References

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Fuchs, M.C., Kreutzer, S., Burow, C., Dietze, M., Fischer, M., Schmidt, C., Fuchs, M., 2015. Data processing in luminescence dating analysis: An exemplary workflow using the R package 'Luminescence'. Quaternary International, 362, pp. 8-13. http://dx.doi.org/10.1016/j.quaint.2014.06.034

Kreutzer, S., Schmidt, C., Fuchs, M.C., Dietze, M., Fischer, M., Fuchs, M., 2012. Introducing an R package for luminescence dating analysis. Ancient TL, 30, pp. 1-8.

analyse\_IRSAR.RF

Analyse IRSAR RF measurements

# Description

Function to analyse IRSAR RF measurements on K-feldspar samples, performed using the protocol according to Erfurt et al. (2003) and beyond.

#### Usage

```
analyse_IRSAR.RF(object, sequence.structure = c("NATURAL", "REGENERATED"),
   RF_nat.lim, RF_reg.lim, method = "FIT", test_parameter, fit.trace = FALSE,
   n.MC = 10, slide.show_density = FALSE, txtProgressBar = TRUE,
   plot = TRUE, ...)
```

# **Arguments**

object RLum. Analysis (**required**): input object containing data for protocol analysis.

The function expects to find at least two curves in the RLum. Analysis object:

(1) RF\_nat, (2) RF\_reg

sequence.structure

vector character (with default): specifies the general sequence structure. Allowed steps are NATURAL, REGENERATED. In addition any other character is allowed in the sequence structure; such curves will be ignored during the analysis.

RF\_nat.lim vector (with default): set minimum and maximum channel range for natural

signal fitting and sliding. If only one value is provided this will be treated as

minimum value and the maximum limit will be added automatically.

RF\_reg.lim vector (with default): set minimum and maximum channel range for regener-

ated signal fitting and sliding. If only one value is provided this will be treated as minimum value and the maximum limit will be added automatically.

method character (with default): setting method applied for the data analysis. Possible

options are "FIT" or "SLIDE".

test\_parameter list (with default): set test parameter Supported parameters are: curves\_ratio,

residuals\_slope (only for method = "SLIDE"), curves\_bounds, dynamic\_ratio, lambda, beta and delta.phi. All input: numeric values, NA and NULL (s. De-

tails)

(see Details for further information)

fit.trace logical (with default): trace fitting (for debugging use)

n.MC numeric (with default): set number of Monte Carlo runs for start parameter

estimation (method = "FIT") or error estimation (method = "SLIDE"). Note:

Large values will significantly increase the computation time

slide.show\_density

logical (with default): enable or disable KDE for MC run results. If the distri-

bution is too narrow nothing is shown

 ${\tt txtProgressBar} \ \ {\tt logical} \ (with \ default) : \ enables \ {\tt TRUE} \ or \ disables \ {\tt FALSE} \ the \ progression \ bar$ 

during MC runs

plot logical (with default): plot output (TRUE or FALSE)

further arguments that will be passed to the plot output. Currently supported ar-

guments are main, xlab, ylab, xlim, ylim, log, legend.pos (passes argument

to x,y in legend)

# Details

The function performs an IRSAR analysis described for K-feldspar samples by Erfurt et al. (2003) assuming a negligible sensitivity change of the RF signal.

General Sequence Structure (according to Erfurt et al. (2003))

- 1. Measuring IR-RF intensity of the natural dose for a few seconds  $(RF_{nat})$
- 2. Bleach the samples under solar conditions for at least 30 min without changing the geometry
- 3. Waiting for at least one hour
- 4. Regeneration of the IR-RF signal to at least the natural level (measuring  $(RF_{reg})$
- 5. Fitting data with a stretched exponential function
- 6. Calculate the the palaeodose  $D_e$  using the parameters from the fitting

Actually two methods are supported to obtain the  $D_e$ : method = "FIT" and method = "SLIDE": method = "FIT"

The principle is described above and follows the original suggestions by Erfurt et al., 2003. For the fitting the mean count value of the RF\_nat curve is used.

Function used for the fitting (according to Erfurt et al. (2003)):

$$\phi(D) = \phi_0 - \Delta\phi(1 - exp(-\lambda * D))^{\beta}$$

with  $\phi(D)$  the dose dependent IR-RF flux,  $\phi_0$  the inital IR-RF flux,  $\Delta \phi$  the dose dependent change of the IR-RF flux,  $\lambda$  the exponential parameter, D the dose and  $\beta$  the dispersive factor.

To obtain the palaeodose  $D_e$  the function is changed to:

$$D_e = ln(-(\phi(D) - \phi_0)/(-\lambda * \phi)^{1/\beta} + 1)/-\lambda$$

The fitting is done using the port algorithm of the nls function.

method = "SLIDE"

For this method the natural curve is slided along the x-axis until congruence with the regenerated curve is reached. Instead of fitting this allows to work with the original data without the need of any physical model. This approach was introduced for RF curves by Buylaert et al., 2012 and Lapp et al., 2012.

Here the sliding is done by searching for the minimum of the squared residuals.

#### **Error estimation**

For method = "FIT" the asymmetric error range is obtained by using the 2.5 % (lower) and the 97.5 % (upper) quantiles of the  $RF_{nat}$  curve for calculating the  $D_e$  error range.

For method = "SLIDE" the error is obtained by bootstrapping the residuals of the slided curve to construct new natural curves for a Monte Carlo simulation. The error is returned in two ways: (a) the standard deviation of the herewith obtained  $D_e$  from the MC runs and (b) the confidence interval using the 2.5 % (lower) and the 97.5 % (upper) quantiles. The results of the MC runs are returned with the function output.

# **Test parameters**

The argument test\_parameters allows to pass some thresholds for several test parameters, which will be evaluated during the function run. If a threshold is set and it will be exceeded the test

parameter status will be set to "FAILED". Intentionally this parameter is not termed 'rejection criteria' as not all test parameters are evaluated for both methods and some parameters are calculated by not evaluated by default. Common for all parameters are the allowed argument options NA and NULL. If the parameter is set to NA the value is calculated but the result will not be evaluated, means it has no effect on the status ("OK" or "FAILED") of the parameter. Setting the parameter to NULL disables the parameter entirely and the parameter will be also removed from the function output. This might be useful in cases where a particular parameter asks for long computation times. Currently supported parameters are:

```
curves_ratio numeric (default: 1.001):
```

The ratio of  $RF_{nat}$  over  $RF_{reg}$  in the range of  $RF_{nat}$  of is calculated and should not exceed the threshold value.

```
residuals_slope numeric (default: NA; only for method = "SLIDE"):
```

A linear function is fitted on the residuals after sliding. The corresponding slope can be used to discard values as a high (positive, negative) slope may indicate that both curves are fundamentally different and the method cannot be applied at all. Per default the value of this parameter is calculated but not evaluated.

```
curves_bounds numeric (default: max(RF_{reg_counts}):
```

This measure uses the maximum time (x) value of the regenerated curve. The maximum time (x) value of the natural curve cannot be larger than this value. However, although this is not recommended the value can be changed or disabled.

```
dynamic_ratio numeric (default: NA):
```

The dynamic ratio of the regenerated curve is calculated as ratio of the minimum and maximum count values.

```
lambda, beta and delta.phi numeric (default: NA; method = "SLIDE"):
```

The stretched exponential function suggested by Erfurt et al. (2003) describing the decay of the RF signal, comprises several parameters that might be useful to evaluate the shape of the curves. For method = "FIT" this parameter is obtained during the fitting, for method = "SLIDE" a rather rough estimation is made using the function nlsLM and the equation given above. Note: As this procedure requests more computation time, setting of one of these three parameters to NULL also prevents a calculation of the remaining two.

#### Value

A plot (optional) and an RLum.Results object is returned. The slot data contains the following elements:

```
$ De. values: data. frame table with De and corresponding values
```

- ..\$ DE: numeric: the obtained equivalent dose
- ..\$ DE.ERROR : numeric: (only method = "SLIDE") standard deviation obtained from MC runs
- ..\$ DE.LOWER : numeric: 2.5% quantile for De values obtained by MC runs
- ..\$ DE.UPPER : numeric: 97.5% quantile for De values obtained by MC runs

..\$ DE.STATUS: character: test parameter status
..\$ RF\_NAT.LIM: character: used RF\_nat curve limits
..\$ RF\_REG.LIM: character: used RF\_reg curve limits
..\$ POSITION: integer: (optional) position of the curves
..\$ DATE: character: (optional) measurement date

..\$ SEQUENCE\_NAME : character: (optional) sequence name

..\$ UID: character: unique data set ID

\$ test\_parameter : data.frame table test parameters

\$ fit: nls nlsModel object

\$ slide: list data from the sliding process \$ call: language-class: the original function call

The output (De. values) should be accessed using the function get\_RLum

# **Function version**

0.4.0 (2015-08-21 14:53:14)

#### Note

# [THIS FUNCTION HAS BETA-STATUS]

This function assumes that there is no sensitivity change during the measurements (natural vs. regenerated signal), which is in contrast to the findings from Buylaert et al. (2012). Furthermore: In course of ongoing research this function has been almost fully re-written, but further thoughtful tests are still pending! However, as a lot new package functionality was introduced with the changes made for this function and to allow a part of such tests the re-newed code was made part of the current package.

#### Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

# References

Buylaert, J.P., Jain, M., Murray, A.S., Thomsen, K.J., Lapp, T., 2012. IR-RF dating of sand-sized K-feldspar extracts: A test of accuracy. Radiation Measurements 44 (5-6), 560-565. doi: 10.1016/j.radmeas.2012.06.021

Erfurt, G., Krbetschek, M.R., 2003. IRSAR - A single-aliquot regenerative-dose dating protocol applied to the infrared radiofluorescence (IR-RF) of coarse- grain K-feldspar. Ancient TL 21, 35-42.

Erfurt, G., 2003. Infrared luminescence of Pb+ centres in potassium-rich feldspars. physica status solidi (a) 200, 429-438.

Erfurt, G., Krbetschek, M.R., 2003. Studies on the physics of the infrared radioluminescence of potassium feldspar and on the methodology of its application to sediment dating. Radiation Measurements 37, 505-510.

Erfurt, G., Krbetschek, M.R., Bortolot, V.J., Preusser, F., 2003. A fully automated multi-spectral radioluminescence reading system for geochronometry and dosimetry. Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms 207, 487-499.

Lapp, T., Jain, M., Thomsen, K.J., Murray, A.S., Buylaert, J.P., 2012. New luminescence measurement facilities in retrospective dosimetry. Radiation Measurements 47, 803-808. doi:10.1016/j.radmeas.2012.02.006

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Trautmann, T., Krbetschek, M.R., Dietrich, A., Stolz, W., 1998. Investigations of feldspar radioluminescence: potential for a new dating technique. Radiation Measurements 29, 421-425.

Trautmann, T., Krbetschek, M.R., Dietrich, A., Stolz, W., 1999. Feldspar radioluminescence: a new dating method and its physical background. Journal of Luminescence 85, 45-58.

Trautmann, T., Krbetschek, M.R., Stolz, W., 2000. A systematic study of the radioluminescence properties of single feldspar grains. Radiation Measurements 32, 685-690.

#### See Also

```
RLum. Analysis, RLum. Results, get_RLum, nls, nlsLM
```

# **Examples**

```
##load data
data(ExampleData.RLum.Analysis, envir = environment())
##perform analysis
temp <- analyse_IRSAR.RF(object = IRSAR.RF.Data)
##show De results and test paramter results
get_RLum(temp, data.object = "De.values")
get_RLum(temp, data.object = "test_parameter")</pre>
```

analyse\_pIRIRSequence Analyse post-IR IRSL sequences

# **Description**

The function performs an analysis of post-IR IRSL sequences including curve fitting on RLum. Analysis objects.

#### Usage

```
analyse_pIRIRSequence(object, signal.integral.min, signal.integral.max,
background.integral.min, background.integral.max, dose.points,
sequence.structure = c("TL", "IR50", "pIRIR225"), plot = TRUE,
plot.single = FALSE, ...)
```

# **Arguments**

```
object RLum.Analysis(required): input object containing data for analysis signal.integral.min

integer (required): lower bound of the signal integral. Provide this value as vector for different integration limits for the different IRSL curves.

signal.integral.max

integer (required): upper bound of the signal integral. Provide this value as vector for different integration limits for the different IRSL curves.
```

background.integral.min

integer (required): lower bound of the background integral. Provide this value as vector for different integration limits for the different IRSL curves.

background.integral.max

integer (required): upper bound of the background integral. Provide this value as vector for different integration limits for the different IRSL curves.

dose.points

numeric (optional): a numeric vector containing the dose points values. Using this argument overwrites dose point values in the signal curves.

sequence.structure

vector character (with default): specifies the general sequence structure. Allowed values are "TL" and any "IR" combination (e.g., "IR50", "pIRIR225"). Additionally a parameter "EXCLUDE" is allowed to exclude curves from the analysis (Note: If a preheat without PMT measurement is used, i.e. preheat as non

TL, remove the TL step.)

plot logical (with default): enables or disables plot output.

plot.single logical (with default): single plot output (TRUE/FALSE) to allow for plotting

the results in single plot windows. Requires plot = TRUE.

further arguments that will be passed to the function analyse\_SAR.CWOSL and

plot\_GrowthCurve

#### **Details**

To allow post-IR IRSL protocol (Thomsen et al., 2008) measurement analysis this function has been written as extended wrapper function for the function analyse\_SAR.CWOSL, facilitating an entire sequence analysis in one run. With this, its functionality is strictly limited by the functionality of the function analyse\_SAR.CWOSL.

# Value

Plots (optional) and an RLum. Results object is returned containing the following elements:

data.frame containing De-values, De-error and further parameters De.values

LnLxTnTx.values

data.frame of all calculated Lx/Tx values including signal, background counts and the dose points.

rejection.criteria

data.frame with values that might by used as rejection criteria. NA is produced if no R0 dose point exists.

The output should be accessed using the function get\_RLum.

#### **Function version**

```
0.1.4 (2015-08-29 13:33:00)
```

# Note

```
Best graphical output can be achieved by using the function pdf with the following options:
pdf(file = "...", height = 15, width = 15)
```

#### Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

#### References

Murray, A.S., Wintle, A.G., 2000. Luminescence dating of quartz using an improved single-aliquot regenerative-dose protocol. Radiation Measurements 32, 57-73. doi:10.1016/S1350-4487(99)00253-X

Thomsen, K.J., Murray, A.S., Jain, M., Boetter-Jensen, L., 2008. Laboratory fading rates of various luminescence signals from feldspar-rich sediment extracts. Radiation Measurements 43, 1474-1486. doi:10.1016/j.radmeas.2008.06.002

#### See Also

 $analyse\_SAR.CWOSL, calc\_OSLLxTxRatio, plot\_GrowthCurve, RLum.Analysis, RLum.Results \\ get\_RLum$ 

# **Examples**

```
### NOTE: For this example existing example data are used. These data are non pIRIR data.
##(1) Compile example data set based on existing example data (SAR quartz measurement)
##(a) Load example data
data(ExampleData.BINfileData, envir = environment())
##(b) Transform the values from the first position in a RLum.Analysis object
object <- Risoe.BINfileData2RLum.Analysis(CWOSL.SAR.Data, pos=1)</pre>
##(c) Grep curves and exclude the last two (one TL and one IRSL)
object <- get_RLum(object, record.id = c(-29, -30))
##(d) Define new sequence structure and set new RLum.Analysis object
sequence.structure <-c(1,2,2,3,4,4)
sequence.structure <- as.vector(sapply(seq(0,length(object)-1,by = 4),
                                        function(x){sequence.structure + x}))
object <- sapply(1:length(sequence.structure), function(x){</pre>
  object[[sequence.structure[x]]]
})
object <- set_RLum(class = "RLum.Analysis", records = object, protocol = "pIRIR")
##(2) Perform pIRIR analysis (for this example with quartz OSL data!)
## Note: output as single plots to avoid problems with this example
results <- analyse_pIRIRSequence(object,</pre>
                             signal.integral.min = 1,
                              signal.integral.max = 2,
                             background.integral.min = 900,
                             background.integral.max = 1000,
                              fit.method = "EXP",
                             sequence.structure = c("TL", "pseudoIRSL1", "pseudoIRSL2"),
                             main = "Pseudo pIRIR data set based on quartz OSL",
```

```
plot.single = TRUE)
```

```
##(3) Perform pIRIR analysis (for this example with quartz OSL data!)
## Alternative for PDF output, uncomment and complete for usage
##
# pdf(file = "...", height = 15, width = 15)
# results <- analyse_pIRIRSequence(object,

# signal.integral.min = 1,
# signal.integral.max = 2,
# background.integral.min = 900,
# background.integral.max = 1000,
# fit.method = "EXP",
# main = "Pseudo pIRIR data set based on quartz OSL")
# dev.off()</pre>
```

analyse\_SAR.CWOSL

Analyse SAR CW-OSL measurements

#### **Description**

The function performs a SAR CW-OSL analysis on an RLum. Analysis object including growth curve fitting.

#### Usage

```
analyse_SAR.CWOSL(object, signal.integral.min, signal.integral.max,
  background.integral.min, background.integral.max, rejection.criteria,
  dose.points, mtext.outer, plot = TRUE, plot.single = FALSE, ...)
```

# **Arguments**

```
object
                 RLum. Analysis (required): input object containing data for analysis, alterna-
                 tively a list of RLum. Analysis objects can be provided.
signal.integral.min
                  integer (required): lower bound of the signal integral. Can be a list of
                  integers, if object is of type list
signal.integral.max
                  integer (required): upper bound of the signal integral. Can be a list of
                  integers, if object is of type list
background.integral.min
                  integer (required): lower bound of the background integral. Can be a list of
                  integers, if object is of type list
background.integral.max
                  integer (required): upper bound of the background integral. Can be a list of
                  integers, if object is of type list
rejection.criteria
```

list (with default): provide a named list and set rejection criteria in percentage
for further calculation. Can be a list in a list, if object is of type list
Allowed #' arguments are recycling.ratio, recuperation.rate, palaeodose.error
and exceed.max.regpoint = TRUE/FALS. Example: rejection.criteria = list(recycling.rate)
Per default all numericla values are set to 10.

dose.points

numeric (optional): a numeric vector containg the dose points values Using this argument overwrites dose point values in the signal curves. Can be a list of numeric vectors, if object is of type list

mtext.outer

character (optional): option to provide an outer margin mtext. Can be a list of characters, if object is of type list

plot

logical (with default): enables or disables plot output.

logical (with default) or numeric (optional): single plot output (TRUE/FALSE) to allow for plotting the results in single plot windows. If a numerice vector is provided the plots can be selected individually, i.e. plot.single =

c(1,2,3,4) will plot the TL and Lx, Tx curves but not the legend (5) or the growth curve (6), (7) and (8) belong to rejection criteria plots. Requires plot = TRUE.

further arguments that will be passed to the function plot\_GrowthCurve or calc\_OSLLxTxRatio (supported: background.count.distribution and sigmab)

#### **Details**

The function performs an analysis for a standard SAR protocol measurements introduced by Murray and Wintle (2000) with CW-OSL curves. For the calculation of the Lx/Tx value the function calc\_OSLLxTxRatio is used. For **changing the way the Lx/Tx error is calculated** use the argument background.count.distribution and sigmab, which will be passed to the function calc\_OSLLxTxRatio.

#### Argument object is of type list

If the argument object is of type list containing **only** RLum. Analysis objects, the function recalls itself as often as elements are in the list. This is usefull if an entire measurement wanted to be analysed without writing separate for-loops. To gain in full control of the parameters (e.g., dose.points) for every aliquot (corresponding to one RLum. Analysis object in the list), in this case the arguments can be provided as list. This list should be of similar length as the list provided with the argument object, otherwise the function will create an own list of the requested length. Function output will be just one single RLum. Results object.

Please be careful when using this option. It may allow a fast an efficient data analysis, but the function may also break with an unclear error message, due to wrong input data.

# Working with IRSL data

The function was originally designed to work just for 'OSL' curves, following the principles of the SAR protocol. An IRSL measurement protocol may follow this procedure, e.g., post-IR IRSL protocol (Thomsen et al., 2008). Therefore this functions has been enhanced to work with IRSL data, however, the function is only capable of analysing curves that follow the SAR protocol structure, i.e., to analyse a post-IR IRSL protocol, curve data have to be pre-selected by the user to fit the standards of the SAR protocol, i.e., Lx,Tx,Lx,Tx and so on.

Example: Imagine the measurement contains pIRIR50 and pIRIR225 IRSL curves. Only one curve type can be analysed at the same time: The pIRIR50 curves or the pIRIR225 curves.

# Supported rejection criteria

'recycling.ratio': calculated for every repeated regeneration dose point.

'recuperation.rate': recuperation rate calculated by comparing the Lx/Tx values of the zero regeneration point with the Ln/Tn value (the Lx/Tx ratio of the natural signal). For methodological background see Aitken and Smith (1988).

'palaeodose.error': set the allowed error for the De value, which per default should not exceed 10%.

#### Value

A plot (optional) and an RLum. Results object is returned containing the following elements:

De. values data.frame containing De-values, De-error and further parameters

LnLxTnTx.values

data.frame of all calculated Lx/Tx values including signal, background counts

and the dose points

rejection.criteria

data.frame with values that might by used as rejection criteria. NA is produced

if no R0 dose point exists.

Formula formula that have been used for the growth curve fitting

The output should be accessed using the function get\_RLum.

# **Function version**

0.6.3 (2015-08-30 19:14:03)

# Note

This function must not be mixed up with the function Analyse\_SAR.OSLdata, which works with Risoe.BINfileData-class objects.

The function currently does only support 'OSL' or 'IRSL' data!

#### Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

# References

Aitken, M.J. and Smith, B.W., 1988. Optical dating: recuperation after bleaching. Quaternary Science Reviews 7, 387-393.

Duller, G., 2003. Distinguishing quartz and feldspar in single grain luminescence measurements. Radiation Measurements, 37 (2), 161-165.

Murray, A.S. and Wintle, A.G., 2000. Luminescence dating of quartz using an improved single-aliquot regenerative-dose protocol. Radiation Measurements 32, 57-73.

Thomsen, K.J., Murray, A.S., Jain, M., Boetter-Jensen, L., 2008. Laboratory fading rates of various luminescence signals from feldspar-rich sediment extracts. Radiation Measurements 43, 1474-1486. doi:10.1016/j.radmeas.2008.06.002

# See Also

```
calc_OSLLxTxRatio, plot_GrowthCurve, RLum.Analysis, RLum.Results get_RLum
```

# **Examples**

```
##load data
##ExampleData.BINfileData contains two BINfileData objects
##CWOSL.SAR.Data and TL.SAR.Data
data(ExampleData.BINfileData, envir = environment())
##transform the values from the first position in a RLum.Analysis object
object <- Risoe.BINfileData2RLum.Analysis(CWOSL.SAR.Data, pos=1)</pre>
##perform SAR analysis
results <- analyse_SAR.CWOSL(object,</pre>
                  signal.integral.min = 1,
                  signal.integral.max = 2,
                  background.integral.min = 900,
                  background.integral.max = 1000,
                  log = "x",
                  fit.method = "EXP")
##show De results
get_RLum(results)
##show LnTnLxTx table
get_RLum(results, data.object = "LnLxTnTx.table")
```

Analyse\_SAR.OSLdata Analyse SAR CW-OSL measurements.

# Description

The function analyses SAR CW-OSL curve data and provides a summary of the measured data for every position. The output of the function is optimised for SAR OSL measurements on quartz.

# Usage

```
Analyse_SAR.OSLdata(input.data, signal.integral, background.integral, position,
  run, set, dtype, keep.SEL = FALSE,
  info.measurement = "unkown measurement", log = "", output.plot = FALSE,
  output.plot.single = FALSE, cex.global = 1, ...)
```

# **Arguments**

input.data Risoe.BINfileData-class (**required**): input data from a Risoe BIN file, produced by the function read\_BIN2R.

signal.integral

vector (required): channels used for the signal integral, e.g. signal.integral=c(1:2)

background.integral

vector (**required**): channels used for the background integral, e.g. background.integral=c(85:100

position  $\frac{\text{vector (optional): reader positions that want to be analysed (e.g. position=<math>c(1:48)$ .

Empty positions are automatically omitted. If no value is given all positions are

analysed by default.

run vector (optional): range of runs used for the analysis. If no value is given the

range of the runs in the sequence is deduced from the Risoe.BINfileData object.

set vector (optional): range of sets used for the analysis. If no value is given the

range of the sets in the sequence is deduced from the Risoe.BINfileData ob-

ject.

dtype character (optional): allows to further limit the curves by their data type

(DTYPE), e.g., dtype = c("Natural", "Dose") limits the curves to this two data types. By default all values are allowed. See Risoe.BINfileData-class for

allowed data types.

keep. SEL logical (default): option allowing to use the SEL element of the Risoe.BINfileData-

class manually. NOTE: In this case any limitation provided by run, set and

dtype are ignored!

info.measurement

character (with default): option to provide information about the measurement

on the plot output (e.g. name of the BIN or BINX file).

log character (with default): a character string which contains "x" if the x axis is to

be logarithmic, "y" if the y axis is to be logarithmic and "xy" or "yx" if both axes

are to be logarithmic. See plot.default.

output.plot logical (with default): plot output (TRUE/FALSE)

output.plot.single

logical (with default): single plot output (TRUE/FALSE) to allow for plotting the

results in single plot windows. Requires output.plot = TRUE.

cex.global numeric (with default): global scaling factor.

#'

... further arguments that will be passed to the function calc\_OSLLxTxRatio (sup-

ported: background.count.distribution and sigmab)

#### **Details**

The function works only for standard SAR protocol measurements introduced by Murray and Wintle (2000) with CW-OSL curves. For the calculation of the Lx/Tx value the function calc\_OSLLxTxRatio is used.

# Provided rejection criteria

'recyling ratio': calculated for every repeated regeneration dose point.

'recuperation': recuperation rate calculated by comparing the Lx/Tx values of the zero regeneration point with the Ln/Tn value (the Lx/Tx ratio of the natural signal). For methodological background see Aitken and Smith (1988)

'IRSL/BOSL': the integrated counts (signal.integral) of an IRSL curve are compared to the integrated counts of the first regenerated dose point. It is assumed that IRSL curves got the same dose as the first regenerated dose point. **Note:** This is not the IR depletation ratio described by Duller (2003).

# Value

A plot (optional) and list is returned containing the following elements:

LnLxTnTx data.frame of all calculated Lx/Tx values including signal, background counts

and the dose points.

RejectionCriteria

data.frame with values that might by used as rejection criteria. NA is produced

if no R0 dose point exists.

SARParameters data.frame of additional measurement parameters obtained from the BIN file,

e.g. preheat or read temperature (not valid for all types of measurements).

#### **Function version**

0.2.16 (2015-08-21 14:53:14)

#### Note

Rejection criteria are calculated but not considered during the analysis to discard values.

The analysis of IRSL data is not directly supported. You may want to consider using the functions analyse\_SAR.CWOSL or analyse\_pIRIRSequence instead.

The development of this function will not be continued. We recommend to use the function analyse\_SAR.CWOSL or instead.

# Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France), Margret C. Fuchs, TU Bergakademie Freiberg (Germany)

R Luminescence Package Team

#### References

Aitken, M.J. and Smith, B.W., 1988. Optical dating: recuperation after bleaching. Quaternary Science Reviews 7, 387-393.

Duller, G., 2003. Distinguishing quartz and feldspar in single grain luminescence measurements. Radiation Measurements, 37 (2), 161-165.

Murray, A.S. and Wintle, A.G., 2000. Luminescence dating of quartz using an improved single-aliquot regenerative-dose protocol. Radiation Measurements 32, 57-73.

#### See Also

calc\_OSLLxTxRatio, Risoe.BINfileData-class, read\_BIN2R and for further analysis plot\_GrowthCurve

analyse\_SAR.TL 19

#### **Examples**

analyse\_SAR.TL

Analyse SAR TL measurements

# **Description**

The function performs a SAR TL analysis on a RLum. Analysis object including growth curve fitting.

#### Usage

```
analyse_SAR.TL(object, object.background, signal.integral.min,
  signal.integral.max, sequence.structure = c("PREHEAT", "SIGNAL",
  "BACKGROUND"), rejection.criteria = list(recycling.ratio = 10,
  recuperation.rate = 10), log = "", ...)
```

# **Arguments**

tion.

```
object
                  RLum. Analysis (required): input object containing data for analysis
object.background
                  currently not used
signal.integral.min
                  integer (required): requires the channel number for the lower signal integral
                  bound (e.g. signal.integral.min = 100)
signal.integral.max
                  integer (required): requires the channel number for the upper signal integral
                  bound (e.g. signal.integral.max = 200)
sequence.structure
                  vector character (with default): specifies the general sequence structure. Three
                  steps are allowed ("PREHEAT", "SIGNAL", "BACKGROUND"), in addition a param-
                  eter "EXCLUDE". This allows excluding TL curves which are not relevant for the
                  protocol analysis. (Note: None TL are removed by default)
rejection.criteria
```

list (with default): list containing rejection criteria in percentage for the calcula-

20 analyse\_SAR.TL

log character (with default): a character string which contains "x" if the x axis is to be logarithmic, "y" if the y axis is to be logarithmic and "xy" or "yx" if both axes

are to be logarithmic. See plot.default).

... further arguments that will be passed to the function plot\_GrowthCurve

# **Details**

This function performs a SAR TL analysis on a set of curves. The SAR procedure in general is given by Murray and Wintle (2000). For the calculation of the Lx/Tx value the function calc\_TLLxTxRatio is used.

# Provided rejection criteria

'recyling.ratio': calculated for every repeated regeneration dose point.

'recuperation.rate': recuperation rate calculated by comparing the Lx/Tx values of the zero regeneration point with the Ln/Tn value (the Lx/Tx ratio of the natural signal). For methodological background see Aitken and Smith (1988)

#### Value

A plot (optional) and an RLum. Results object is returned containing the following elements:

De. values data.frame containing De-values and further parameters

LnLxTnTx.values

data.frame of all calculated Lx/Tx values including signal, background counts and the dose points.

rejection.criteria

data.frame with values that might by used as rejection criteria. NA is produced if no R0 dose point exists.

**note:** the output should be accessed using the function get\_RLum

# **Function version**

0.1.4 (2015-08-21 14:53:14)

# Note

# THIS IS A BETA VERSION

None TL curves will be removed from the input object without further warning.

#### Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

#### References

Aitken, M.J. and Smith, B.W., 1988. Optical dating: recuperation after bleaching. Quaternary Science Reviews 7, 387-393.

Murray, A.S. and Wintle, A.G., 2000. Luminescence dating of quartz using an improved single-aliquot regenerative-dose protocol. Radiation Measurements 32, 57-73.

# See Also

```
calc_TLLxTxRatio, plot_GrowthCurve, RLum. Analysis, RLum. Results get_RLum
```

# **Examples**

apply\_CosmicRayRemoval

Function to remove cosmic rays from an RLum.Data.Spectrum S4 class object

# **Description**

The function provides several methods for cosmic ray removal and spectrum smoothing for an RLum.Data.Spectrum S4 class object

# Usage

```
apply_CosmicRayRemoval(object, method = "Pych", method.Pych.smoothing = 2,
    silent = FALSE, plot = FALSE, ...)
```

# **Arguments**

object method RLum.Data.Spectrum (**required**): S4 object of class RLum.Data.Spectrum character (with default): Defines method that is applied for cosmic ray removal. Allowed methods are smooth (smooth), smooth.spline (smooth.spline) and Pych (default). See details for further information.

method.Pych.smoothing

integer (with default): Smoothing parameter for cosmic ray removal according to Pych (2003). The value defines how many neighboring values in each frame are used for smoothing (e.g., 2 means that the two previous and two following values are used).

silent logical (with default): Option to suppress terminal output.,

plot logical (with default): If TRUE the histograms used for the cosmic-ray removal

are returned as plot including the used threshold. Note: A separat plot is returned for each frame! Currently only for method = "Pych" a graphical output is

provided.

... further arguments and graphical parameters that will be passed to the smooth

function.

#### **Details**

```
method = "Pych"
```

This method applies the cosmic-ray removal algorithm described by Pych (2003). Some aspects that are different to the publication:

- For interpolation between neighbouring values the median and not the mean is used.
- The number of breaks to construct the histogram is set to: length(number.of.input.values)/2

For further details see references below.

```
method = "smooth"
```

Method uses the function smooth to remove cosmic rays.

Arguments that can be passed are: kind, twiceit

```
method = "smooth.spline"
Method uses the function smooth.spline to remove cosmic rays.
Arguments that can be passed are: spar
```

#### How to combine methods?

Different methods can be combined by applying the method repeatedly to the dataset (see example).

# Value

Returns same object as input (RLum. Data. Spectrum)

# **Function version**

```
0.1.3 (2015-08-21 14:53:14)
```

## Note

-

# Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

### References

Pych, W., 2003. A Fast Algorithm for Cosmic-Ray Removal from Single Images. Astrophysics 116, 148-153. http://arxiv.org/pdf/astro-ph/0311290.pdf?origin=publication\_detail

#### See Also

RLum.Data.Spectrum, smooth, smooth.spline, apply\_CosmicRayRemoval

# **Examples**

```
##(1) - use with your own data and combine (uncomment for usage)
## run two times the default method and smooth with another method
## your.spectrum <- apply_CosmicRayRemoval(your.spectrum, method = "Pych")
## your.spectrum <- apply_CosmicRayRemoval(your.spectrum, method = "Pych")
## your.spectrum <- apply_CosmicRayRemoval(your.spectrum, method = "smooth")</pre>
```

```
apply_EfficiencyCorrection
```

Function to apply spectral efficiency correction to RLum.Data.Spectrum S4 class objects

# Description

The function allows spectral efficiency corrections for RLum.Data.Spectrum S4 class objects

# Usage

```
apply_EfficiencyCorrection(object, spectral.efficiency)
```

# **Arguments**

```
object RLum.Data.Spectrum (required): S4 object of class RLum.Data.Spectrum spectral.efficiency data.frame (required): Data set containing wavelengths (x-column) and relative spectral response values (y-column) in percentage
```

# **Details**

The efficiency correction is based on a spectral response dataset provided by the user. Usually the data set for the quantum efficiency is of lower resolution and values are interpolated for the required spectral resolution.

# Value

Returns same object as input (RLum. Data. Spectrum)

# **Function version**

```
0.1 (2015-08-21 14:53:14)
```

#### Note

Please note that the spectral efficiency data from the camera may not sufficiently correct for spectral efficiency of the entire optical system (e.g., spectrometer, camera ...).

This function has BETA status.

# Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France), Johannes Friedrich, University of Bayreuth (Germany) R Luminescence Package Team

#### References

\_

#### See Also

```
RLum.Data.Spectrum
```

# **Examples**

```
##(1) - use with your own data (uncomment for usage)
## spectral.efficiency <- read.csv("your data")
##
## your.spectrum <- apply_EfficiencyCorrection(your.spectrum, )</pre>
```

BaseDataSet.CosmicDoseRate

Base data set for cosmic dose rate calculation

# **Description**

Collection of data from various sources needed for cosmic dose rate calculation

# **Format**

values.cosmic.Softcomp: values.factor.Altitude: values.par.FJH: data frame containing cosmic dose rates for shallow depths (< 167 g cm^-2) obtained using data frame containing altitude factors for adjusting geomagnetic field-change factors. Value data frame containing values for parameters F, J and H (read from Fig. 2 in Prescott & Hut

$$Dc = D0 * (F + J * exp((altitude/1000)/H))$$

# Version

0.1

# **Source**

The following data were carefully read from figures in mentioned sources and used for fitting procedures. The derived expressions are used in the function calc\_CosmicDoseRate.

# values.cosmic.Softcomp

Program: "AGE" Reference: Gruen (2009)

Fit: Polynomials in the form of

For depths between 40-167 g cm^-2:

$$y = 2 * 10^- 6 * x^2 - 0.0008 * x + 0.2535$$

(For depths  $<40 \text{ g cm}^2$ )

$$y = -6 * 10^{-}8 * x^{3} + 2 * 10^{-}5 * x^{2} - 0.0025 * x + 0.2969$$

# values.factor.Altitude

Reference: Prescott & Hutton (1994)

Page: 499 Figure: 1

Fit: 2-degree polynomial in the form of

$$y = -0.026 * x^2 + 0.6628 * x + 1.0435$$

# values.par.FJH

Reference: Prescott & Hutton (1994)

Page: 500 Figure: 2

Fits: 3-degree polynomials and linear fits

F (non-linear part,  $\lambda$  < 36.5 deg.):

$$y = -7 * 10^{-}7 * x^{3} - 8 * 10^{-}5 * x^{2} - 0.0009 * x + 0.3988$$

F (linear part,  $\lambda > 36.5$  deg.):

$$y = -0.0001 * x + 0.2347$$

J (non-linear part,  $\lambda$  < 34 deg.):

$$y = 5 * 10^{-}6 * x^{3} - 5 * 10^{-}5 * x^{2} + 0.0026 * x + 0.5177$$

J (linear part,  $\lambda > 34$  deg.):

$$y = 0.0005 * x + 0.7388$$

H (non-linear part,  $\lambda$  < 36 deg.):

26 calc\_AliquotSize

$$y = -3 * 10^{-}6 * x^{3} - 5 * 10^{-}5 * x^{2} - 0.0031 * x + 4.398$$

H (linear part,  $\lambda > 36$  deg.):

$$y = 0.0002 * x + 4.0914$$

#### References

Gruen, R., 2009. The "AGE" program for the calculation of luminescence age estimates. Ancient TL, 27, pp. 45-46.

Prescott, J.R., Hutton, J.T., 1988. Cosmic ray and gamma ray dosimetry for TL and ESR. Nuclear Tracks and Radiation Measurements, 14, pp. 223-227.

Prescott, J.R., Hutton, J.T., 1994. Cosmic ray contributions to dose rates for luminescence and ESR dating: large depths and long-term time variations. Radiation Measurements, 23, pp. 497-500.

# **Examples**

```
##load data
data(BaseDataSet.CosmicDoseRate)
```

calc\_AliquotSize

Estimate the amount of grains on an aliquot

# **Description**

Estimate the number of grains on an aliquot. Alternatively, the packing density of an aliquot is computed.

# Usage

```
calc_AliquotSize(grain.size, sample.diameter, packing.density = 0.65,
   MC = TRUE, grains.counted, plot = TRUE, ...)
```

# **Arguments**

grain.size

numeric (**required**): mean grain size (microns) or a range of grain sizes from which the mean grain size is computed (e.g. c(100, 200)).

sample.diameter

numeric (required): diameter (mm) of the targeted area on the sample carrier.

packing.density

numeric (with default) empirical value for mean packing density.

If packing density = "inf" a hexagonal structure on an infinite plane with a packing density of 0.906... is assumed.

MC

logical (optional): if TRUE the function performs a monte carlo simulation for estimating the amount of grains on the sample carrier and assumes random errors in grain size distribution and packing density. Requires a vector with min and max grain size for grain.size. For more information see details.

calc\_AliquotSize 27

grains.counted numeric (optional) grains counted on a sample carrier. If a non-zero positive

integer is provided this function will calculate the packing density of the aliquot. If more than one value is provided the mean packing density and its standard

deviation is calculated. Note that this overrides packing.density.

plot logical (with default): plot output (TRUE/FALSE)

... further arguments to pass (main, xlab, MC.iter).

#### **Details**

This function can be used to either estimate the number of grains on an aliquot or to compute the packing density depending on the the arguments provided.

The following function is used to estimate the number of grains n:

$$n = (\pi * x^2)/(\pi * y^2) * d$$

where x is the radius of the aliquot size (microns), y is the mean radius of the mineral grains (mm) and d is the packing density (value between 0 and 1).

# Packing density

The default value for packing.density is 0.65, which is the mean of empirical values determined by Heer et al. (2012) and unpublished data from the Cologne luminescence laboratory. If packing.density = "inf" a maximum density of  $\pi/\sqrt{12} = 0.9068\ldots$  is used. However, note that this value is not appropriate as the standard preparation procedure of aliquots resembles a PECC ("Packing Equal Circles in a Circle") problem where the maximum packing density is asymptotic to about 0.87.

# **Monte Carlo simulation**

The number of grains on an aliquot can be estimated by Monte Carlo simulation when setting MC = TRUE. Each of the parameters necessary to calculate n (x, y, d) are assumed to be normally distributed with means  $\mu_x$ ,  $\mu_y$ ,  $\mu_d$  and standard deviations  $\sigma_x$ ,  $\sigma_y$ ,  $\sigma_d$ .

For the mean grain size random samples are taken first from  $N(\mu_y, \sigma_y)$ , where  $\mu_y = mean.grain.size$  and  $\sigma_y = (max.grain.size - min.grain.size)/4$  so that 95% of all grains are within the provided the grain size range. This effectively takes into account that after sieving the sample there is still a small chance of having grains smaller or larger than the used mesh sizes. For each random sample the mean grain size is calculated, from which random subsamples are drawn for the Monte Carlo simulation.

The packing density is assumed to be normally distributed with an empirically determined  $\mu=0.65$  (or provided value) and  $\sigma=0.18$ . The normal distribution is truncated at d = 0.87 as this is approximately the maximum packing density that can be achieved in PECC problem.

The sample diameter has  $\mu = sample.diameter$  and  $\sigma = 0.2$  to take into account variations in sample disc preparation (i.e. applying silicon spray to the disc). A lower truncation point at x = 0.5 is used, which assumes that aliquouts with smaller sample diameters of 0.5 mm are discarded. Likewise, the normal distribution is truncated at 9.8 mm, which is the diameter of the sample disc.

For each random sample drawn from the normal distributions the amount of grains on the aliquot is calculated. By default, 10^5 iterations are used, but can be reduced/increased with MC.iter (see ...). The results are visualised in a bar- and boxplot together with a statistical summary.

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#### Value

Returns a terminal output. In addition an RLum.Results object is returned containing the following element:

summary data.frame summary of all relevant calculation results.

args list used arguments
call call the function call

MC list results of the Monte Carlo simulation

The output should be accessed using the function get\_RLum

#### **Function version**

```
0.31 (2015-08-21 14:53:14)
```

# Author(s)

```
Christoph Burow, University of Cologne (Germany)
R Luminescence Package Team
```

#### References

Duller, G.A.T., 2008. Single-grain optical dating of Quaternary sediments: why aliquot size matters in luminescence dating. Boreas 37, 589-612.

Heer, A.J., Adamiec, G., Moska, P., 2012. How many grains are there on a single aliquot?. Ancient TL 30, 9-16.

# **Further reading**

Chang, H.-C., Wang, L.-C., 2010. A simple proof of Thue's Theorem on Circle Packing. http://arxiv.org/pdf/1009.4322v1.pdf, 2013-09-13.

Graham, R.L., Lubachevsky, B.D., Nurmela, K.J., Oestergard, P.R.J., 1998. Dense packings of congruent circles in a circle. Discrete Mathematics 181, 139-154.

Huang, W., Ye, T., 2011. Global optimization method for finding dense packings of equal circles in a circle. European Journal of Operational Research 210, 474-481.

# **Examples**

calc\_CentralDose 29

calc_CentralDose	Apply the central age model (CAM) after Galbraith et al. (1999) to a given De distribution
------------------	--

# Description

This function calculates the central dose and dispersion of the De distribution, their standard errors and the profile log likelihood function for sigma.

# Usage

```
calc_CentralDose(data, sigmab, plot = TRUE, ...)
```

# **Arguments**

data	RLum.Results or data.frame ( <b>required</b> ): for data.frame: two columns with De (data[,1]) and De error (values[,2])
sigmab	numeric (with default): spread in De values given as a fraction (e.g. 0.2). This value represents the expected overdispersion in the data should the sample be well-bleached (Cunningham & Walling 2012, p. 100).
plot	logical (with default): plot output
	further arguments (trace, verbose).

# **Details**

This function uses the equations of Galbraith et al. (1999, 358-359). The parameter sigma is estimated using the maximum likelihood approach. A detailed explanation on maximum likelihood estimation can be found in the appendix of Galbraith & Laslett (1993, 468-470)

# Value

Returns a plot (optional) and terminal output. In addition an RLum.Results object is returned containing the following element:

summary	data.frame summary of all relevant model results.
data	data.frame original input data
args	list used arguments
call	call the function call
profile	data.frame the log likelihood profile for sigma

The output should be accessed using the function get\_RLum

# **Function version**

```
1.3.1 (2015-08-21 14:53:14)
```

30 calc\_CentralDose

#### Author(s)

Christoph Burow, University of Cologne (Germany) Based on a rewritten S script of Rex Galbraith, 2010

R Luminescence Package Team

#### References

Galbraith, R.F. & Laslett, G.M., 1993. Statistical models for mixed fission track ages. Nuclear Tracks Radiation Measurements 4, 459-470.

Galbraith, R.F., Roberts, R.G., Laslett, G.M., Yoshida, H. & Olley, J.M., 1999. Optical dating of single grains of quartz from Jinmium rock shelter, northern Australia. Part I: experimental design and statistical models. Archaeometry 41, 339-364.

Galbraith, R.F. & Roberts, R.G., 2012. Statistical aspects of equivalent dose and error calculation and display in OSL dating: An overview and some recommendations. Quaternary Geochronology 11, 1-27.

# **Further reading**

Arnold, L.J. & Roberts, R.G., 2009. Stochastic modelling of multi-grain equivalent dose (De) distributions: Implications for OSL dating of sediment mixtures. Quaternary Geochronology 4, 204-230.

Bailey, R.M. & Arnold, L.J., 2006. Statistical modelling of single grain quartz De distributions and an assessment of procedures for estimating burial dose. Quaternary Science Reviews 25, 2475-2502.

Cunningham, A.C. & Wallinga, J., 2012. Realizing the potential of fluvial archives using robust OSL chronologies. Quaternary Geochronology 12, 98-106.

Rodnight, H., Duller, G.A.T., Wintle, A.G. & Tooth, S., 2006. Assessing the reproducibility and accuracy of optical dating of fluvial deposits. Quaternary Geochronology, 1 109-120.

Rodnight, H., 2008. How many equivalent dose values are needed to obtain a reproducible distribution?. Ancient TL 26, 3-10.

# See Also

plot, calc\_CommonDose, calc\_FiniteMixture, calc\_FuchsLang2001, calc\_MinDose

# **Examples**

```
##load example data
data(ExampleData.DeValues, envir = environment())
##apply the central dose model
calc_CentralDose(ExampleData.DeValues$CA1)
```

calc\_CommonDose 31

calc_CommonDose Apply the (un-)logged common age model after Galbraith to a given De distribution	ı et al. (1999)
---	-----------------

# **Description**

Function to calculate the common dose of a De distribution.

# Usage

```
calc_CommonDose(data, sigmab, log = TRUE, ...)
```

# **Arguments**

data	RLum.Results or data.frame (required): for data.frame: two columns with De (data[,1]) and De error (values[,2])
sigmab	numeric (with default): spread in De values given as a fraction (e.g. 0.2). This value represents the expected overdispersion in the data should the sample be well-bleached (Cunningham & Walling 2012, p. 100).
log	logical (with default): fit the (un-)logged common age model to De data
	currently not used.

# **Details**

# (Un-)logged model

When log = TRUE this function calculates the weighted mean of logarithmic De values. Each of the estimates is weighted by the inverse square of its relative standard error. The weighted mean is then transformed back to the dose scale (Galbraith & Roberts 2012, p. 14).

The log transformation is not applicable if the De estimates are close to zero or negative. In this case the un-logged model can be applied instead (log = FALSE). The weighted mean is then calculated using the un-logged estimates of De and their absolute standard error (Galbraith & Roberts 2012, p. 14).

# Value

Returns a terminal output. In addition an RLum. Results object is returned containing the following element:

summary data.frame summary of all relevant model results.

data data.frame original input data

args list used arguments call call the function call

The output should be accessed using the function get\_RLum

# **Function version**

```
0.1 (2015-08-21 14:53:14)
```

#### Author(s)

Christoph Burow, University of Cologne (Germany) R Luminescence Package Team

#### References

Galbraith, R.F. & Laslett, G.M., 1993. Statistical models for mixed fission track ages. Nuclear Tracks Radiation Measurements 4, 459-470.

Galbraith, R.F., Roberts, R.G., Laslett, G.M., Yoshida, H. & Olley, J.M., 1999. Optical dating of single grains of quartz from Jinmium rock shelter, northern Australia. Part I: experimental design and statistical models. Archaeometry 41, 339-364.

Galbraith, R.F. & Roberts, R.G., 2012. Statistical aspects of equivalent dose and error calculation and display in OSL dating: An overview and some recommendations. Quaternary Geochronology 11, 1-27.

# **Further reading**

Arnold, L.J. & Roberts, R.G., 2009. Stochastic modelling of multi-grain equivalent dose (De) distributions: Implications for OSL dating of sediment mixtures. Quaternary Geochronology 4, 204-230.

Bailey, R.M. & Arnold, L.J., 2006. Statistical modelling of single grain quartz De distributions and an assessment of procedures for estimating burial dose. Quaternary Science Reviews 25, 2475-2502.

Cunningham, A.C. & Wallinga, J., 2012. Realizing the potential of fluvial archives using robust OSL chronologies. Quaternary Geochronology 12, 98-106.

Rodnight, H., Duller, G.A.T., Wintle, A.G. & Tooth, S., 2006. Assessing the reproducibility and accuracy of optical dating of fluvial deposits. Quaternary Geochronology 1, 109-120.

Rodnight, H., 2008. How many equivalent dose values are needed to obtain a reproducible distribution?. Ancient TL 26, 3-10.

# See Also

```
calc_CentralDose, calc_FiniteMixture, calc_FuchsLang2001, calc_MinDose
```

# **Examples**

```
## load example data
data(ExampleData.DeValues, envir = environment())
## apply the common dose model
calc_CommonDose(ExampleData.DeValues$CA1)
```

# **Description**

This function calculates the cosmic dose rate taking into account the soft- and hard-component of the cosmic ray flux and allows corrections for geomagnetic latitude, altitude above sea-level and geomagnetic field changes.

# Usage

```
calc_CosmicDoseRate(depth, density, latitude, longitude, altitude,
  corr.fieldChanges = FALSE, est.age = NA, half.depth = FALSE,
  error = 10)
```

# **Arguments**

depth	numeric ( <b>required</b> ): depth of overburden (m). For more than one absorber use $c(depth_1, depth_2,, depth_n)$
density	numeric ( <b>required</b> ): average overburden density (g/cm^3). For more than one absorber use
	c(density_1,density_2,, density_n)
latitude	numeric (required): latitude (decimal degree), N positive
longitude	numeric (required): longitude (decimal degree), E positive
altitude	numeric (required): altitude (m above sea-level)
corr.fieldChanges	
	logical (with default): correct for geomagnetic field changes after Prescott & Hutton (1994). Apply only when justified by the data.
est.age	numeric (with default): estimated age range (ka) for geomagnetic field change correction (0-80 ka allowed)
half.depth	logical (with default): How to overcome with varying overburden thickness. If TRUE only half the depth is used for calculation. Apply only when justified, i.e. when a constant sedimentation rate can safely be assumed.
error	numeric (with default): general error (percentage) to be implemented on corrected cosmic dose rate estimate

# **Details**

This function calculates the total cosmic dose rate considering both the soft- and hard-component of the cosmic ray flux.

# **Internal calculation steps**

(1) Calculate total depth of all absorber in hg/cm<sup>2</sup> (1 hg/cm<sup>2</sup> = 100 g/cm<sup>2</sup>)

```
absorber = depth_1 * density_1 + depth_2 * density_2 + ... + depth_n * density_n
```

(2) If half.depth = TRUE

```
absorber = absorber/2
```

- (3) Calculate cosmic dose rate at sea-level and 55 deg. latitude
- a) If absorber is > 167 g/cm<sup>2</sup> (only hard-component; Allkofer et al. 1975): apply equation given by Prescott & Hutton (1994) (c.f. Barbouti & Rastin 1983)

$$D0 = C/(((absorber + d)^{\alpha} + a) * (absober + H)) * exp(-B * absorber)$$

- b) If absorber is < 167 g/cm<sup>2</sup> (soft- and hard-component): derive D0 from Fig. 1 in Prescott & Hutton (1988).
- (4) Calculate geomagnetic latitude (Prescott & Stephan 1982, Prescott & Hutton 1994)

```
\lambda = arcsin(0.203 * cos(latitude) * cos(longitude - 291) + 0.979 * sin(latitude))
```

(5) Apply correction for geomagnetic latitude and altitude above sea-level. Values for F, J and H were read from Fig. 3 shown in Prescott & Stephan (1982) and fitted with 3-degree polynomials for lambda < 35 degree and a linear fit for lambda > 35 degree.

$$Dc = D0 * (F + J * exp((altitude/1000)/H))$$

(6) Optional: Apply correction for geomagnetic field changes in the last 0-80 ka (Prescott & Hutton 1994). Correction and altitude factors are given in Table 1 and Fig. 1 in Prescott & Hutton (1994). Values for altitude factor were fitted with a 2-degree polynomial. The altitude factor is operated on the decimal part of the correction factor.

$$Dc' = Dc * correctionFactor$$

# Usage of depth and density

- (1) If only one value for depth and density is provided, the cosmic dose rate is calculated for exactly one sample and one absorber as overburden (i.e. depth\*density).
- (2) In some cases it might be useful to calculate the cosmic dose rate for a sample that is overlain by more than one absorber, e.g. in a profile with soil layers of different thickness and a distinct difference in density. This can be calculated by providing a matching number of values for depth and density (e.g. depth = c(1, 2), density = c(1.7, 2.4))
- (3) Another possibility is to calculate the cosmic dose rate for more than one sample of the same profile. This is done by providing more than one values for depth and only one for density. For example, depth = c(1, 2, 3), density = 1.7 will calculate the cosmic dose rate for three samples in 1, 2 and 3 m depth in a sediment of density 1.7 g/cm<sup>3</sup>.

# Value

Returns a terminal output. In addition an RLum.Results object is returned containing the following element:

summary data.frame summary of all relevant calculation results.

args list used arguments call call the function call

The output should be accessed using the function get\_RLum

#### **Function version**

0.5.2 (2015-08-21 14:53:14)

#### Note

Despite its universal use the equation to calculate the cosmic dose rate provided by Prescott & Hutton (1994) is falsely stated to be valid from the surface to 10<sup>4</sup> hg/cm<sup>2</sup> of standard rock. The original expression by Barbouti & Rastin (1983) only considers the muon flux (i.e. hard-component) and is by their own definition only valid for depths between 10-10<sup>4</sup> hg/cm<sup>2</sup>.

Thus, for near-surface samples (i.e. for depths <  $167 \text{ g/cm}^2$ ) the equation of Prescott & Hutton (1994) underestimates the total cosmic dose rate, as it neglects the influence of the soft-component of the cosmic ray flux. For samples at zero depth and at sea-level the underestimation can be as large as  $\sim 0.1 \text{ Gy/ka}$ . In a previous article, Prescott & Hutton (1988) give another approximation of Barbouti & Rastins equation in the form of

$$D = 0.21 * exp(-0.070 * absorber + 0.0005 * absorber^{2})$$

which is valid for depths between 150-5000 g/cm<sup>2</sup>. For shallower depths (< 150 g/cm<sup>2</sup>) they provided a graph (Fig. 1) from which the dose rate can be read.

As a result, this function employs the equation of Prescott & Hutton (1994) only for depths > 167 g/cm<sup>2</sup>, i.e. only for the hard-component of the cosmic ray flux. Cosmic dose rate values for depths < 167 g/cm<sup>2</sup> were obtained from the "AGE" programm (Gruen 2009) and fitted with a 6-degree polynomial curve (and hence reproduces the graph shown in Prescott & Hutton 1988). However, these values assume an average overburden density of 2 g/cm<sup>3</sup>.

It is currently not possible to obtain more precise cosmic dose rate values for near-surface samples as there is no equation known to the author of this function at the time of writing.

## Author(s)

Christoph Burow, University of Cologne (Germany) R Luminescence Package Team

#### References

Allkofer, O.C., Carstensen, K., Dau, W.D., Jokisch, H., 1975. Letter to the editor. The absolute cosmic ray flux at sea level. Journal of Physics G: Nuclear and Particle Physics 1, L51-L52.

Barbouti, A.I., Rastin, B.C., 1983. A study of the absolute intensity of muons at sea level and under various thicknesses of absorber. Journal of Physics G: Nuclear and Particle Physics 9, 1577-1595.

Crookes, J.N., Rastin, B.C., 1972. An investigation of the absolute intensity of muons at sea-level. Nuclear Physics B 39, 493-508.

Gruen, R., 2009. The "AGE" program for the calculation of luminescence age estimates. Ancient TL 27, 45-46.

Prescott, J.R., Hutton, J.T., 1988. Cosmic ray and gamma ray dosimetry for TL and ESR. Nuclear Tracks and Radiation Measurements 14,

223-227. Prescott, J.R., Hutton, J.T., 1994. Cosmic ray contributions to dose rates for luminescence and ESR dating: large depths and long-term time variations. Radiation Measurements 23, 497-500.

Prescott, J.R., Stephan, L.G., 1982. The contribution of cosmic radiation to the environmental dose for thermoluminescence dating. Latitude, altitude and depth dependences. PACT 6, 17-25.

36 calc\_FadingCorr

#### See Also

BaseDataSet.CosmicDoseRate

#### **Examples**

```
##(1) calculate cosmic dose rate (one absorber)
calc_CosmicDoseRate(depth = 2.78, density = 1.7,
                    latitude = 38.06451, longitude = 1.49646,
                    altitude = 364, error = 10)
##(2a) calculate cosmic dose rate (two absorber)
calc\_CosmicDoseRate(depth = c(5.0, 2.78), density = c(2.65, 1.7),
                    latitude = 38.06451, longitude = 1.49646,
                    altitude = 364, error = 10)
##(2b) calculate cosmic dose rate (two absorber) and
##correct for geomagnetic field changes
calc_CosmicDoseRate(depth = c(5.0, 2.78), density = c(2.65, 1.7),
                    latitude = 12.04332, longitude = 4.43243,
                    altitude = 364, corr.fieldChanges = TRUE,
                    est.age = 67, error = 15)
##(3) calculate cosmic dose rate and export results to .csv file
#calculate cosmic dose rate and save to variable
results<- calc_CosmicDoseRate(depth = 2.78, density = 1.7,</pre>
                              latitude = 38.06451, longitude = 1.49646,
                              altitude = 364, error = 10)
# the results can be accessed by
get_RLum(results, "summary")
#export results to .csv file - uncomment for usage
#write.csv(results, file = "c:/users/public/results.csv")
##(4) calculate cosmic dose rate for 6 samples from the same profile
      and save to .csv file
#calculate cosmic dose rate and save to variable
results<- calc_CosmicDoseRate(depth = c(0.1, 0.5, 2.1, 2.7, 4.2, 6.3),
                              density = 1.7, latitude = 38.06451,
                              longitude = 1.49646, altitude = 364,
                              error = 10)
#export results to .csv file - uncomment for usage
#write.csv(results, file = "c:/users/public/results_profile.csv")
```

calc\_FadingCorr

Apply a fading correction according to Huntley & Lamothe (2001) for a given g-value.

# **Description**

This function runs the iterations that are needed to calculate the corrected age including the error for a given g-value according to Huntley & Lamothe (2001).

calc\_FadingCorr 37

### **Usage**

```
calc_FadingCorr(g_value, tc, age.faded, n.MCruns = 10000, seed,
 txtProgressBar = TRUE)
```

## **Arguments**

g\_value vector (required): g-value and error obtained from separate fading measurements (see example) numeric (required): time in seconds (time between irradiation and the prompt tc measurement, cf. Huntely & Lamothe 2001) numeric vector (**required**): uncorrected age with error in ka (see example) age.faded n.MCruns integer (with default): number of Monte Carlo simulation runs for error estimation. If n.MCruns = 'auto' is used the function tries to find a 'stable' error for the age. Note: This may take a while! integer (optional): sets the seed for the random number generator in R using seed set.seed

txtProgressBar logical (with default): enables or disables txtProgressBar

### **Details**

The error of the fading-corrected age is determined using a Monte Carlo simulation approach. Solving of the equation is realised using uniroot. Large values for n.MCruns will significantly increase the computation time.

```
n.MCruns = 'auto'
```

The error estimation based on a stochastic process, i.e. for a small number of MC runs the calculated error varies considerably every time the function is called, even with the same input values. The argument option n.MCruns = 'auto' tries to find a stable value for the standard error, i.e. the standard deviation of values calculated during the MC runs (age.corr.MC), within a given precision (2 digits) by increasing the number of MC runs stepwise and calculating the corresponding error.

If the determined error does not differ from the 9 values calculated previously within a precision of (here) 3 digits the calculation is stopped as it is assumed that the error is stable. Please note that (a) the duration depends on the input values as well as on the provided computation ressources and it may take a while, (b) the length (size) of the output vector age.corr.MC, where all the single values produced during the MC runs are stored, equals the number of MC runs (here termed observations).

To avoid an endless loop the calculation is stopped if the number of observations exceeds 10^7. This limitation can be overwritten by setting the number of MC runs manually, e.g. n.MCruns = 10000001. Note: For this case the function is not checking whether the calculated error is stable.

### seed

This option allows to recreate previously calculated results by setting the seed for the R random number generator (see set.seed for details). This option should not be mixed up with the option n.MCruns = 'auto'. The results may appear similar, but they are not comparable!

## Value

Returns an S4 object of type RLum.Results. Slot data contains a list with the following struc-

\$ age.corr (data.frame)

- .. \$ age
- .. \$ age.error
- .. \$ age.faded
- .. \$ age.faded.error
- .. \$ g\_value
- .. \$ g\_value.error
- .. \$ tc
- .. \$ n.MCruns
- .. \$ observations
- .. \$ seed

\$ age.corr.MC (numeric)

Age.corr.MC contain all possible ages from the Monte Carlo (error) simulation.

## **Function version**

```
0.3.0 (2015-08-21 14:53:14)
```

## Note

The upper age limit is set to 500 ka!

## Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne R Luminescence Package Team

## References

Huntley, D.J., Lamothe, M., 2001. Ubiquity of anomalous fading in K-feldspars and the measurement and correction for it in optical dating. Canadian Journal of Earth Sciences, 38, 1093-1106.

# See Also

```
RLum.Results, get_RLum, uniroot
```

## **Examples**

 ${\tt calc\_FiniteMixture}$ 

Apply the finite mixture model (FMM) after Galbraith (2005) to a given De distribution

## **Description**

This function fits a k-component mixture to a De distribution with differing known standard errors. Parameters (doses and mixing proportions) are estimated by maximum likelihood assuming that the log dose estimates are from a mixture of normal distributions.

## Usage

```
calc_FiniteMixture(data, sigmab, n.components, grain.probability = FALSE,
  dose.scale, pdf.weight = TRUE, pdf.sigma = "sigmab",
  pdf.colors = "gray", pdf.scale, plot.proportions = TRUE, plot = TRUE,
  ...)
```

## **Arguments**

rg	guments	
	data	RLum.Results or data.frame ( <b>required</b> ): for data.frame: two columns with De (data[,1]) and De error (values[,2])
	sigmab	numeric ( <b>required</b> ): spread in De values given as a fraction (e.g. 0.2). This value represents the expected overdispersion in the data should the sample be well-bleached (Cunningham & Wallinga 2012, p. 100).
	n.components	numeric ( <b>required</b> ): number of components to be fitted. If a vector is provided (e.g. $c(2:8)$ ) the finite mixtures for 2, 3 8 components are calculated and a plot and a statistical evaluation of the model performance (BIC score and maximum log-likelihood) is provided.
grain.probability		
		logical (with default): prints the estimated probabilities of which component each grain is in
	dose.scale	$\begin{array}{l} \text{numeric: manually set the scaling of the $y$-axis of the first plot with a vector in the form of $c(\min,\max)$ } \end{array}$
	pdf.weight	logical (with default): weight the probability density functions by the components proportion (applies only when a vector is provided for n.components)
	pdf.sigma	character (with default): if "sigmab" the components normal distributions are plotted with a common standard deviation (i.e. sigmab) as assumed by the FFM. Alternatively, "se" takes the standard error of each component for the sigma parameter of the normal distribution
	pdf.colors	character (with default): color coding of the components in the the plot. Possible options are "gray", "colors" and "none"
	pdf.scale	<pre>numeric: manually set the max density value for proper scaling of the x-axis of the first plot</pre>
	plot.proportion	ns
		logical (with default): plot barplot showing the proportions of components
	plot	logical (with default): plot output
		further arguments to pass. See details for their usage.

## **Details**

This model uses the maximum likelihood and Bayesian Information Criterion (BIC) approaches.

Indications of overfitting are:

- increasing BIC
- repeated dose estimates
- covariance matrix not positive definite
- covariance matrix produces NaNs
- convergence problems

### Plot

If a vector (c(k.min:k.max)) is provided for n. components a plot is generated showing the the k components equivalent doses as normal distributions. By default pdf.weight is set to FALSE, so that the area under each normal distribution is always 1. If TRUE, the probability density functions are weighted by the components proportion for each iteration of k components, so the sum of areas of each component equals 1. While the density values are on the same scale when no weights are used, the y-axis are individually scaled if the probability density are weighted by the components proportion.

The standard deviation (sigma) of the normal distributions is by default determined by a common sigmab (see pdf.sigma). For pdf.sigma = "se" the standard error of each component is taken instead

The stacked barplot shows the proportion of each component (in per cent) calculated by the FFM. The last plot shows the achieved BIC scores and maximum log-likelihood estimates for each iteration of k.

### Value

Returns a plot (optional) and terminal output. In addition an RLum.Results object is returned containing the following elements:

summary data.frame summary of all relevant model results.

data data.frame original input data

args list used arguments
call call the function call

mle covariance matrices of the log likelhoods

BIC BIC score

11ik maximum log likelihood

grain.probability

probabilities of a grain belonging to a component

components matrix estimates of the de, de error and proportion for each component

single.comp data.frame single componente FFM estimate

If a vector for n.components is provided (e.g. c(2:8)), mle and grain.probability are lists containing matrices of the results for each iteration of the model.

The output should be accessed using the function get\_RLum

# **Function version**

```
0.4 (2015-08-21 14:53:14)
```

### Author(s)

Christoph Burow, University of Cologne (Germany) Based on a rewritten S script of Rex Galbraith, 2006.

R Luminescence Package Team

#### References

Galbraith, R.F. & Green, P.F., 1990. Estimating the component ages in a finite mixture. Nuclear Tracks and Radiation Measurements 17, 197-206.

Galbraith, R.F. & Laslett, G.M., 1993. Statistical models for mixed fission track ages. Nuclear Tracks Radiation Measurements 4, 459-470.

Galbraith, R.F. & Roberts, R.G., 2012. Statistical aspects of equivalent dose and error calculation and display in OSL dating: An overview and some recommendations. Quaternary Geochronology 11, 1-27.

Roberts, R.G., Galbraith, R.F., Yoshida, H., Laslett, G.M. & Olley, J.M., 2000. Distinguishing dose populations in sediment mixtures: a test of single-grain optical dating procedures using mixtures of laboratory-dosed quartz. Radiation Measurements 32, 459-465.

Galbraith, R.F., 2005. Statistics for Fission Track Analysis, Chapman & Hall/CRC, Boca Raton.

## **Further reading**

Arnold, L.J. & Roberts, R.G., 2009. Stochastic modelling of multi-grain equivalent dose (De) distributions: Implications for OSL dating of sediment mixtures. Quaternary Geochronology 4, 204-230.

Cunningham, A.C. & Wallinga, J., 2012. Realizing the potential of fluvial archives using robust OSL chronologies. Quaternary Geochronology 12, 98-106.

Rodnight, H., Duller, G.A.T., Wintle, A.G. & Tooth, S., 2006. Assessing the reproducibility and accuracy of optical dating of fluvial deposits. Quaternary Geochronology 1, 109-120.

Rodnight, H. 2008. How many equivalent dose values are needed to obtain a reproducible distribution?. Ancient TL 26, 3-10.

# See Also

```
calc_CentralDose, calc_CommonDose, calc_FuchsLang2001, calc_MinDose
```

### **Examples**

```
## show structure of the results
FMM

## show the results on equivalent dose, standard error and proportion of
## fitted components
get_RLum(object = FMM, data.object = "components")
```

calc\_FuchsLang2001

Apply the model after Fuchs & Lang (2001) to a given De distribution.

## **Description**

This function applies the method according to Fuchs & Lang (2001) for heterogeneously bleached samples with a given coefficient of variation threshold.

## Usage

```
calc_FuchsLang2001(data, cvThreshold = 5, startDeValue = 1, plot = TRUE,
    ...)
```

## **Arguments**

data	RLum.Results or data.frame ( <b>required</b> ): for data.frame: two columns with De (data[,1]) and De error (values[,2])
cvThreshold	<ul><li>numeric (with default): coefficient of variation in percent, as threshold for the method, e.g. cvThreshold = 3. See details.</li></ul>
startDeValue	numeric (with default): number of the first aliquot that is used for the calculations
plot	logical (with default): plot output TRUE/FALSE
	further arguments and graphical parameters passed to plot

## **Details**

### Used values

If the coefficient of variation (c[v]) of the first two values is larger than the threshold  $c[v\_threshold]$ , the first value is skipped. Use the startDeValue argument to define a start value for calculation (e.g. 2nd or 3rd value).

# Basic steps of the approach

- (1) Estimate natural relative variation of the sample using a dose recovery test
- (2) Sort the input values ascendingly
- (3) Calculate a running mean, starting with the lowermost two values and add values iteratively.
- (4) Stop if the calculated c[v] exceeds the specified cvThreshold

calc\_FuchsLang2001 43

### Value

Returns a plot (optional) and terminal output. In addition an RLum.Results object is returned containing the following elements:

summary data.frame summary of all relevant model results.

data data.frame original input data

args list used arguments
call call the function call

usedDeValues data.frame containing the used values for the calculation

## **Function version**

```
0.4.1 (2015-08-21 14:53:14)
```

## Note

Please consider the requirements and the constraints of this method (see Fuchs & Lang, 2001)

## Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) Christoph Burow, University of Cologne (Germany)
R Luminescence Package Team

### References

Fuchs, M. & Lang, A., 2001. OSL dating of coarse-grain fluvial quartz using single-aliquot protocols on sediments from NE Peloponnese, Greece. In: Quaternary Science Reviews 20, 783-787.

Fuchs, M. & Wagner, G.A., 2003. Recognition of insufficient bleaching by small aliquots of quartz for reconstructing soil erosion in Greece. Quaternary Science Reviews 22, 1161-1167.

### See Also

```
plot, calc_MinDose, calc_FiniteMixture, calc_CentralDose, calc_CommonDose, RLum.Results
```

# **Examples**

```
##load example data
data(ExampleData.DeValues, envir = environment())

##calculate De according to Fuchs & Lang (2001)
temp<- calc_FuchsLang2001(ExampleData.DeValues$BT998, cvThreshold = 5)</pre>
```

44 calc\_gSGC

cal	_	gSGC

Calculate De value based on the gSGC by Li et al., 2015

## **Description**

Function returns De value and De value error using the global standardised growth curve (gSGC) assumption proposed by Li et al., 2015 for OSL dating of sedimentary quartz

## Usage

```
calc_gSGC(data, gSGC.type = "0-250", gSGC.parameters, n.MC = 100,
  verbose = TRUE, plot = TRUE)
```

## **Arguments**

data data. frame (required): input data of prodiding the following columns: 'LnTn',

'LnTn.error', Lr1Tr1', 'Lr1Tr1.error', 'Dr1' Note: column names are not re-

quired the function, expect the input data in the given order

gSGC. type character (with default): define the function parameters that should be used for

the iteration procedure: Li et al., 2015 (Table 2) presented function parameters

for two dose ranges: "0-450" and "0-250"

gSGC.parameters

list (optional): option to provide own function parameters used for #' fitting as

named list. Nomenclature follows Li et al., 2015, i.e. list(A, A. error, D0, D0. error, c, c. error, Y

range requires a vector for the range the function is considered as valid, e.g.

range = c(0, 250)

Using this option overwrites the default parameter list of the gSGC, meaning the

argument gSGC. type will be without effect

n.MC integer (with default): number of Monte Carlo simulation runs for error esti-

mation, s. details.

verbose logical: enable or disable terminal output

plot logical: enable or disable graphical feedback as plot

## **Details**

The error of the De value is determined using a Monte Carlo simulation approach. Solving of the equation is realised using uniroot. Large values for n.MC will significantly increase the computation time.

### Value

 $Returns\ an\ S4\ object\ of\ type\ RLum.\ Results.\ Slot\ data\ contains\ a\ list\ with\ the\ following\ structure:$ 

- \$ De.value (data.frame)
- .. \$ De
- .. \$ De.error
- .. \$ Eta
- \$ De.MC (list) contains the matricies from the error estimation.
- \$ uniroot (list) contains the uniroot outputs of the De estimations

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## **Function version**

```
0.1 (2015-08-21 14:53:14)
```

## Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montagine (France)

R Luminescence Package Team

## References

Li, B., Roberts, R.G., Jacobs, Z., Li, S.-H., 2015. Potential of establishing a 'global standardised growth curve' (gSGC) for optical dating of quartz from sediments. Quaternary Geochronology 27, 94-104. doi:10.1016/j.quageo.2015.02.011

### See Also

```
RLum.Results, get_RLum, uniroot
```

# **Examples**

```
results <- calc_gSGC(data = data.frame(
LnTn = 2.361, LnTn.error = 0.087,
Lr1Tr1 = 2.744, Lr1Tr1.error = 0.091,
Dr1 = 34.4))
get_RLum(results, data.object = "De")</pre>
```

calc\_HomogeneityTest Apply a simple homogeneity test after Galbraith (2003)

## **Description**

A simple homogeneity test for De estimates

## Usage

```
calc_HomogeneityTest(data, log = TRUE, ...)
```

## **Arguments**

data	RLum.Results or data.frame ( <b>required</b> ): for data.frame: two columns with De (data[,1]) and De error (values[,2])
log	logical (with default): peform the homogeniety test with (un-)logged data
	further arguments (for internal compatibility only).

## **Details**

For details see Galbraith (2003).

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### Value

Returns a terminal output. In addition an RLum.Results object is returned containing the following element:

summary data.frame summary of all relevant model results.

data data.frame original input data

args list used arguments
call call the function call

The output should be accessed using the function get\_RLum

## **Function version**

```
0.2 (2015-08-21 14:53:14)
```

## Author(s)

```
Christoph Burow, University of Cologne (Germany)
R Luminescence Package Team
```

### References

Galbraith, R.F., 2003. A simple homogeneity test for estimates of dose obtained using OSL. Ancient TL 21, 75-77.

# See Also

```
pchisq
```

# **Examples**

```
## load example data
data(ExampleData.DeValues, envir = environment())
## apply the homogeneity test
calc_HomogeneityTest(ExampleData.DeValues$BT998)
```

calc\_IEU Apply the internal-external-uncertainty (IEU) model after Thomsen et al. (2007) to a given De distribution

# **Description**

Function to calculate the IEU De for a De data set.

# Usage

```
calc_IEU(data, a, b, interval, decimal.point = 2, plot = TRUE, ...)
```

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## **Arguments**

data	RLum.Results or data.frame ( <b>required</b> ): for data.frame: two columns with De (data[,1]) and De error (values[,2])
а	numeric: slope
b	numeric: intercept
interval	<pre>numeric: fixed interval (e.g. 5 Gy) used for iteration of Dbar, from the mean to Lowest.De used to create Graph.IEU [Dbar.Fixed vs Z]</pre>
decimal.point	<pre>numeric (with default): number of decimal points for rounding calculations (e.g. 2)</pre>
plot	logical (with default): plot output
• • •	further arguments (trace, verbose).

## **Details**

This function uses the equations of Thomsen et al. (2007). The parameters a and b are estimated from dose-recovery experiments.

### Value

Returns a plot (optional) and terminal output. In addition an RLum.Results object is returned containing the following element:

summary data.frame summary of all relevant model results.

data data.frame original input data

args list used arguments call call the function call

tables list a list of data frames containing all calculation tables

The output should be accessed using the function get\_RLum.

# **Function version**

```
0.1.0 (2015-08-21 14:53:14)
```

## Author(s)

Rachel Smedley, Geography & Earth Sciences, Aberystwyth University (United Kingdom) Based on an excel spreadsheet and accompanying macro written by Kristina Thomsen. R Luminescence Package Team

### References

Smedley, R.K., 2015. A new R function for the Internal External Uncertainty (IEU) model. Ancient TL 33, 16-21.

Thomsen, K.J., Murray, A.S., Boetter-Jensen, L. & Kinahan, J., 2007. Determination of burial dose in incompletely bleached fluvial samples using single grains of quartz. Radiation Measurements 42, 370-379.

## See Also

plot, calc\_CommonDose, calc\_CentralDose, calc\_FiniteMixture, calc\_FuchsLang2001, calc\_MinDose

48 calc\_MaxDose

## **Examples**

```
## load data
data(ExampleData.DeValues, envir = environment())
## apply the IEU model
ieu <- calc_IEU(ExampleData.DeValues$CA1, a = 0.2, b = 1.9, interval = 1)</pre>
```

calc\_MaxDose

Apply the maximum age model to a given De distribution

# Description

Function to fit the maximum age model to De data. This is a wrapper function that calls calc\_MinDose() and applies a similiar approach as described in Olley et al. (2006).

## Usage

```
calc_MaxDose(data, sigmab, log = TRUE, par = 3, bootstrap = FALSE,
  init.values, plot = TRUE, ...)
```

# **Arguments**

data	RLum.Results or data.frame (required): for data.frame: two columns with De (data[,1]) and De error (values[,2])
sigmab	numeric ( <b>required</b> ): spread in De values given as a fraction (e.g. 0.2). This value represents the expected overdispersion in the data should the sample be well-bleached (Cunningham & Walling 2012, p. 100).
log	logical (with default): fit the (un-)logged three parameter minimum dose model to De data
par	<pre>numeric (with default): apply the 3- or 4-parametric minimum age model (par=3 or par=4).</pre>
bootstrap	logical (with default): apply the recycled bootstrap approach of Cunningham & Wallinga (2012).
init.values	numeric (with default): starting values for gamma, sigma, p0 and mu. Custom values need to be provided in a vector of length three in the form of c(gamma, sigma, p0).
plot	logical (with default): plot output (TRUE/FALSE)
•••	further arguments for bootstrapping (bs.M, bs.N, bs.h,sigmab.sd). See details for their usage.

## **Details**

### **Data transformation**

To estimate the maximum dose population and its standard error, the three parameter minimum age model of Galbraith et al. (1999) is adapted. The measured De values are transformed as follows:

- 1. convert De values to natural logs
- 2. multiply the logged data to creat a mirror image of the De distribution

calc\_MaxDose 49

- 3. shift De values along x-axis by the smallest x-value found to obtain only positive values
- 4. combine in quadrature the measurement error associated with each De value with a relative error specified by sigmab
- 5. apply the MAM to these data

When all calculations are done the results are then converted as follows

- 1. subtract the x-offset
- 2. multiply the natural logs by -1
- 3. take the exponent to obtain the maximum dose estimate in Gy

### **Further documentation**

Please see calc\_MinDose.

## Value

Please see calc\_MinDose.

### **Function version**

0.3 (2015-08-21 14:53:14)

### Author(s)

Christoph Burow, University of Cologne (Germany) Based on a rewritten S script of Rex Galbraith, 2010

R Luminescence Package Team

### References

Arnold, L.J., Roberts, R.G., Galbraith, R.F. & DeLong, S.B., 2009. A revised burial dose estimation procedure for optical dating of young and modern-age sediments. Quaternary Geochronology 4, 306-325.

Galbraith, R.F. & Laslett, G.M., 1993. Statistical models for mixed fission track ages. Nuclear Tracks Radiation Measurements 4, 459-470.

Galbraith, R.F., Roberts, R.G., Laslett, G.M., Yoshida, H. & Olley, J.M., 1999. Optical dating of single grains of quartz from Jinmium rock shelter, northern Australia. Part I: experimental design and statistical models. Archaeometry 41, 339-364.

Galbraith, R.F., 2005. Statistics for Fission Track Analysis, Chapman & Hall/CRC, Boca Raton.

Galbraith, R.F. & Roberts, R.G., 2012. Statistical aspects of equivalent dose and error calculation and display in OSL dating: An overview and some recommendations. Quaternary Geochronology 11, 1-27.

Olley, J.M., Roberts, R.G., Yoshida, H., Bowler, J.M., 2006. Single-grain optical dating of grave-infill associated with human burials at Lake Mungo, Australia. Quaternary Science Reviews 25, 2469-2474.

### **Further reading**

Arnold, L.J. & Roberts, R.G., 2009. Stochastic modelling of multi-grain equivalent dose (De) distributions: Implications for OSL dating of sediment mixtures. Quaternary Geochronology 4, 204-230.

Bailey, R.M. & Arnold, L.J., 2006. Statistical modelling of single grain quartz De distributions and an assessment of procedures for estimating burial dose. Quaternary Science Reviews 25, 2475-2502.

Cunningham, A.C. & Wallinga, J., 2012. Realizing the potential of fluvial archives using robust OSL chronologies. Quaternary Geochronology 12, 98-106.

Rodnight, H., Duller, G.A.T., Wintle, A.G. & Tooth, S., 2006. Assessing the reproducibility and accuracy of optical dating of fluvial deposits. Quaternary Geochronology 1, 109-120.

Rodnight, H., 2008. How many equivalent dose values are needed to obtain a reproducible distribution? Ancient TL 26, 3-10.

## See Also

calc\_CentralDose, calc\_CommonDose, calc\_FiniteMixture, calc\_FuchsLang2001, calc\_MinDose

## **Examples**

```
## load example data
data(ExampleData.DeValues, envir = environment())
# apply the maximum dose model
calc_MaxDose(ExampleData.DeValues$CA1, sigmab = 0.2, par = 3)
```

calc\_MinDose

Apply the (un-)logged minimum age model (MAM) after Galbraith et al. (1999) to a given De distribution

# **Description**

Function to fit the (un-)logged three or four parameter minimum dose model (MAM-3/4) to De data.

# Usage

```
calc_MinDose(data, sigmab, log = TRUE, par = 3, bootstrap = FALSE,
  init.values, plot = TRUE, multicore = FALSE, ...)
```

## **Arguments**

data

RLum.Results or data.frame (**required**): for data.frame: two columns with De (data[ ,1]) and De error (values[ ,2])

sigmab numeric (**required**): spread in De values given as a fraction (e.g. 0.2). This

value represents the expected overdispersion in the data should the sample be

well-bleached (Cunningham & Walling 2012, p. 100).

log logical (with default): fit the (un-)logged minimum dose model to De data

par numeric (with default): apply the 3- or 4-parametric minimum age model (par=3

or par=4). The MAM-3 is used by default.

bootstrap logical (with default): apply the recycled bootstrap approach of Cunningham

& Wallinga (2012).

init.values numeric (optional): a named list with starting values for gamma, sigma, p0 and

 $mu\;(e.g.\;list(gamma=100\;sigma=1.5,\;p0=0.1,\;mu=100)).$  If no values are

provided reasonable values are tried to be estimated from the data.

plot logical (with default): plot output (TRUE/FALSE)

multicore logical (with default): enable parallel computation of the bootstrap by creating

a multicore SNOW cluster. Depending on the number of available logical CPU cores this will drastically reduce the computation time. Note that this option is

highly experimental and not work for all machines. (TRUE/FALSE)

... (optional) further arguments for bootstrapping (bs.M, bs.N, bs.h, sigmab.sd).

See details for their usage. Further arguments are verbose to de-/activate console output (logical), debug for extended console output (logical) and cores (integer) to manually specify the number of cores to be used when multicore=TRUE.

## **Details**

#### **Parameters**

This model has four parameters:

gamma: minimum dose on the log scale

mu: mean of the non-truncated normal distribution

sigma: spread in ages above the minimum p0: proportion of grains at gamma

If par=3 (default) the 3-parametric minimum age model is applied, where gamma=mu. For par=4 the 4-parametric model is applied instead.

# (Un-)logged model

In the original version of the three-parameter minimum dose model, the basic data are the natural logarithms of the De estimates and relative standard errors of the De estimates. This model will be applied if log=TRUE.

If log=FALSE, the modified un-logged model will be applied instead. This has essentially the same form as the original version. gamma and sigma are in Gy and gamma becomes the minimum true dose in the population.

While the original (logged) version of the mimimum dose model may be appropriate for most samples (i.e. De distributions), the modified (un-logged) version is specially designed for modern-age

and young samples containing negative, zero or near-zero De estimates (Arnold et al. 2009, p. 323).

#### Initial values & boundaries

The log likelihood calculations use the nlminb function for box-constrained optimisation using PORT routines. Accordingly, initial values for the four parameters can be specified via init.values. If no values are provided for init.values reasonable starting values are estimated from the input data. If the final estimates of gamma, mu, sigma and p0 are totally off target, consider providing custom starting values via init.values.

In contrast to previous versions of this function the boundaries for the individual model parameters can no longer be specified. Appropriate boundary are now hard-coded and are valid for all input data sets.

### **Bootstrap**

When bootstrap=TRUE the function applies the bootstrapping method as described in Wallinga & Cunningham (2012). By default, the minimum age model produces 1000 first level and 3000 second level bootstrap replicates (actually, the number of second level bootstrap replicates is three times the number of first level replicates unless specified otherwise). The uncertainty on sigmab is 0.04 by default. These values can be changed by using the arguments bs.M (first level replicates), bs.N (second level replicates) and sigmab.sd (error on sigmab). With bs.h the bandwidth of the kernel density estimate can be specified. By default, h is calculated as

$$h = (2 * \sigma_{DE})/\sqrt{n}$$

## Multicore support

This function supports parallel computing and can be activated by multicore=TRUE. By default, the number of available logical CPU cores is determined automatically, but can be changed with cores. The multicore support is only available when bootstrap=TRUE and spawns n R instances for each core to get MAM estimates for each of the N and M boostrap replicates. Note that this option is highly experimental and may or may not work for your machine. Also the performance gain increases for larger number of bootstrap replicates. Also note that with each additional core and hence R instance and depending on the number of bootstrap replicates the memory usage can significantly increase. Make sure that memory is always availabe, otherwise there will be a massive perfomance hit.

# Value

Returns a plot (optional) and terminal output. In addition an RLum.Results object is returned containing the following elements:

summary	data.frame summary of all relevant model results.
data	data.frame original input data
args	list used arguments
call	call the function call
mle	mle2 object containing the maximum log likelhood functions for all parameters
BIC	numeric BIC score
confint	data.frame confidence intervals for all parameters
profile	profile.mle2 the log likelihood profiles

bootstrap list bootstrap results

The output should be accessed using the function get\_RLum

#### **Function version**

0.4.1 (2015-08-21 14:53:14)

#### Note

The default starting values for gamma, mu, sigma and p0 may only be appropriate for some De data sets and may need to be changed for other data. This is especially true when the un-logged version is applied.

Also note that all R warning messages are suppressed when running this function. If the results seem odd consider re-running the model with debug=TRUE which provides extended console output and forwards all internal warning messages.

### Author(s)

Christoph Burow, University of Cologne (Germany)

Based on a rewritten S script of Rex Galbraith, 2010

The bootstrap approach is based on a rewritten MATLAB script of Alastair Cunningham.

Alastair Cunningham is thanked for his help in implementing and cross-checking the code.

R Luminescence Package Team

#### References

Arnold, L.J., Roberts, R.G., Galbraith, R.F. & DeLong, S.B., 2009. A revised burial dose estimation procedure for optical dating of young and modern-age sediments. Quaternary Geochronology 4, 306-325.

Galbraith, R.F. & Laslett, G.M., 1993. Statistical models for mixed fission track ages. Nuclear Tracks Radiation Measurements 4, 459-470.

Galbraith, R.F., Roberts, R.G., Laslett, G.M., Yoshida, H. & Olley, J.M., 1999. Optical dating of single grains of quartz from Jinmium rock shelter, northern Australia. Part I: experimental design and statistical models. Archaeometry 41, 339-364.

Galbraith, R.F., 2005. Statistics for Fission Track Analysis, Chapman & Hall/CRC, Boca Raton.

Galbraith, R.F. & Roberts, R.G., 2012. Statistical aspects of equivalent dose and error calculation and display in OSL dating: An overview and some recommendations. Quaternary Geochronology 11, 1-27.

## **Further reading**

Arnold, L.J. & Roberts, R.G., 2009. Stochastic modelling of multi-grain equivalent dose (De) distributions: Implications for OSL dating of sediment mixtures. Quaternary Geochronology 4, 204-230.

Bailey, R.M. & Arnold, L.J., 2006. Statistical modelling of single grain quartz De distributions and an assessment of procedures for estimating burial dose. Quaternary Science Reviews 25, 2475-2502.

Cunningham, A.C. & Wallinga, J., 2012. Realizing the potential of fluvial archives using robust

OSL chronologies. Quaternary Geochronology 12, 98-106.

Rodnight, H., Duller, G.A.T., Wintle, A.G. & Tooth, S., 2006. Assessing the reproducibility and accuracy of optical dating of fluvial deposits. Quaternary Geochronology 1, 109-120.

Rodnight, H., 2008. How many equivalent dose values are needed to obtain a reproducible distribution?. Ancient TL 26, 3-10.

### See Also

calc\_CentralDose, calc\_CommonDose, calc\_FiniteMixture, calc\_FuchsLang2001, calc\_MaxDose

## **Examples**

```
## Load example data
data(ExampleData.DeValues, envir = environment())
# (1) Apply the minimum age model with minimum required parameters.
# By default, this will apply the un-logged 3-parametric MAM.
calc_MinDose(data = ExampleData.DeValues$CA1, sigmab = 0.1)
# (2) Re-run the model, but save results to a variable and turn
# plotting of the log-likelihood profiles off.
mam <- calc_MinDose(data = ExampleData.DeValues$CA1,</pre>
                    sigmab = 0.1,
                    plot = FALSE)
# Show structure of the RLum.Results object
mam
# Show summary table that contains the most relevant results
res <- get_RLum(mam, "summary")</pre>
res
# Plot the log likelihood profiles retroactively, because before
\# we set plot = FALSE
plot_RLum.Results(mam)
# Plot the dose distribution in an abanico plot and draw a line
# at the minimum dose estimate
plot_AbanicoPlot(data = ExampleData.DeValues$CA1,
                 main = "3-parameter Minimum Age Model",
                 line = mam,polygon.col = "none",
                 hist = TRUE,
                 rug = TRUE,
                 summary = c("n", "mean", "mean.weighted", "median", "in.ci"),
                 centrality = res$de,
                 line.col = "red",
                 grid.col = "none",
                 line.label = paste0(round(res$de, 1), "\U00B1",
                                     round(res$de_err, 1), " Gy"),
                 bw = 0.1,
                 ylim = c(-25, 18),
                 summary.pos = "topleft",
```

calc\_OSLLxTxRatio 55

```
mtext = bquote("Parameters: " ~
                                   sigma[b] == .(get_RLum(mam, "args")$sigmab) ~ ", " ~
                                   gamma == .(round(log(res$de), 1)) ~ ", ~ " ~
                                   sigma == .(round(res$sig, 1)) \sim ", " \sim
                                   rho == .(round(res$p0, 2))))
# (3) Run the minimum age model with bootstrap
# NOTE: Bootstrapping is computationally intensive, which is why the
# following example is commented out. To run the examples just
# uncomment the code.
# (3.1) run the minimum age model with default values for bootstrapping
#calc_MinDose(data = ExampleData.DeValues$CA1,
              sigmab = 0.15,
#
              bootstrap = TRUE)
# (3.2) Bootstrap control parameters
#mam <- calc_MinDose(data = ExampleData.DeValues$CA1,</pre>
                     sigmab = 0.15,
#
#
                     bootstrap = TRUE,
#
                     bs.M = 300,
#
                     bs.N = 500,
#
                     bs.h = 4,
#
                     sigmab.sd = 0.06,
                     plot = FALSE)
# Plot the results
#plot_RLum(mam)
# save bootstrap results in a separate variable
#bs <- get_RLum(mam, "bootstrap")</pre>
# show structure of the bootstrap results
#str(bs, max.level = 2, give.attr = FALSE)
# print summary of minimum dose and likelihood pairs
#summary(bs$pairs$gamma)
# Show polynomial fits of the bootstrap pairs
#bs$poly.fits$poly.three
# Plot various statistics of the fit using the generic plot() function
#par(mfcol=c(2,2))
#plot(bs$poly.fits$poly.three, ask = FALSE)
# Show the fitted values of the polynomials
#summary(bs$poly.fits$poly.three$fitted.values)
```

calc\_OSLLxTxRatio

Calculate Lx/Tx ratio for CW-OSL curves

## **Description**

Calculate Lx/Tx ratios from a given set of CW-OSL curves.

56 calc\_OSLLxTxRatio

### Usage

calc\_OSLLxTxRatio(Lx.data, Tx.data, signal.integral, background.integral,
background.count.distribution = "non-poisson", sigmab)

## **Arguments**

Lx.data RLum.Data.Curve or data.frame (required): requires a CW-OSL shine down

curve (x = time, y = counts)

Tx.data RLum.Data.Curve or data.frame (optional): requires a CW-OSL shine down

curve (x = time, y = counts). If no input is given the Tx.data will be treated as

NA and no Lx/Tx ratio is calculated.

signal.integral

vector (required): vector with the limits for the signal integral.

background.integral

vector (required): vector with the bounds for the background integral.

background.count.distribution

character (with default): Sets the count distribution assumed for the error calculation. Possible arguments poisson or non-poisson. See details for further

information

sigmab numeric (optional): Option to set a manual value for the overdispersion (for

LnTx and TnTx), used for the Lx/Tx error calculation. The value should be provided as absolute squared count values, e.g. sigmab = c(300, 300). Note: If only one value is provided this value is taken for both (LnTx and TnTx) signals.

### **Details**

The integrity of the chosen values for the signal and background integral is checked by the function; the signal integral limits have to be lower than the background integral limits. If a vector is given as input instead of a data.frame, an artificial data.frame is produced. The error calculation is done according to Galbraith (2002).

## background.count.distribution

This argument allows selecting the distribution assumption that is used for the error calculation. According to Galbraith (2002, 2014) the background counts may be overdispersed (i.e. do not follow a poisson distribution, which is assumed for the photomultiplier counts). In that case (might be the normal case) it has to be accounted for the overdispersion by estimating  $\sigma^2$  (i.e. the overdispersion value). Therefore the relative standard error is calculated as:

(a) poisson

$$rse(\mu_S) \approx \sqrt{(Y_0 + Y_1/k^2)/Y_0 - Y_1/k}$$

(b) non-poisson

$$rse(\mu_S) \approx \sqrt{(Y_0 + Y_1/k^2 + \sigma^2(1 + 1/k))/Y_0 - Y_1/k}$$

Please note that when using the early background subtraction method in combination with the 'non-poisson' distribution argument, the corresponding Lx/Tx error may considerably increase due to a high sigmab value. Please check whether this is valid for your data set and if necessary consider to provide an own sigmab value using the corresponding argument sigmab.

calc\_OSLLxTxRatio 57

#### Value

Returns an S4 object of type RLum. Results. Slot data contains a list with the following structure: \$LxTx.table (data.frame) .. \$LnLx

- .. \$ LnLx.BG
- .. \$ TnTx
- .. \$ TnTx.BG
- .. \$ Net\_LnLx
- .. \$ Net\_LnLx.Error
- .. \$ Net\_TnTx.Error
- .. \$ LxTx
- .. \$ LxTx.Error
- \$ calc.parameters (list)
- .. \$ sigmab.LnTx
- .. \$ sigmab.TnTx
- .. \$ k

## **Function version**

```
0.5.1 (2015-08-21 14:53:14)
```

#### Note

The results of this function have been cross-checked with the Analyst (vers. 3.24b). Access to the results object via get\_RLum.

## Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

## References

 $\label{lem:condition} Duller, G., 2007. \ Analyst. \ http://www.nutech.dtu.dk/english/~/media/Andre_Universitetsenheder/Nutech/Produkter%20og%20services/Dosimetri/radiation_measurement_instruments/tl_osl_reader/Manuals/analyst_manual_v3_22b.ashx$ 

Galbraith, R.F., 2002. A note on the variance of a background-corrected OSL count. Ancient TL, 20 (2), 49-51.

Galbraith, R.F., 2014. A further note on the variance of a background-corrected OSL count. Ancient TL, 31 (2), 1-3.

# See Also

# **Examples**

58 calc\_SourceDoseRate

```
##get results object
get_RLum(results)
```

calc\_SourceDoseRate

Calculation of the source dose rate via the date of measurement

## **Description**

Calculating the dose rate of the irradiation source via the date of measurement based on: source calibration date, source dose rate, dose rate error. The function returns a data frame that provides the input argument dose\_rate for the function Second2Gray.

# Usage

```
calc_SourceDoseRate(measurement.date, calib.date, calib.dose.rate, calib.error,
  source.type = "Sr-90", dose.rate.unit = "Gy/s", predict = NULL)
```

## **Arguments**

measurement.date

character or Date (required): date of measurement in "YYYY-MM-DD". Exceptionally, if no value is provided, the date will be set to today. The argument can be provided as vector.

calib.date character or Date (required): date of source calibration in "YYYY-MM-DD"

calib.dose.rate

numeric (required): dose rate at date of calibration in Gy/s or Gy/min

numeric (required): error of dose rate at date of calibration Gy/s or Gy/min calib.error character (with default): specify irrdiation source (Sr-90 or Co-60 or Am-214), source.type

see details for further information

dose.rate.unit character (with default): specify dose rate unit for input (Gy/min or Gy/s), the

output is given in Gy/s as valid for the function Second2Gray

predict integer (with default): option allowing to predicit the dose rate of the source

> over time in days set by the provided value. Starting date is the value set with measurement.date, e.g., calc\_SourceDoseRate(...,predict = 100) cal-

culates the source dose rate for the next 100 days.

### **Details**

Calculation of the source dose rate based on the time elapsed since the last calibration of the irradiation source. Decay parameters assume a Sr-90 beta source.

$$dose.rate = D0 * exp(-log(2)/T.1/2 * t)$$

with: D0 <- calibration dose rate T.1/2 <- half-life of the source nuclide (here in days) t <- time since source calibration (in days) log(2) / T.1/2 equals the decay constant lambda

Information on the date of measurements may be taken from the data's original .BIN file (using e.g., BINfile <- readBIN2R() and the slot BINfile@METADATA\$DATE)

## Allowed source types and related values

calc\_SourceDoseRate 59

#	Source type	T.1/2	Reference
[1]	Sr-90	28.90 y	NNDC, Brookhaven National Laboratory
[2]	Am-214	432.6 y	NNDC, Brookhaven National Laboratory
[3]	Co-60	5.274 y	NNDC, Brookhaven National Laboratory

## Value

Returns an S4 object of type RLum.Results. Slot data contains a list with the following structure:

\$ dose.rate (data.frame)

- .. \$ dose.rate
- .. \$ dose.rate.error
- .. \$ date (corresponding measurement date)
- \$ parameters (list)
- .. \$ source.type
- .. \$ halflife
- .. \$ dose.rate.unit

\$ call (the original function call)

The output should be accessed using the function get\_RLum. A plot method of the output is provided via plot\_RLum

## **Function version**

0.3.0 (2015-08-30 16:29:29)

## Note

Please be careful when using the option predict, especially when a multiple set for measurement.date and calib.date is provided. For the source dose rate prediction the function takes the last value measurement.date and predicts from that the source source dose rate for the number of days requested, means: the (multiple) orignal input will be replaced. However, the function do not change entries for the calibration dates, but mix them up. Therefore, it is not recommended to use this option when multiple calibration dates (calib.date) are provided.

# Author(s)

Margret C. Fuchs, HZDR, Helmholtz-Institute Freiberg for Resource Technology (Germany), Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

## References

 $NNDC, Brookhaven\ National\ Laboratory\ (http://www.nndc.bnl.gov/)$ 

# See Also

Second2Gray, get\_RLum, plot\_RLum

60 calc\_Statistics

### **Examples**

```
##(1) Simple function usage
##Basic calculation of the dose rate for a specific date
dose.rate <- calc_SourceDoseRate(measurement.date = "2012-01-27",</pre>
                                   calib.date = "2014-12-19",
                                   calib.dose.rate = 0.0438,
                                   calib.error = 0.0019)
##show results
get_RLum(dose.rate)
##(2) Usage in combination with another function (e.g., Second2Gray() )
## load example data
data(ExampleData.DeValues, envir = environment())
## use the calculated variable dose.rate as input argument
## to convert De(s) to De(Gy)
Second2Gray(ExampleData.DeValues$BT998, dose.rate)
##(3) source rate prediction and plotting
dose.rate <- calc_SourceDoseRate(measurement.date = "2012-01-27",</pre>
                                   calib.date = "2014-12-19",
                                   calib.dose.rate = 0.0438,
                                   calib.error = 0.0019,
                                   predict = 1000)
plot_RLum(dose.rate)
##(4) export output to a LaTeX table (example using the package 'xtable')
## Not run:
xtable::xtable(get_RLum(dose.rate))
## End(Not run)
```

calc\_Statistics

Function to calculate statistic measures

# **Description**

This function calculates a number of descriptive statistics for De-data, most fundamentally using error-weighted approaches.

## Usage

```
calc_Statistics(data, weight.calc = "square", na.rm = TRUE)
```

# Arguments

data data.frame or RLum.Results object (required): for data.frame two columns: De (data[,1]) and De error (data[,2]). To plot several data sets in one plot

the data sets must be provided as list, e.g. list(data.1, data.2).

weight.calc character: type of weight calculation. One out of "reciprocal" (weight is

1/error), "square" (weight is 1/error^2). Default is "square".

calc\_TLLxTxRatio 61

na.rm

logical (with default): indicating whether NA values should be stripped before the computation proceeds.

## Value

Returns a list with weighted and unweighted statistic measures.

## **Function version**

```
0.1.3 (2015-08-21 14:53:14)
```

## Author(s)

```
Michael Dietze, GFZ Potsdam (Germany)
R Luminescence Package Team
```

# **Examples**

calc\_TLLxTxRatio

Calculate the Lx/Tx ratio for a given set of TL curves [beta version]

# Description

Calculate Lx/Tx ratio for a given set of TL curves.

## Usage

```
calc_TLLxTxRatio(Lx.data.signal, Lx.data.background, Tx.data.signal,
   Tx.data.background, signal.integral.min, signal.integral.max)
```

# **Arguments**

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## **Details**

-

## Value

Returns an S4 object of type RLum. Results. Slot data contains a list with the following structure:

- \$ LxTx.table
- .. \$ LnLx
- .. \$ LnLx.BG
- .. \$ TnTx
- .. \$ TnTx.BG
- .. \$ Net\_LnLx
- .. \$ Net\_LnLx.Error

# **Function version**

```
0.3.0 (2015-08-21 14:53:14)
```

## Note

## This function has still BETA status!

## Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne #' (France), Christoph Schmidt, University of Bayreuth (Germany)
R Luminescence Package Team

## References

-

## See Also

```
RLum.Results, analyse_SAR.TL
```

CW2pHMi 63

### **Examples**

```
##load package example data
 data(ExampleData.BINfileData, envir = environment())
 ##convert Risoe.BINfileData into a curve object
 temp <- Risoe.BINfileData2RLum.Analysis(TL.SAR.Data, pos = 3)</pre>
 Lx.data.signal <- get_RLum(temp, record.id=1)</pre>
 Lx.data.background <- get_RLum(temp, record.id=2)</pre>
 Tx.data.signal <- get_RLum(temp, record.id=3)</pre>
 Tx.data.background <- get_RLum(temp, record.id=4)</pre>
 signal.integral.min <- 210
 signal.integral.max <- 230</pre>
 output <- calc_TLLxTxRatio(Lx.data.signal,</pre>
                              Lx.data.background,
                              Tx.data.signal, Tx.data.background,
                              signal.integral.min, signal.integral.max)
 get_RLum(output)
CW2pHMi
                           Transform a CW-OSL curve into a pHM-OSL curve via interpolation
```

## **Description**

This function transforms a conventionally measured continuous-wave (CW) OSL-curve to a pseudo hyperbolic modulated (pHM) curve under hyperbolic modulation conditions using the interpolation procedure described by Bos & Wallinga (2012).

under hyperbolic modulation conditions

## Usage

```
CW2pHMi(values, delta)
```

# **Arguments**

 ${\tt values} \qquad \qquad {\tt RLum.Data.Curve\ or\ data.frame\ (\textbf{required}):\ RLum.Data.Curve\ or\ data.frame}$ 

with measured curve data of type stimulation time (t) (values[,1]) and mea-

sured counts (cts) (values[,2]).

delta vector (optional): stimulation rate parameter, if no value is given, the optimal

value is estimated automatically (see details). Smaller values of delta produce

more points in the rising tail of the curve.

## **Details**

The complete procedure of the transformation is described in Bos & Wallinga (2012). The input data. frame consists of two columns: time (t) and count values (CW(t))

## **Internal transformation steps**

64 CW2pHMi

- (1) log(CW-OSL) values
- (2) Calculate t' which is the transformed time:

$$t' = t - (1/\delta) * log(1 + \delta * t)$$

- (3) Interpolate CW(t'), i.e. use the log(CW(t)) to obtain the count values for the transformed time
- (t'). Values beyond min(t) and max(t) produce NA values.
- (4) Select all values for t' < min(t), i.e. values beyond the time resolution of t. Select the first two values of the transformed data set which contain no NA values and use these values for a linear fit using 1m.
- (5) Extrapolate values for t' < min(t) based on the previously obtained fit parameters.
- (6) Transform values using

$$pHM(t) = (\delta * t/(1 + \delta * t)) * c * CW(t')$$
 
$$c = (1 + \delta * P)/\delta * P$$
 
$$P = length(stimulation\ period)$$

(7) Combine all values and truncate all values for t' > max(t)

The number of values for  $t' < \min(t)$  depends on the stimulation rate parameter delta. To avoid the production of too many artificial data at the raising tail of the determined pHM curve, it is recommended to use the automatic estimation routine for delta, i.e. provide no value for delta.

## Value

The function returns the same data type as the input data type with the transformed curve values.

package Neum object with two additional info ciements.

\$CW2pHMi.x.t : transformed time values \$CW2pHMi.method : used method for the production of the new data points

list(list("data.frame"))

with four columns:

\$x : time

\$y.t : transformed count values\$x.t : transformed time values

\$method : used method for the production of the new data points

## **Function version**

0.2.2 (2015-08-21 14:53:14)

## Note

According to Bos & Wallinga (2012), the number of extrapolated points should be limited to avoid artificial intensity data. If delta is provided manually and more than two points are extrapolated, a

CW2pHMi 65

warning message is returned.

The function approx may produce some Inf and NaN data. The function tries to manually interpolate these values by calculating the mean using the adjacent channels. If two invalid values are succeeding, the values are removed and no further interpolation is attempted. In every case a warning message is shown.

## Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France)

Based on comments and suggestions from: Adrie J.J. Bos, Delft University of Technology, The Netherlands

R Luminescence Package Team

## References

Bos, A.J.J. & Wallinga, J., 2012. How to visualize quartz OSL signal components. Radiation Measurements, 47, 752-758.

## **Further Reading**

Bulur, E., 1996. An Alternative Technique For Optically Stimulated Luminescence (OSL) Experiment. Radiation Measurements, 26, 701-709.

Bulur, E., 2000. A simple transformation for converting CW-OSL curves to LM-OSL curves. Radiation Measurements, 32, 141-145.

## See Also

```
CW2pLM, CW2pLMi, CW2pPMi, fit_LMCurve, lm, RLum.Data.Curve
```

## **Examples**

66 CW2pLM

```
,"ID"]
curve.HIGH<-CWOSL.SAR.Data@METADATA[CWOSL.SAR.Data@METADATA[,"ID"]==curve.ID[1]</pre>
                                      ,"HIGH"]
curve.NPOINTS<-CWOSL.SAR.Data@METADATA[CWOSL.SAR.Data@METADATA[,"ID"]==curve.ID[1]</pre>
                                         ,"NPOINTS"]
##combine curve to data set
curve<-data.frame(x = seq(curve.HIGH/curve.NPOINTS,curve.HIGH,</pre>
                           by = curve.HIGH/curve.NPOINTS),
                   y=unlist(CWOSL.SAR.Data@DATA[curve.ID[1]]))
##transform values
curve.transformed <- CW2pHMi(curve)</pre>
##plot curve
plot(curve.transformed$x, curve.transformed$y.t, log = "x")
##(3) - produce Fig. 4 from Bos & Wallinga (2012)
##load data
data(ExampleData.CW_OSL_Curve, envir = environment())
values <- CW_Curve.BosWallinga2012</pre>
##open plot area
plot(NA, NA,
     xlim=c(0.001,10),
     ylim=c(0,8000),
     ylab="pseudo OSL (cts/0.01 s)",
     xlab="t [s]",
     log="x",
     main="Fig. 4 - Bos & Wallinga (2012)")
values.t<-CW2pLMi(values, P=1/20)</pre>
lines(values[1:length(values.t[,1]),1],CW2pLMi(values, P=1/20)[,2],\\
      col="red" ,lwd=1.3)
text(0.03,4500,"LM", col="red",cex=.8)
values.t<-CW2pHMi(values, delta=40)</pre>
lines(values[1:length(values.t[,1]),1],CW2pHMi(values, delta=40)[,2],
      col="black", lwd=1.3)
```

lines(values[1:length(values.t[,1]),1],CW2pPMi(values, P=1/10)[,2],

text(0.005,3000,"HM", cex=.8)

values.t<-CW2pPMi(values, P=1/10)</pre>

col="blue", lwd=1.3)
text(0.5,6500,"PM", col="blue" ,cex=.8)

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## **Description**

Transforms a conventionally measured continuous-wave (CW) curve into a pseudo linearly modulated (pLM) curve using the equations given in Bulur (2000).

## Usage

```
CW2pLM(values)
```

# **Arguments**

values

RLum.Data.Curve or data.frame (**required**): RLum.Data.Curve data object. Alternatively, a data.frame of the measured curve data of type stimulation time (t) (values[,1]) and measured counts (cts) (values[,2]) can be provided.

## **Details**

According to Bulur (2000) the curve data are transformed by introducing two new parameters P (stimulation period) and u (transformed time):

$$P = 2 * max(t)$$

$$u = \sqrt{(2 * t * P)}$$

The new count values are then calculated by

$$ctsNEW = cts(u/P)$$

and the returned data. frame is produced by: data.frame(u,ctsNEW)

## Value

The function returns the same data type as the input data type with the transformed curve values.

## **Function version**

```
0.4.1 (2015-08-21 14:53:14)
```

## Note

The transformation is recommended for curves recorded with a channel resolution of at least 0.05 s/channel.

## Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

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#### References

Bulur, E., 2000. A simple transformation for converting CW-OSL curves to LM-OSL curves. Radiation Measurements, 32, 141-145.

## **Further Reading**

Bulur, E., 1996. An Alternative Technique For Optically Stimulated Luminescence (OSL) Experiment. Radiation Measurements, 26, 701-709.

### See Also

```
CW2pHMi, CW2pLMi, CW2pPMi, fit_LMCurve, lm, RLum.Data.Curve
The output of the function can be further used for LM-OSL fitting: CW2pLMi, CW2pHMi, CW2pPMi, fit_LMCurve, RLum.Data.Curve, plot_RLum
```

## **Examples**

CW2pLMi

Transform a CW-OSL curve into a pLM-OSL curve via interpolation under linear modulation conditions

## Description

Transforms a conventionally measured continuous-wave (CW) OSL-curve into a pseudo linearly modulated (pLM) curve under linear modulation conditions using the interpolation procedure described by Bos & Wallinga (2012).

## Usage

```
CW2pLMi(values, P)
```

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## **Arguments**

values RLum.Data.Curve or data.frame (**required**): RLum.Data.Curve or data.frame

with measured curve data of type stimulation time (t) (values[,1]) and mea-

sured counts (cts) (values[,2])

P vector (optional): stimulation time in seconds. If no value is given the optimal

value is estimated automatically (see details). Greater values of P produce more

points in the rising tail of the curve.

## **Details**

The complete procedure of the transformation is given in Bos & Wallinga (2012). The input data. frame consists of two columns: time (t) and count values (CW(t))

### Nomenclature

P = stimulation time (s) 1/P = stimulation rate (1/s)

## **Internal transformation steps**

- (1) log(CW-OSL) values
- (2) Calculate t' which is the transformed time:

$$t' = 1/2 * 1/P * t^2$$

- (3) Interpolate CW(t'), i.e. use the log(CW(t)) to obtain the count values for the transformed time
- (t'). Values beyond min(t) and max(t) produce NA values.
- (4) Select all values for t' < min(t), i.e. values beyond the time resolution of t. Select the first two values of the transformed data set which contain no NA values and use these values for a linear fit using 1m.
- (5) Extrapolate values for t' < min(t) based on the previously obtained fit parameters.
- (6) Transform values using

$$pLM(t) = t/P * CW(t')$$

(7) Combine values and truncate all values for t' > max(t)

The number of values for  $t' < \min(t)$  depends on the stimulation period (P) and therefore on the stimulation rate 1/P. To avoid the production of too many artificial data at the raising tail of the determined pLM curves it is recommended to use the automatic estimation routine for P, i.e. provide no own value for P.

## Value

The function returns the same data type as the input data type with the transformed curve values.

list(list("RLum.Data.Curve"))

package RLum object with two additional info elements:

70 CW2pLMi

```
$CW2pLMi.x.t : transformed time values
```

\$CW2pLMi.method : used method for the production of the new data points

## **Function version**

```
0.3.1 (2015-08-21 14:53:14)
```

### Note

According to Bos & Wallinga (2012) the number of extrapolated points should be limited to avoid artificial intensity data. If P is provided manually and more than two points are extrapolated, a warning message is returned.

## Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne

Based on comments and suggestions from:

Adrie J.J. Bos, Delft University of Technology, The Netherlands

R Luminescence Package Team

### References

Bos, A.J.J. & Wallinga, J., 2012. How to visualize quartz OSL signal components. Radiation Measurements, 47, 752-758.

## **Further Reading**

Bulur, E., 1996. An Alternative Technique For Optically Stimulated Luminescence (OSL) Experiment. Radiation Measurements, 26, 701-709.

Bulur, E., 2000. A simple transformation for converting CW-OSL curves to LM-OSL curves. Radiation Measurements, 32, 141-145.

# See Also

```
CW2pLM, CW2pHMi, CW2pPMi, fit_LMCurve, RLum.Data.Curve
```

# **Examples**

```
##(1)
##load CW-OSL curve data
data(ExampleData.CW_OSL_Curve, envir = environment())
##transform values
values.transformed <- CW2pLMi(ExampleData.CW_OSL_Curve)
##plot
plot(values.transformed$x, values.transformed$y.t, log = "x")
##(2) - produce Fig. 4 from Bos & Wallinga (2012)
##load data
data(ExampleData.CW_OSL_Curve, envir = environment())
values <- CW_Curve.BosWallinga2012</pre>
```

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```
##open plot area
plot(NA, NA,
     xlim = c(0.001, 10),
     ylim = c(0,8000),
     ylab = "pseudo OSL (cts/0.01 s)",
     xlab = "t [s]",
     log = "x",
     main = "Fig. 4 - Bos & Wallinga (2012)")
values.t <- CW2pLMi(values, P = 1/20)</pre>
lines(values[1:length(values.t[,1]),1],CW2pLMi(values, P = 1/20)[,2],
      col = "red", lwd = 1.3)
text(0.03,4500,"LM", col = "red", cex = .8)
values.t <- CW2pHMi(values, delta = 40)</pre>
lines(values[1:length(values.t[,1]),1],CW2pHMi(values, delta = 40)[,2],
      col = "black", lwd = 1.3)
text(0.005,3000,"HM", cex =.8)
values.t <- CW2pPMi(values, P = 1/10)</pre>
lines(values[1:length(values.t[,1]),1], CW2pPMi(values, P = 1/10)[,2],
      col = "blue", lwd = 1.3)
text(0.5,6500,"PM", col = "blue", cex = .8)
```

CW2pPMi

Transform a CW-OSL curve into a pPM-OSL curve via interpolation under parabolic modulation conditions

# **Description**

Transforms a conventionally measured continuous-wave (CW) OSL-curve into a pseudo parabolic modulated (pPM) curve under parabolic modulation conditions using the interpolation procedure described by Bos & Wallinga (2012).

## Usage

```
CW2pPMi(values, P)
```

# **Arguments**

values

RLum.Data.Curve or data.frame (**required**): RLum.Data.Curve or data.frame with measured curve data of type stimulation time (t) (values[,1]) and measured counts (cts) (values[,2])

Ρ

vector (optional): stimulation period in seconds. If no value is given, the optimal value is estimated automatically (see details). Greater values of P produce more points in the rising tail of the curve.

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### **Details**

The complete procedure of the transformation is given in Bos & Wallinga (2012). The input data. frame consists of two columns: time (t) and count values (CW(t))

### **Nomenclature**

```
P = stimulation time (s)
1/P = stimulation rate (1/s)
```

## **Internal transformation steps**

- (1) log(CW-OSL) values
- (2) Calculate t' which is the transformed time:

$$t' = (1/3) * (1/P^2)t^3$$

- (3) Interpolate CW(t'), i.e. use the log(CW(t)) to obtain the count values for the transformed time
- (t'). Values beyond min(t) and max(t) produce NA values.
- (4) Select all values for t' < min(t), i.e. values beyond the time resolution of t. Select the first two values of the transformed data set which contain no NA values and use these values for a linear fit using 1m.
- (5) Extrapolate values for t' < min(t) based on the previously obtained fit parameters. The extrapolation is limited to two values. Other values at the beginning of the transformed curve are set to 0.
- (6) Transform values using

$$pLM(t) = t^2/P^2 * CW(t')$$

(7) Combine all values and truncate all values for t' > max(t)

The number of values for  $t' < \min(t)$  depends on the stimulation period P. To avoid the production of too many artificial data at the raising tail of the determined pPM curve, it is recommended to use the automatic estimation routine for P, i.e. provide no value for P.

## Value

The function returns the same data type as the input data type with the transformed curve values.

\$CW2pPMi.x.t : transformed time values \$CW2pPMi.method : used method for the production of the new data points

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\$x: time

\$y.t : transformed count values\$x.t : transformed time values

\$method : used method for the production of the new data points

#### **Function version**

```
0.2.1 (2015-08-21 14:53:14)
```

#### Note

According to Bos & Wallinga (2012), the number of extrapolated points should be limited to avoid artificial intensity data. If P is provided manually, not more than two points are extrapolated.

## Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France)

Based on comments and suggestions from:

Adrie J.J. Bos, Delft University of Technology, The Netherlands

R Luminescence Package Team

#### References

Bos, A.J.J. & Wallinga, J., 2012. How to visualize quartz OSL signal components. Radiation Measurements, 47, 752-758.

#### **Further Reading**

Bulur, E., 1996. An Alternative Technique For Optically Stimulated Luminescence (OSL) Experiment. Radiation Measurements, 26, 701-709.

Bulur, E., 2000. A simple transformation for converting CW-OSL curves to LM-OSL curves. Radiation Measurements, 32, 141-145.

#### See Also

```
CW2pLM, CW2pLMi, CW2pHMi, fit_LMCurve, RLum.Data.Curve
```

```
##(1)
##load CW-OSL curve data
data(ExampleData.CW_OSL_Curve, envir = environment())
##transform values
values.transformed <- CW2pPMi(ExampleData.CW_OSL_Curve)
##plot
plot(values.transformed$x,values.transformed$y.t, log = "x")
##(2) - produce Fig. 4 from Bos & Wallinga (2012)
##load data</pre>
```

```
data(ExampleData.CW_OSL_Curve, envir = environment())
values <- CW_Curve.BosWallinga2012</pre>
##open plot area
plot(NA, NA,
     xlim = c(0.001, 10),
     ylim = c(0,8000),
     ylab = "pseudo OSL (cts/0.01 s)",
     xlab = "t [s]",
     log = "x",
     main = "Fig. 4 - Bos & Wallinga (2012)")
values.t <- CW2pLMi(values, P = 1/20)</pre>
lines(values[1:length(values.t[,1]),1],CW2pLMi(values, P = 1/20)[,2],
      col = "red", lwd = 1.3)
text(0.03,4500,"LM", col = "red", cex = .8)
values.t <- CW2pHMi(values, delta = 40)</pre>
lines(values[1:length(values.t[,1]),1], CW2pHMi(values, delta = 40)[,2],
      col = "black", lwd = 1.3)
text(0.005,3000,"HM", cex = .8)
values.t <- CW2pPMi(values, P = 1/10)</pre>
lines(values[1:length(values.t[,1]),1], CW2pPMi(values, P = 1/10)[,2],
      col = "blue", lwd = 1.3)
text(0.5,6500,"PM", col = "blue", cex = .8)
```

ExampleData.BINfileData

Example data from a SAR OSL and SAR TL measurement for the package Luminescence

## **Description**

Example data from a SAR OSL and TL measurement for package Luminescence directly extracted from a Risoe BIN-file and provided in an object of type Risoe.BINfileData-class

### **Format**

```
CWOSL.SAR.Data: SAR OSL measurement data TL.SAR.Data: SAR TL measurement data
```

Each class object contains two slots: (a) METADATA is a data.frame with all metadata stored in the BIN file of the measurements and (b) DATA contains a list of vectors of the measured data (usually count values).

## Version

0.1

#### Note

Please note that this example data cannot be exported to a BIN-file using the function writeR2BIN as it was generated and implemented in the package long time ago. In the meantime the BIN-file format changed.

### CWOSL.SAR.Data

Lab: Luminescence Laboratory Bayreuth

Lab-Code: BT607

Location: Saxony/Germany

Material: Middle grain quartz measured

on aluminum cups on a Risoe TL/OSL DA-15 reader

Reference: unpublished

### TL.SAR.Data

Lab: Luminescence Laboratory of Cologne

Lab-Code: LP1\_5 Location: Spain Material: Flint

Setup: Risoe TL/OSL DA-20 reader

(Filter: Semrock Brightline,

HC475/50, N2, unpolished steel discs)

Reference: unpublished

Remarks: dataset limited to one position

#### References

CWOSL.SAR.Data: unpublished data

TL.SAR.Data: unpublished data

## **Examples**

##show first 5 elements of the METADATA and DATA elements in the terminal
data(ExampleData.BINfileData, envir = environment())
CWOSL.SAR.Data@METADATA[1:5,]
CWOSL.SAR.Data@DATA[1:5]

ExampleData.CW\_OSL\_Curve

Example CW-OSL curve data for the package Luminescence

## **Description**

data.frame containing CW-OSL curve data (time, counts)

#### **Format**

Data frame with 1000 observations on the following 2 variables:

list("x") a numeric vector, time
list("y") a numeric vector, counts

# $Example Data. CW\_OSL\_Curve$

Lab: Luminescence Laboratory Bayreuth

Lab-Code: BT607

Location: Saxony/Germany

Material: Middle grain quartz measured on aluminum cups on a Risoe TL/OSL DA-15 reader.

Reference: unpublished data

## CW\_Curve.BosWallinga2012

Lab: Netherlands Centre for Luminescence Dating (NCL)

Lab-Code: NCL-2108077

Location: Guadalentin Basin, Spain Material: Coarse grain quartz

Reference: Bos & Wallinga (2012) and Baartman et al. (2011)

## References

Baartman, J.E.M., Veldkamp, A., Schoorl, J.M., Wallinga, J., Cammeraat, L.H., 2011. Unravelling Late Pleistocene and Holocene landscape dynamics: The Upper Guadalentin Basin, SE Spain. Geomorphology, 125, 172-185.

Bos, A.J.J. & Wallinga, J., 2012. How to visualize quartz OSL signal components. Radiation Measurements, 47, 752-758.

## **Examples**

```
data(ExampleData.CW_OSL_Curve, envir = environment())
plot(ExampleData.CW_OSL_Curve)
```

ExampleData.DeValues Example De data sets for the package Luminescence

### **Description**

Equivalent dose (De) values measured for a fine grain quartz sample from a loess section in Rottewitz (Saxony/Germany) and for a coarse grain quartz sample from a fluvial deposit in the rock shelter of Cueva Anton (Murcia/Spain).

## Usage

ExampleData.DeValues

## Format

A list with two elements, each containing a two column data.frame:

\$BT998: De and De error values for a fine grain quartz sample from a loess section in Rotte-witz.

\$CA1: Single grain De and De error values for a coarse grain quartz sample from a fluvial deposit in the rock shelter of Cueva Anton

### **BT998**

Lab: Luminescence Laboratory Bayreuth

Lab-Code: BT998

Location: Rottewitz (Saxony/Germany)

Material: Fine grain quartz measured on aluminum discs on a Risoe TL/OSL DA-15 reader

Units: Values are given in seconds

Dose Rate: Dose rate of the beta-source at measurement ca. 0.0438 Gy/s +/- 0.0019 Gy/s

Measurement Date: 2012-01-27

## CA<sub>1</sub>

Lab: Cologne Luminescence Laboratory (CLL)

Lab-Code: C-L2941

Location: Cueva Anton (Murcia/Spain)

Material: Coarse grain quartz (200-250 microns) measured on single grain discs on a Risoe TL/OSL DA-20 r

Units: Values are given in Gray

Measurement Date: 2012

#### References

## **BT998**

Unpublished data

#### CA<sub>1</sub>

Burow, C., Kehl, M., Hilgers, A., Weniger, G.-C., Angelucci, D., Villaverde, V., Zapata, J. and Zilhao, J. (accepted). Luminescence dating of fluvial deposits in the rock shelter of Cueva Anton, Spain. Geochronometria.

ExampleData.FittingLM Example data for fit\_LMCurve() in the package Luminescence

# **Description**

Lineraly modulated (LM) measurement data from a quartz sample from Norway including background measurement. Measurements carried out in the luminescence laboratory at the University of Bayreuth.

### **Format**

Two objects (data.frames) with two columns (time and counts).

#### **Source**

Lab: Luminescence Laboratory Bayreuth

Lab-Code: BT900 Location: Norway

Material: Beach deposit, coarse grain quartz measured on aluminum discs on a Risoe TL/OSL DA-15 reader

#### References

Fuchs, M., Kreutzer, S., Fischer, M., Sauer, D., Soerensen, R., 2012. OSL and IRSL dating of raised beach sand deposits along the southeastern coast of Norway. Quaternary Geochronology, 10, 195-200.

# **Examples**

```
##show LM data
data(ExampleData.FittingLM, envir = environment())
plot(values.curve,log="x")
```

ExampleData.LxTxData Example Lx/Tx data from CW-OSL SAR measurement

# Description

LxTx data from a SAR measurement for the package Luminescence.

#### **Format**

A data.frame with 4 columns (Dose, LxTx, LxTx.Error, TnTx).

Lab: Luminescence Laboratory Bayreuth

Lab-Code: BT607

Location: Ostrau (Saxony-Anhalt/Germany)

Material: Middle grain (38-63  $\mu$ m) quartz measured on a Risoe TL/OSL DA-15 reader.

### References

unpublished data

# **Examples**

```
##plot Lx/Tx data vs dose [s]
data(ExampleData.LxTxData, envir = environment())
plot(LxTxData$Dose,LxTxData$LxTx)
```

 ${\tt ExampleData.LxTxOSLData}$ 

Example Lx and Tx curve data from an artificial OSL measurement

# Description

Lx and Tx data of continous wave (CW-) OSL signal curves.

## **Format**

Two data. frames containing time and count values.

# Source

Arbitrary OSL measurement.

## References

unpublished data

```
##load data
data(ExampleData.LxTxOSLData, envir = environment())
##plot data
plot(Lx.data)
plot(Tx.data)
```

ExampleData.RLum.Analysis

Example data as RLum. Analysis objects

## **Description**

Collection of different RLum. Analysis objects for protocol analysis.

### **Format**

IRSAR.RF.Data: IRSAR.RF.Data on coarse grain feldspar Each object contains data needed for the given protocol analysis.

#### Version

0.1

#### Source

## IRSAR.RF.Data

These data were kindly provided by Tobias Lauer and Matthias Krbetschek.

Lab: Luminescence Laboratory TU Bergakademie Freiberg

Lab-Code: ZEU/SA1

Location: Zeuchfeld (Zeuchfeld Sandur; Saxony-Anhalt/Germany)

Material: K-feldspar (130-200  $\mu$ m) Reference: Kreutzer et al. (2014)

## References

## IRSAR.RF.Data

Kreutzer, S., Lauer, T., Meszner, S., Krbetschek, M.R., Faust, D., Fuchs, M., 2014. Chronology of the Quaternary profile Zeuchfeld in Saxony-Anhalt / Germany - a preliminary luminescence dating study. Zeitschrift fuer Geomorphologie 58, 5-26. doi: 10.1127/0372-8854/2012/S-00112

## **Examples**

```
##load data
data(ExampleData.RLum.Analysis, envir = environment())
##plot data
plot_RLum(IRSAR.RF.Data)
```

ExampleData.RLum.Data.Image

Example data as RLum. Data. Image objects

ExampleData.XSYG 81

# **Description**

Measurement of Princton Instruments camera imported with the function read\_SPE2R to R to produce an RLum.Data.Image object.

#### **Format**

```
Object of class RLum. Data. Image
```

### Version

0.1

#### Source

## ExampleData.RLum.Data.Image

These data were kindly provided by Regina DeWitt.

Lab.: Department of Physics, East-Carolina University, NC, USA

Lab-Code: -Location: -Material: -Reference: -

Image data is a measurement of fluorescent ceiling lights with a cooled Princeton Instruments (TM) camera fitted on Risoe DA-20 TL/OSL reader.

# **Examples**

```
##load data
data(ExampleData.RLum.Data.Image, envir = environment())
##plot data
plot_RLum(ExampleData.RLum.Data.Image)
```

ExampleData.XSYG

Example data for a SAR OSL measurement and a TL spectrum using a lexsyg reader

## **Description**

Example data from a SAR OSL measurement and a TL spectrum for package Luminescence imported from a Freiberg Instruments XSYG file using the function read\_XSYG2R.

### **Format**

OSL. SARMeasurement: SAR OSL measurement data

The data contain two elements: (a) \$Sequence. Header is a data.frame with metadata from the measurement, (b) Sequence. Object contains an RLum. Analysis object for further analysis.

TL. Spectrum: TL spectrum data

82 ExampleData.XSYG

RLum.Data.Spectrum object for further analysis. The spectrum was cleaned from cosmic-rays using the function apply\_CosmicRayRemoval. Note that no quantum efficiency calibration was performed.

#### Version

0.1

### **Source**

## **OSL.SARMeasurement**

Lab: Luminescence Laboratory Giessen

Lab-Code: no code
Location: not specified
Material: Coarse grain quartz

on steel cups on lexsyg research reader

Reference: unpublished

## **TL.Spectrum**

Lab: Luminescence Laboratory Giessen

Lab-Code: BT753

Location: Dolni Vestonice/Czech Republic

Material: Fine grain polymineral

on steel cups on lexsyg rearch reader

Reference: Fuchs et al., 2013

Spectrum: Integration time 19 s, channel time 20 s

Heating: 1 K/s, up to 500 deg. C

# References

Unpublished data measured to serve as example data for that package. Location origin of sample BT753 is given here:

Fuchs, M., Kreutzer, S., Rousseau, D.D., Antoine, P., Hatte, C., Lagroix, F., Moine, O., Gauthier, C., Svoboda, J., Lisa, L., 2013. The loess sequence of Dolni Vestonice, Czech Republic: A new OSL-based chronology of the Last Climatic Cycle. Boreas, 42, 664–677.

## See Also

```
read_XSYG2R, RLum.Analysis,
RLum.Data.Spectrum, plot_RLum,
plot_RLum.Analysis, plot_RLum.Data.Spectrum
```

```
OSL.SARMeasurement$Sequence.Object
##grep OSL curves and plot the first curve
OSLcurve <- get_RLum(OSL.SARMeasurement$Sequence.Object,
recordType="0SL")[[1]]
plot_RLum(OSLcurve)
##(2) TL.Spectrum
TL.Spectrum
##plot simple spectrum (2D)
plot_RLum.Data.Spectrum(TL.Spectrum,
                      plot.type="contour",
                      xlim = c(310,750),
                      ylim = c(0,300),
                      bin.rows=10,
                      bin.cols = 1)
##plot 3d spectrum (uncomment for usage)
# plot_RLum.Data.Spectrum(TL.Spectrum, plot.type="persp",
\# x \lim = c(310,750), y \lim = c(0,300), bin.rows=10,
# bin.cols = 1)
```

extract\_IrradiationTimes

Extract irradiation times from an XSYG file

# Description

Extracts irradiation times, dose and times since last irradiation, from a Freiberg Instruments XSYG-file. These information can be further used to update an existing BINX-file

## Usage

```
extract_IrradiationTimes(object, file.BINX, recordType = c("irradiation (NA)",
   "IRSL (UVVIS)", "OSL (UVVIS)", "TL (UVVIS)"), compatibility.mode = TRUE,
   txtProgressBar = TRUE)
```

#### **Arguments**

object

character (**required**) or RLum. Analysis object: path and file name of the XSYG file or an RLum. Analysis produced by the function read\_XSYG2R.

**Note**: If an RLum. Analysis is used, any input for the arguments file.BINX and recordType will be ignored!

file.BINX

character (optional): path and file name of an existing BINX-file. If a file name is provided the file will be updated with the information from the XSYG file in the same folder as the original BINX-file.

Note: The XSYG and the BINX-file have to be originate from the same measurement!

recordType

character (with default): select relevant curves types from the XSYG file or RLum. Analysis object. As the XSYG-file format comprises much more information than usually needed for routine data analysis and allowed in the BINXfile format, only the relevant curves are selected by using the function get\_RLum. The argument recordType works as described for this function.

Note: A wrong selection will causes a function error. Please change this argument only if you have reasons to do so.

compatibility.mode

logical (with default): this option is parsed only if a BIN/BINX file is produced and it will reset all position values to a max. value of 48, cf.write\_R2BIN

txtProgressBar logical (with default): enables TRUE or disables FALSE the progression bars during import and export

#### **Details**

The function was written to compensate missing information in the BINX-file output of Freiberg Instruments lexsyg readers. As all information are available within the XSYG-file anyway, these information can be extracted and used for further analysis or/and to stored in a new BINX-file, which can be further used by other software, e.g. Analyst (Geoff Duller).

Typical application example: g-value estimation from fading measurements using the Analyst or any other self written script.

Beside the some simple data transformation steps the function applies the functions read\_XSYG2R, read\_BIN2R, write\_R2BIN for data import and export.

## Value

An RLum. Results object is returned with the following structure: .. \$irr.times (data.frame)

If a BINX-file path and name is set, the output will be additionally transferred to a new BINX-file with the function name as suffix. For the output the path of the input BINX-file itself is used. Note that this will not work if the input object is a file path to an XSYG-file. In this case the argument input is ignored.

# **Function version**

0.2.1 (2015-08-21 14:53:14)

#### Note

The produced output object contains still the irradiation steps to keep the output transparent. However, for the BINX-file export this steps are removed as the BINX-file format description does not allow irradiations as separat sequences steps.

Know issue: The 'fading correction' menu in the Analyst will not work appear with the produced BIN/BINX-file due to hidden bits, which are not reproduced by the function write\_R2BIN() or if it appears it stops with a floating point error.

Negative values for TIMESINCELAS.STEP? Yes, this is possible and no bug, as in the XSYG file multiple curves are stored for one step. Example: A TL step may comprise three curves: (a) counts vs. time, (b) measured temperature vs. time and (c) predefined temperature vs. time. Three curves, but they are all belonging to one TL measurement step, but with regard to the time stamps this could produce negative values as the important function (read\_XSYG2R) do not change the order of entries for one step towards a correct time order.

## Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

#### References

Duller, G., 2007. Analyst.

#### See Also

RLum.Analysis, RLum.Results, Risoe.BINfileData, read\_XSYG2R, read\_BIN2R, write\_R2BIN

## **Examples**

```
## (1) - example for your own data
## set files and run function
#
   file.XSYG <- file.choose()</pre>
#
   file.BINX <- file.choose()</pre>
#
#
      output <- extract_IrradiationTimes(file.XSYG = file.XSYG, file.BINX) = file.BINX)
#
      get_RLum(output)
## export results additionally to a CSV.file in the same directory as the XSYG-file
#
        write.table(x = get_RLum(output),
#
                     file = paste0(file.BINX, "_extract_IrradiationTimes.csv"),
                     sep = ";",
#
#
                     row.names = FALSE)
```

fit\_CWCurve

Nonlinear Least Squares Fit for CW-OSL curves [beta version]

#### **Description**

The function determines the weighted least-squares estimates of the component parameters of a CW-OSL signal for a given maximum number of components and returns various component parameters. The fitting procedure uses the nls function with the port algorithm.

## Usage

```
fit_CWCurve(values, n.components.max, fit.failure_threshold = 5,
  fit.method = "port", fit.trace = FALSE, fit.calcError = FALSE,
  LED.power = 36, LED.wavelength = 470, cex.global = 0.6,
  sample_code = "Default", output.path, output.terminal = TRUE,
  output.terminalAdvanced = TRUE, plot = TRUE, ...)
```

## **Arguments**

values RLum. Data. Curve or data.frame (**required**): x, y data of measured values (time

and counts). See examples.

n.components.max

vector (optional): maximum number of components that are to be used for fit-

ting. The upper limit is 7.

 $fit.failure\_threshold$ 

vector (with default): limits the failed fitting attempts.

fit.method character (with default): select fit method, allowed values: 'port' and 'LM'.

'port' uses the 'port' routine usint the funtion nls 'LM' utilises the function nlsLM from the package minpack.lm and with that the Levenberg-Marquardt

algorithm.

fit.trace logical (with default): traces the fitting process on the terminal.

fit.calcError logical (with default): calculate 1-sigma error range of components using confint

LED. power numeric (with default): LED power (max.) used for intensity ramping in mW/cm^2.

**Note:** The value is used for the calculation of the absolute photoionisation cross

section.

LED.wavelength numeric (with default): LED wavelength used for stimulation in nm. Note: The

value is used for the calculation of the absolute photoionisation cross section.

cex.global numeric (with default): global scaling factor.

sample\_code character (optional): sample code used for the plot and the optional output table

(mtext).

output.path character (optional): output path for table output containing the results of the fit.

The file name is set automatically. If the file already exists in the directory, the

values are appended.

output.terminal

logical (with default): terminal ouput with fitting results.

output.terminalAdvanced

logical (with default): enhanced terminal output. Requires output.terminal = TRUE.

If output.terminal = FALSE no advanced output is possible.

plot logical (with default): returns a plot of the fitted curves.

... further arguments and graphical parameters passed to plot.

#### **Details**

### **Fitting function**

The function for the CW-OSL fitting has the general form:

$$y = I0_1 * \lambda_1 * exp(-\lambda_1 * x) + \dots + I0_i * \lambda_i * exp(-\lambda_i * x)$$

where 0 < i < 8

and  $\lambda$  is the decay constant and N0 the intial number of trapped electrons. (for the used equation cf. Boetter-Jensen et al., 2003)

### Start values

Start values are estimated automatically by fitting a linear function to the logarithmized input data set. Currently, there is no option to manually provide start parameters.

#### Goodness of fit

The goodness of the fit is given as pseudoR^2 value (pseudo coefficient of determination). According to Lave (1970), the value is calculated as:

$$pseudoR^2 = 1 - RSS/TSS$$

where RSS = Residual Sum of Squaresand TSS = Total Sum of Squares

## Error of fitted component parameters

The 1-sigma error for the components is calculated using the function confint. Due to considerable calculation time, this option is deactived by default. In addition, the error for the components can be estimated by using internal R functions like summary. See the nls help page for more information.

For details on the nonlinear regression in R, see Ritz & Streibig (2008).

## Value

(optional) the fitted CW-OSL curves are returned as plot. plot

table (optional) an output table (\*.csv) with parameters of the fitted components is

provided if the output.path is set.

list(list("RLum.Results"))

beside the plot and table output options, an RLum. Results object is returned.

fit: an nls object (\$fit) for which generic R functions are provided, e.g. summary, confint, profile. For more details, see nls.

output.table: a data.frame containing the summarised parameters including the error

component.contribution.matrix: matrix containing the values for the component to sum contribution plot (\$component.contribution.matrix).

Matrix structure:

Column 1 and 2: time and rev(time) values

Additional columns are used for the components, two for each component, containing I0 and n0. The last columns cont. provide information on the relative component contribution for each time interval including the row sum for this

values.

object

beside the plot and table output options, an RLum. Results object is returned.

fit: an nls object (\$fit) for which generic R functions are provided, e.g. summary, confint, profile. For more details, see nls.

output.table: a data.frame containing the summarised parameters including the error

component.contribution.matrix: matrix containing the values for the component to sum contribution plot (\$component.contribution.matrix).

Matrix structure:

Column 1 and 2: time and rev(time) values

Additional columns are used for the components, two for each component, containing I0 and n0. The last columns cont. provide information on the relative component contribution for each time interval including the row sum for this values.

#### **Function version**

```
0.5.1 (2015-08-21 14:53:14)
```

#### Note

Beta version - This function has not been properly tested yet and should therefore not be used for publication purposes!

The pseudo- $R^2$  may not be the best parameter to describe the goodness of the fit. The trade off between the n. components and the pseudo- $R^2$  value is currently not considered.

The function **does not** ensure that the fitting procedure has reached a global minimum rather than a local minimum!

## Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

#### References

Boetter-Jensen, L., McKeever, S.W.S., Wintle, A.G., 2003. Optically Stimulated Luminescence Dosimetry. Elsevier Science B.V.

Lave, C.A.T., 1970. The Demand for Urban Mass Transportation. The Review of Economics and Statistics, 52 (3), 320-323.

Ritz, C. & Streibig, J.C., 2008. Nonlinear Regression with R. In: R. Gentleman, K. Hornik, G. Parmigiani, eds., Springer, p. 150.

## See Also

```
fit_LMCurve, plot,nls, RLum.Data.Curve, RLum.Results, get_RLum, nlsLM
```

fit_LMCurve	Nonlinear Least Squares Fit for LM-OSL curves
-------------	---

## **Description**

The function determines weighted nonlinear least-squares estimates of the component parameters of an LM-OSL curve (Bulur 1996) for a given number of components and returns various component parameters. The fitting procedure uses the function nls with the port algorithm.

# Usage

```
fit_LMCurve(values, values.bg, n.components = 3, start_values,
  input.dataType = "LM", fit.method = "port", sample_code = "",
  sample_ID = "", LED.power = 36, LED.wavelength = 470,
  fit.trace = FALSE, fit.advanced = FALSE, fit.calcError = FALSE,
  bg.subtraction = "polynomial", verbose = TRUE, plot = TRUE,
  plot.BG = FALSE, ...)
```

## **Arguments**

values	RLum.Data.Curve or data.frame ( <b>required</b> ): x,y data of measured values (time and counts). See examples.
values.bg	RLum.Data.Curve or data.frame (optional): x,y data of measured values (time and counts) for background subtraction.
n.components	integer (with default): fixed number of components that are to be recognised during fitting (min = $1$ , max = $7$ ).
start_values	data.frame (optional): start parameters for lm and xm data for the fit. If no start values are given, an automatic start value estimation is attempted (see details).
input.dataType	character (with default): alter the plot output depending on the input data: "LM" or "pLM" (pseudo-LM). See: CW2pLM
fit.method	character (with default): select fit method, allowed values: 'port' and 'LM'. 'port' uses the 'port' routine usint the funtion nls 'LM' utilises the function nlsLM from the package minpack.lm and with that the Levenberg-Marquardt algorithm.
sample_code	character (optional): sample code used for the plot and the optional output table (mtext).
sample_ID	character (optional): additional identifier used as column header for the table output.
LED.power	numeric (with default): LED power (max.) used for intensity ramping in mW/cm^2. <b>Note:</b> This value is used for the calculation of the absolute photoionisation cross section.
LED.wavelength	numeric (with default): LED wavelength in nm used for stimulation. <b>Note:</b> This value is used for the calculation of the absolute photoionisation cross section.
fit.trace	logical (with default): traces the fitting process on the terminal.
fit.advanced	logical (with default): enables advanced fitting attempt for automatic start parameter recognition. Works only if no start parameters are provided. <b>Note:</b> It may take a while and it is not compatible with fit.method = "LM".

fit.calcError logical (with default): calculate 1-sigma error range of components using con-

fint.

bg. subtraction character (with default): specifies method for background subtraction (polynomial,

linear, channel, see Details). **Note:** requires input for values.bg.

verbose logical (with default): terminal output with fitting results.

plot logical (with default): returns a plot of the fitted curves.

plot.BG logical (with default): returns a plot of the background values with the fit used

for the background subtraction.

... Further arguments that may be passed to the plot output, e.g. xlab, xlab, main,

log.

#### **Details**

# **Fitting function**

The function for the fitting has the general form:

$$y = (exp(0.5)*Im_1*x/xm_1)*exp(-x^2/(2*xm_1^2))+, \dots, +exp(0.5)*Im_i*x/xm_i)*exp(-x^2/(2*xm_i^2))$$

where 1 < i < 8

This function and the equations for the conversion to b (detrapping probability) and n0 (proportional to initially trapped charge) have been taken from Kitis et al. (2008):

$$xm_i = \sqrt{max(t)/b_i}$$

$$Im_i = exp(-0.5)n0/xm_i$$

## **Background subtraction**

Three methods for background subtraction are provided for a given background signal (values.bg). polynomial: default method. A polynomial function is fitted using glm and the resulting function is used for background subtraction:

$$y = a * x^4 + b * x^3 + c * x^2 + d * x + e$$

linear: a linear function is fitted using glm and the resulting function is used for background subtraction:

$$y = a * x + b$$

channel: the measured background signal is subtracted channelwise from the measured signal.

#### **Start values**

The choice of the initial parameters for the nls-fitting is a crucial point and the fitting procedure may mainly fail due to ill chosen start parameters. Here, three options are provided:

(a) If no start values (start\_values) are provided by the user, a cheap guess is made by using the detrapping values found by Jain et al. (2003) for quartz for a maximum of 7 components. Based on these values, the pseudo start parameters xm and Im are recalculated for the given data set. In all cases, the fitting starts with the ultra-fast component and (depending on n.components) steps

through the following values. If no fit could be achieved, an error plot (for plot = TRUE) with the pseudo curve (based on the pseudo start parameters) is provided. This may give the opportunity to identify appropriate start parameters visually.

- (b) If start values are provided, the function works like a simple nls fitting approach.
- (c) If no start parameters are provided and the option fit.advanced = TRUE is chosen, an advanced start parameter estimation is applied using a stochastical attempt. Therefore, the recalculated start parameters (a) are used to construct a normal distribution. The start parameters are then sampled randomly from this distribution. A maximum of 100 attempts will be made. **Note:** This process may be time consuming.

#### Goodness of fit

The goodness of the fit is given by a pseudoR^2 value (pseudo coefficient of determination). According to Lave (1970), the value is calculated as:

$$pseudoR^2 = 1 - RSS/TSS$$

where  $RSS = Residual\ Sum\ of\ Squares$  and  $TSS = Total\ Sum\ of\ Squares$ 

## Error of fitted component parameters

The 1-sigma error for the components is calculated using the function confint. Due to considerable calculation time, this option is deactived by default. In addition, the error for the components can be estimated by using internal R functions like summary. See the nls help page for more information.

For more details on the nonlinear regression in R, see Ritz & Streibig (2008).

#### Value

Various types of plots are returned. For details see above.

Furthermore an RLum. Results object is returned with the following structure:

## data:

- .. \$fit: nls (nls object)
- .. \$output.table : data.frame with fitting results
- .. \$component.contribution.matrix: list component distribution matrix
- .. \$call: call the original function call

Matrix structure for the distribution matrix:

Column 1 and 2: time and rev(time) values

Additional columns are used for the components, two for each component, containing I0 and n0. The last columns cont. provide information on the relative component contribution for each time interval including the row sum for this values.

# **Function version**

0.3.0 (2015-08-21 14:53:14)

#### Note

The pseudo- $R^2$  may not be the best parameter to describe the goodness of the fit. The trade off between the n. components and the pseudo- $R^2$  value currently remains unconsidered.

The function **does not** ensure that the fitting procedure has reached a global minimum rather than a local minimum! In any case of doubt, the use of manual start values is highly recommended.

## Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

#### References

Bulur, E., 1996. An Alternative Technique For Optically Stimulated Luminescence (OSL) Experiment. Radiation Measurements, 26, 5, 701-709.

Jain, M., Murray, A.S., Boetter-Jensen, L., 2003. Characterisation of blue-light stimulated luminescence components in different quartz samples: implications for dose measurement. Radiation Measurements, 37 (4-5), 441-449.

Kitis, G. & Pagonis, V., 2008. Computerized curve deconvolution analysis for LM-OSL. Radiation Measurements, 43, 737-741.

Lave, C.A.T., 1970. The Demand for Urban Mass Transportation. The Review of Economics and Statistics, 52 (3), 320-323.

Ritz, C. & Streibig, J.C., 2008. Nonlinear Regression with R. R. Gentleman, K. Hornik, & G. Parmigiani, eds., Springer, p. 150.

#### See Also

```
fit_CWCurve, plot, nls, nlsLM, get_RLum
```

```
##(1) fit LM data without background subtraction
data(ExampleData.FittingLM, envir = environment())
fit_LMCurve(values = values.curve, n.components = 3, log = "x")
##(2) fit LM data with background subtraction and export as JPEG
## -alter file path for your preferred system
##jpeg(file = "~/Desktop/Fit_Output\%03d.jpg", quality = 100,
## height = 3000, width = 3000, res = 300)
data(ExampleData.FittingLM, envir = environment())
fit_LMCurve(values = values.curve, values.bg = values.curveBG,
            n.components = 2, log = "x", plot.BG = TRUE)
##dev.off()
##(3) fit LM data with manual start parameters
data(ExampleData.FittingLM, envir = environment())
fit_LMCurve(values = values.curve,
            values.bg = values.curveBG,
            n.components = 3,
            log = "x",
            start_values = data.frame(Im = c(170, 25, 400), xm = c(56, 200, 1500)))
```

get\_Layout 93

get\_Layout

Collection of layout definitions

#### **Description**

This helper function returns a list with layout definitions for homogeneous plotting.

#### Usage

```
get_Layout(layout)
```

### **Arguments**

layout

character or list object (required): name of the layout definition to be returned. If name is provided the respective definition is returned. One of the following supported layout definitions is possible: "default", "journal.1", "small", "empty". User-specific layout definitions must be provided as a list object of predefined structure, see details.

#### **Details**

The easiest way to create a user-specific layout definition is perhaps to create either an empty or a default layout object and fill/modify the definitions (user.layout <- get\_Layout(data = "empty")).

### Value

A list object with layout definitions for plot functions.

## **Function version**

```
0.1 (2015-08-21 14:53:14)
```

## Author(s)

```
Michael Dietze, GFZ Potsdam (Germany)
R Luminescence Package Team
```

```
## read example data set
data(ExampleData.DeValues, envir = environment())

## show structure of the default layout definition
layout.default <- get_Layout(layout = "default")
str(layout.default)

## show colour definitions for Abanico plot, only
layout.default$abanico$colour

## set Abanico plot title colour to orange
layout.default$abanico$colour$main <- "orange"

## create Abanico plot with modofied layout definition</pre>
```

94 get\_Quote

get\_Quote

Function to return essential quotes

## **Description**

This function returns one of the collected essential quotes in the growing library. If called without any parameters, a random quote is returned.

## Usage

```
get_Quote(ID, author, separated = FALSE)
```

# **Arguments**

ID character, qoute ID to be returned.

author character, all quotes by specified author. separated logical, return result in separated form.

# Value

Returns a character with quote and respective (false) author.

## **Function version**

```
0.1.1 (2015-08-21 14:53:14)
```

# Author(s)

```
Michael Dietze, GFZ Potsdam (Germany)
R Luminescence Package Team
```

```
## ask for an arbitrary qoute
get_Quote()
```

get\_Risoe.BINfileData 95

get\_Risoe.BINfileData General accessor function for RLum S4 class objects

# **Description**

Function calls object-specific get functions for RisoeBINfileData S4 class objects.

## Usage

```
get_Risoe.BINfileData(object)
```

## **Arguments**

object Risoe.BINfileData (required): S4 object of class RLum

... further arguments that one might want to pass to the specific get function

## **Details**

The function provides a generalised access point for specific Risoe.BINfileData objects. Depending on the input object, the corresponding get function will be selected. Allowed arguments can be found in the documentations of the corresponding Risoe.BINfileData class.

## Value

Return is the same as input objects as provided in the list.

## **Function version**

```
0.1 (2015-08-21 14:53:14)
```

# Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

# See Also

Risoe.BINfileData

96 get\_RLum

get\_RLum

General accessor function for RLum S4 class objects

## **Description**

Function calls object-specific get functions for RLum S4 class objects.

## Usage

```
get_RLum(object, ...)
## S4 method for signature 'list'
get_RLum(object, ...)
```

## **Arguments**

object RLum (**required**): S4 object of class RLum or an object of type list containing only objects of type RLum

... further arguments that will be passed to the object specific methods. For furter details on the supported arguments please see the class documentation: RLum.Data.Curve, RLum.Data.Spectrum, RLum.Data.Image, RLum.Analysis and RLum.Results

#### **Details**

The function provides a generalised access point for specific RLum objects.

Depending on the input object, the corresponding get function will be selected. Allowed arguments can be found in the documentations of the corresponding RLum class.

# Value

Return is the same as input objects as provided in the list.

## Methods (by class)

• list: Returns a list of RLum objects that had been passed to get\_RLum

#### **Function version**

```
0.2.0 (2015-08-21 14:53:14)
```

#### Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

### See Also

```
RLum.Data.Curve, RLum.Data.Image, RLum.Data.Spectrum, RLum.Analysis, RLum.Results
```

length\_RLum 97

#### **Examples**

```
##Example based using data and from the calc_CentralDose() function
##load example data
data(ExampleData.DeValues, envir = environment())
##apply the central dose model 1st time
temp1 <- calc_CentralDose(ExampleData.DeValues$CA1)
##get results and store them in a new object
temp.get <- get_RLum(object = temp1)</pre>
```

length\_RLum

General accessor function for RLum S4 class objects

### **Description**

Function calls object-specific get functions for RLum S4 class objects.

## Usage

```
length_RLum(object)
```

## **Arguments**

object RLum (required): S4 object of class RLum

## **Details**

The function provides a generalised access point for specific RLum objects.

Depending on the input object, the corresponding get function will be selected. Allowed arguments can be found in the documentations of the corresponding RLum class.

## Value

Return is the same as input objects as provided in the list.

### **Function version**

```
0.1 (2015-08-21 14:53:14)
```

# Author(s)

```
Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team
```

# See Also

RLum.Data.Curve, RLum.Data.Image, RLum.Data.Spectrum, RLum.Analysis, RLum.Results

```
merge_Risoe.BINfileData
```

Merge Risoe.BINfileData objects or Risoe BIN-files

## Description

Function allows merging Risoe BIN/BINX files or Risoe.BINfileData objects.

### Usage

```
merge_Risoe.BINfileData(input.objects, output.file,
 keep.position.number = FALSE, position.number.append.gap = 0)
```

## **Arguments**

```
input.objects
                 character or Risoe. BINfileData (required): Character vector with path and
                 files names (e.g. input.objects = c("path/file1.bin", "path/file2.bin")
                 orRisoe.BINfileData objects (e.g. input.objects = c(object1, object2))
                 character (optional): File output path and name.
output.file
```

If no value is given, a Risoe.BINfileData is returned instead of a file.

keep.position.number

logical (with default): Allows keeping the original position numbers of the input objects. Otherwise the position numbers are recalculated.

position.number.append.gap

integer (with default): Set the position number gap between merged BIN-file sets, if the option keep.position.number = FALSE is used. See details for further information.

### **Details**

The function allows merging different measurements to one file or one object.

The record IDs are recalculated for the new object. Other values are kept for each object. The number of input objects is not limited.

```
position.number.append.gap option
```

If the option keep.position.number = FALSE is used, the position numbers of the new data set are recalculated by adding the highest position number of the previous data set to the each position number of the next data set. For example: The highest position number is 48, then this number will be added to all other position numbers of the next data set (e.g. 1 + 48 = 49)

However, there might be cases where an additional addend (summand) is needed before the next position starts. Example:

```
Position number set (A): 1,3,5,7
Position number set (B): 1, 3, 5, 7
```

With no additional summand the new position numbers would be: 1,3,5,7,8,9,10,11. That might be unwanted. Using the argument position.number.append.gap = 1 it will become: 1,3,5,7,9,11,13,15,17.

merge\_RLum 99

### Value

Returns a file or a Risoe.BINfileData object.

#### **Function version**

```
0.2.3 (2015-08-21 14:53:14)
```

### Note

The validity of the output objects is not further checked.

## Author(s)

```
Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team
```

## References

```
Duller, G., 2007. Analyst.
```

#### See Also

```
Risoe.BINfileData, read_BIN2R, write_R2BIN
```

# **Examples**

```
##merge two objects
data(ExampleData.BINfileData, envir = environment())

object1 <- CWOSL.SAR.Data
object2 <- CWOSL.SAR.Data

object.new <- merge_Risoe.BINfileData(c(object1, object2))</pre>
```

merge\_RLum

General merge function for RLum S4 class objects

# Description

Function calls object-specific merge functions for RLum S4 class objects.

# Usage

```
merge_RLum(objects, ...)
```

### **Arguments**

```
objects list of RLum (required): list of S4 object of class RLum
... further arguments that one might want to pass to the specific merge function
```

100 merge\_RLum

#### **Details**

The function provides a generalised access point for merge specific RLum objects.

Depending on the input object, the corresponding merge function will be selected. Allowed arguments can be found in the documentations of each merge function. Empty list elements (NULL) are automatically removed from the input list.

object corresponding merge function

RLum.Results : merge\_RLum

### Value

Return is the same as input objects as provided in the list.

#### **Function version**

```
0.1.2 (2015-08-30 19:11:03)
```

#### Note

So far not for every RLum object a merging function exists.

## Author(s)

```
Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team
```

## References

#

## See Also

```
RLum.Results,
```

```
##Example based using data and from the calc_CentralDose() function
##load example data
data(ExampleData.DeValues, envir = environment())

##apply the central dose model 1st time
temp1 <- calc_CentralDose(ExampleData.DeValues$CA1)

##apply the central dose model 2nd time
temp2 <- calc_CentralDose(ExampleData.DeValues$CA1)

##merge the results and store them in a new object
temp.merged <- get_RLum(merge_RLum(objects = list(temp1, temp2)))</pre>
```

merge\_RLum.Analysis

Merge function for RLum. Analysis S4 class objects

## **Description**

Function allows merging of RLum. Analysis objects and adding of allowed objects to an RLum. Analysis.

## Usage

```
merge_RLum.Analysis(objects)
```

## **Arguments**

objects

list of RLum. Analysis (**required**): list of S4 objects of class RLum. Analysis. Furthermore other objects of class RLum can be added, see details.

### **Details**

This function simply allowing to merge RLum. Analysis objects. Additionally other RLum objects can be added to an existing RLum. Analysis object. Supported objects to be added are: RLum. Data. Curve, RLum. Data. Spectrum and RLum. Data. Image.

The order in the new RLum. Analysis object is the object order provided with the input list.

## Value

Return an RLum. Analysis object.

# **Function version**

```
0.1 (2015-08-21 14:53:14)
```

## Note

The information for the slot 'protocol' is taken from the first RLum. Analysis object in the input list. Therefore at least one object of type RLum. Analysis has to be provided.

## Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

## References

\_

### See Also

merge\_RLum, RLum.Analysis, RLum.Data.Curve, RLum.Data.Spectrum, RLum.Data.Image, RLum

#### **Examples**

```
##merge different RLum objects from the example data
data(ExampleData.RLum.Analysis, envir = environment())
data(ExampleData.BINfileData, envir = environment())

object <- Risoe.BINfileData2RLum.Analysis(CWOSL.SAR.Data, pos=1)
curve <- get_RLum(object)[[2]]

temp.merged <- merge_RLum.Analysis(list(curve, IRSAR.RF.Data, IRSAR.RF.Data))</pre>
```

merge\_RLum.Data.Curve Merge function for RLum.Data.Curve S4 class objects

# **Description**

Function allows merging of RLum.Data.Curve objects in different ways

## Usage

```
merge_RLum.Data.Curve(object, merge.method = "mean", method.info)
```

## **Arguments**

object list of RLum.Data.Curve (**required**): list of S4 objects of class RLum.Curve.

merge.method character (**required**): method for combining of the objects, e.g. 'mean',
 'sum', see details for further information and allowed methods. Note: Elements

in slot info will be taken from the first curve in the list.

method.info numeric (optional): allows to specify how info elements of the input objects are combined, e.g. 1 means that just the elements from the first object are kept, 2

keeps only the info elements from the 2 object etc. If nothing is provided all

elements are combined.

## Details

This function simply allowing to merge RLum. Data. Curve objects without touching the objects itself. Merging is always applied on the 2nd colum of the data matrix of the object.

# Supported merge operations are RLum. Data. Curve

```
"sum"
```

All count values will be summed up using the function rowSums.

"mean"

The mean over the count values is calculated using the function rowMeans.

"-"

The row sums of the last objects are subtracted from the first object.

```
"*"
```

The row sums of the last objects are mutliplied with the first object.

```
"/"
```

Values of the first object are divided by row sums of the last objects.

#### Value

Return an RLum. Data. Curve object.

## **Function version**

```
0.1.1 (2015-08-21 14:53:14)
```

#### Note

The information from the slot 'recordType' is taken from the first RLum.Data.Curve object in the input list. The slot 'curveType' is filled with the name merged.

### Author(s)

```
Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team
```

## References

\_

## See Also

```
merge_RLum, RLum.Data.Curve
```

```
##load example data
data(ExampleData.XSYG, envir = environment())

##grep first and 3d TL curves
TL.curves <- get_RLum(OSL.SARMeasurement$Sequence.Object, recordType = "TL (UVVIS)")
TL.curve.1 <- TL.curves[[1]]
TL.curve.3 <- TL.curves[[3]]

##plot single curves
plot_RLum(TL.curve.1)
plot_RLum(TL.curve.3)

##subtract the 1st curve from the 2nd and plot
TL.curve.merged <- merge_RLum.Data.Curve(list(TL.curve.3, TL.curve.1), merge.method = "/")
plot_RLum(TL.curve.merged)</pre>
```

merge\_RLum.Results

General accessor function for RLum S4 class objects

## **Description**

Function calls object-specific get functions for RLum S4 class objects.

## Usage

```
merge_RLum.Results(object.list)
```

## **Arguments**

```
object.list RLum (required): a list of S4 objects of class RLum
```

### **Details**

The function provides a generalised access point for specific RLum objects.

Depending on the input object, the corresponding merge function will be selected. Allowed arguments can be found in the documentations of the corresponding RLum class.

## Value

Return is the same as input objects as provided in the list.

# **Function version**

0.1

# Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

## See Also

RLum.Data.Curve, RLum.Data.Image, RLum.Data.Spectrum, RLum.Analysis, RLum.Results

plot\_AbanicoPlot

Function to create an Abanico Plot.

# Description

A plot is produced which allows comprehensive presentation of data precision and its dispersion around a central value as well as illustration of a kernel density estimate, histogram and/or dot plot of the dose values.

## Usage

```
plot_AbanicoPlot(data, na.rm = TRUE, log.z = TRUE, z.0 = "mean.weighted",
    dispersion = "qr", plot.ratio = 0.75, rotate = FALSE, mtext, summary,
    summary.pos, legend, legend.pos, stats, rug = FALSE, kde = TRUE,
    hist = FALSE, dots = FALSE, y.axis = TRUE, error.bars = FALSE, bar,
    bar.col, polygon.col, line, line.col, line.label, grid.col, frame = 1,
    bw = "SJ", output = FALSE, ...)
```

# **Arguments**

data	<pre>data.frame or RLum.Results object (required): for data.frame two columns: De (data[,1]) and De error (data[,2]). To plot several data sets in one plot the data sets must be provided as list, e.g. list(data.1, data.2).</pre>
na.rm	logical (with default): exclude NA values from the data set prior to any further operations.
log.z	${f logical}$ (with default): Option to display the z-axis in logarithmic scale. Default is TRUE.
z.0	character or numeric: User-defined central value, used for centering of data. One out of "mean", "mean.weighted" and "median" or a numeric value (not its logarithm). Default is "mean.weighted".
dispersion	character (with default): measure of dispersion, used for drawing the scatter polygon. One out of "qr" (quartile range), "pnn" (symmetric percentile range with nn the lower percentile, e.g. "p05" depicting the range between 5 and 95 "sd" (standard deviation) and "2sd" (2 standard deviations), default is "qr". Note that "sd" and "2sd" are only meaningful in combination with "z.0 = 'mean'" because the unweighted mean is used to center the polygon.
plot.ratio	<pre>numeric: Relative space, given to the radial versus the cartesian plot part, deault is 0.75.</pre>
rotate	logical: Option to turn the plot by 90 degrees.
mtext	character: additional text below the plot title.
summary	character (optional): add statistic measures of centrality and dispersion to the plot. Can be one or more of several keywords. See details for available keywords.
summary.pos	numeric or character (with default): optional position coordinates or keyword (e.g. "topright") for the statistical summary. Alternatively, the keyword "sub" may be specified to place the summary below the plot header. However, this latter option in only possible if mtext is not used.
legend	character vector (optional): legend content to be added to the plot.
legend.pos	<pre>numeric or character (with default): optional position coordinates or keyword (e.g. "topright") for the legend to be plotted.</pre>
stats	character: additional labels of statistically important values in the plot. One or more out of the following: "min", "max", "median".
rug	logical: Option to add a rug to the KDE part, to indicate the location of individual values.
kde	logical: Option to add a KDE plot to the dispersion part, default is TRUE.
hist	logical: Option to add a histogram to the dispersion part. Only meaningful when not more than one data set is plotted.

dots logical: Option to add a dot plot to the dispersion part. If number of dots

exceeds space in the dispersion part, a square indicates this.

y.axis logical: Option to hide y-axis labels. Useful for data with small scatter.

error.bars logical: Option to show De-errors as error bars on De-points. Useful in com-

bination with y.axis = FALSE, bar.col = "none".

bar numeric (with default): option to add one or more dispersion bars (i.e., bar

showing the 2-sigma range) centered at the defined values. By default a bar is

drawn according to "z.0". To omit the bar set "bar = FALSE".

bar.col character or numeric (with default): colour of the dispersion bar. Default is

"grey60".

polygon.col character or numeric (with default): colour of the polygon showing the data

scatter. Sometimes this polygon may be omitted for clarity. To disable it use

FALSE or polygon = FALSE. Default is "grey80".

line numeric: numeric values of the additional lines to be added.

line.col character or numeric: colour of the additional lines.

line.label character: labels for the additional lines.

grid.col character or numeric (with default): colour of the grid lines (originating at

[0,0] and strechting to the z-scale). To disable grid lines use FALSE. Default is

"grey".

frame numeric (with default): option to modify the plot frame type. Can be one out

of 0 (no frame), 1 (frame originates at 0,0 and runs along min/max isochrons), 2 (frame embraces the 2-sigma bar), 3 (frame embraces the entire plot as a rect-

angle). Default is 1.

bw character (with default): bin-width for KDE, choose a numeric value for man-

ual setting.

output logical: Optional output of numerical plot parameters. These can be useful to

reproduce similar plots. Default is FALSE.

... Further plot arguments to pass. xlab must be a vector of length 2, specifying

the upper and lower x-axes labels.

#### **Details**

The Abanico Plot is a combination of the classic Radial Plot (plot\_RadialPlot) and a kernel density estimate plot (e.g plot\_KDE). It allows straightforward visualisation of data precision, error scatter around a user-defined central value and the combined distribution of the values, on the actual scale of the measured data (e.g. seconds, equivalent dose, years). The principle of the plot is shown in Galbraith & Green (1990). The function authors are thankful for the thoughtprovocing figure in this article.

The semi circle (z-axis) of the classic Radial Plot is bent to a straight line here, which actually is the basis for combining this polar (radial) part of the plot with any other cartesian visualisation method (KDE, histogram, PDF and so on). Note that the plot allows dispaying two measures of distribution. One is the 2-sigma bar, which illustrates the spread in value errors, and the other is the polygon, which stretches over both parts of the Abanico Plot (polar and cartesian) and illustrates the actual spread in the values themselfes.

Since the 2-sigma-bar is a polygon, it can be (and is) filled with shaded lines. To change density (lines per inch, default is 15) and angle (default is 45 degrees) of the shading lines, specify these parameters. See ?polygon() for further help.

The Abanico Plot supports other than the weighted mean as measure of centrality. When it is obvious that the data is not (log-)normally distributed, the mean (weighted or not) cannot be a valid measure of centrality and hence central dose. Accordingly, the median and the weighted median can be

chosen as well to represent a proper measure of centrality (e.g. centrality = "median.weighted"). Also user-defined numeric values (e.g. from the central age model) can be used if this appears appropriate.

The proportion of the polar part and the cartesian part of the Abanico Plot can be modified for display reasons (plot.ratio = 0.75). By default, the polar part spreads over 75 % and leaves 25 % for the part that shows the KDE graph.

A statistic summary, i.e. a collection of statistic measures of centrality and dispersion (and further measures) can be added by specifying one or more of the following keywords: "n" (number of samples), "mean" (mean De value), "mean.weighted" (error-weighted mean), "median" (median of the De values), "sdrel" (relative standard deviation in percent), "sdrel.weighted" (error-weighted relative standard deviation in percent), "sdabs" (absolute standard deviation), "sdabs.weighted" (error-weighted absolute standard deviation), "serel" (relative standard error), "serel.weighted" (error-weighted relative standard error), "seabs" (absolute standard error), "seabs.weighted" (error-weighted absolute standard error), "in.2s" (percent of samples in 2-sigma range), "kurtosis" (kurtosis) and "skewness" (skewness).

The optional parameter layout allows to modify the entire plot more sophisticated. Each element of the plot can be addressed and its properties can be defined. This includes font type, size and decoration, colours and sizes of all plot items. To infer the definition of a specific layout style cf. get\_Layout() or type eg. for the layout type "journal" get\_Layout("journal"). A layout type can be modified by the user by assigning new values to the list object.

It is possible for the z-scale to specify where ticks are to be drawn by using the parameter at, e.g. at = seq(80, 200, 20), cf. function documentation of axis. Specifying tick positions manually overrides a zlim-definition.

### Value

returns a plot object and, optionally, a list with plot calculus data.

# **Function version**

0.1.2 (2015-08-21 14:53:14)

# Author(s)

Michael Dietze, GFZ Potsdam (Germany), Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) Inspired by a plot introduced by Galbraith & Green (1990) R Luminescence Package Team

#### References

Galbraith, R. & Green, P., 1990. Estimating the component ages in a finite mixture. International Journal of Radiation Applications and Instrumentation. Part D. Nuclear Tracks and Radiation Measurements, 17 (3), pp. 197-206.

### See Also

```
plot_RadialPlot, plot_KDE, plot_Histogram
```

```
## store original graphics parameters
par.old <- par(no.readonly = TRUE)</pre>
## load example data and recalculate to Gray
data(ExampleData.DeValues, envir = environment())
ExampleData.DeValues <- ExampleData.DeValues$CA1</pre>
## plot the example data straightforward
plot_AbanicoPlot(data = ExampleData.DeValues)
## now with linear z-scale
plot_AbanicoPlot(data = ExampleData.DeValues,
                 log.z = FALSE)
## now with output of the plot parameters
plot1 <- plot_AbanicoPlot(data = ExampleData.DeValues,</pre>
                          output = TRUE)
str(plot1)
plot1$zlim
## now with adjusted z-scale limits
plot_AbanicoPlot(data = ExampleData.DeValues,
                 zlim = c(10, 200))
## now with adjusted x-scale limits
plot_AbanicoPlot(data = ExampleData.DeValues,
                 xlim = c(0, 20)
## now with rug to indicate individual values in KDE part
plot_AbanicoPlot(data = ExampleData.DeValues,
                 rug = TRUE)
## now with a smaller bandwidth for the KDE plot
plot_AbanicoPlot(data = ExampleData.DeValues,
                 bw = 0.04)
## now with a histogram instead of the KDE plot
plot_AbanicoPlot(data = ExampleData.DeValues,
                 hist = TRUE,
                 kde = FALSE)
## now with a KDE plot and histogram with manual number of bins
plot_AbanicoPlot(data = ExampleData.DeValues,
                 hist = TRUE,
                 breaks = 20)
## now with a KDE plot and a dot plot
plot_AbanicoPlot(data = ExampleData.DeValues,
                 dots = TRUE)
## now with user-defined plot ratio
plot_AbanicoPlot(data = ExampleData.DeValues,
                 plot.ratio = 0.5)
## now with user-defined central value
plot_AbanicoPlot(data = ExampleData.DeValues,
```

```
z.0 = 70)
## now with weighted median as central value
plot_AbanicoPlot(data = ExampleData.DeValues,
                 z.0 = "median")
## now with the 17-83 percentile range as definition of scatter
plot_AbanicoPlot(data = ExampleData.DeValues,
                 z.0 = "median".
                 dispersion = "p17")
## now with user-defined green line for minimum age model
CAM <- calc_CentralDose(ExampleData.DeValues,</pre>
                        plot = FALSE)
plot_AbanicoPlot(data = ExampleData.DeValues,
                 line = CAM,
                 line.col = "darkgreen",
                 line.label = "CAM")
## now create plot with legend, colour, different points and smaller scale
plot_AbanicoPlot(data = ExampleData.DeValues,
                 legend = "Sample 1",
                 col = "tomato4",
                 bar.col = "peachpuff",
                 pch = "R",
                 cex = 0.8)
## now without 2-sigma bar, polygon, grid lines and central value line
plot_AbanicoPlot(data = ExampleData.DeValues,
                 bar.col = FALSE,
                 polygon.col = FALSE,
                 grid.col = FALSE,
                 y.axis = FALSE,
                 1wd = 0)
## now with direct display of De errors, without 2-sigma bar
plot_AbanicoPlot(data = ExampleData.DeValues,
                 bar.col = FALSE,
                 ylab = "".
                 y.axis = FALSE,
                 error.bars = TRUE)
## now with user-defined axes labels
plot_AbanicoPlot(data = ExampleData.DeValues,
                 xlab = c("Data error (%)",
                          "Data precision"),
                 ylab = "Scatter",
                 zlab = "Equivalent dose (Gy)")
## now with minimum, maximum and median value indicated
plot_AbanicoPlot(data = ExampleData.DeValues,
                 stats = c("min", "max", "median"))
## now with a brief statistical summary
plot_AbanicoPlot(data = ExampleData.DeValues,
                 summary = c("n", "in.2s")
```

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```
## now with another statistical summary as subheader
plot_AbanicoPlot(data = ExampleData.DeValues,
                 summary = c("mean.weighted", "median"),
                 summary.pos = "topleft")
## now a plot with two 2-sigma bars for one data set
plot_AbanicoPlot(data = ExampleData.DeValues,
                 bar = c(30, 100)
## now the data set is split into sub-groups, one is manipulated
data.1 <- ExampleData.DeValues[1:30,]</pre>
data.2 <- ExampleData.DeValues[31:62,] * 1.3</pre>
## now a common dataset is created from the two subgroups
data.3 <- list(data.1, data.2)</pre>
## now the two data sets are plotted in one plot
plot_AbanicoPlot(data = data.3)
## now with some graphical modification
plot_AbanicoPlot(data = data.3,
                 z.0 = "median"
                 col = c("steelblue4", "orange4"),
                 bar.col = c("steelblue3", "orange3"),
                 polygon.col = c("steelblue1", "orange1"),
                 pch = c(2, 6),
                 angle = c(30, 50),
                 summary = c("n", "in.2s", "median"))
## create Abanico plot with predefined layout definition
plot_AbanicoPlot(data = ExampleData.DeValues,
                 layout = "journal")
## now with predefined layout definition and further modifications
plot_AbanicoPlot(data = data.3,
                 z.0 = "median",
                 layout = "journal",
                 col = c("steelblue4", "orange4"),
                 bar.col = adjustcolor(c("steelblue3", "orange3"),
                                       alpha.f = 0.5),
                 polygon.col = c("steelblue3", "orange3"))
## for further information on layout definitions see documentation
## of function get_Layout()
## restore original graphical parameters
par(par.old)
```

plot\_DRTResults

Visualise dose recovery test results

# **Description**

The function provides a standardised plot output for dose recovery test measurements.

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# Usage

```
plot_DRTResults(values, given.dose, error.range = 10, preheat,
  boxplot = FALSE, mtext, summary, summary.pos, legend, legend.pos,
  par.local = TRUE, na.rm = FALSE, ...)
```

### **Arguments**

rguments	
values	RLum.Results or data.frame, ( <b>required</b> ): input values containing at least De and De error. To plot more than one data set in one figure, a list of the individual data sets must be provided (e.g. list(dataset.1, dataset.2)).
given.dose	numeric (optional): given dose used for the dose recovery test to normalise data. If only one given dose is provided this given dose is valid for all input data sets (i.e., values is a list). Otherwise a given dose for each input data set has to be provided (e.g., given.dose = c(100,200)). If no given.dose values are plotted without normalisation (might be useful for preheat plateau tests). Note: Unit has to be the same as from the input values (e.g., Seconds or Gray).
error.range	numeric: symmetric error range in percent will be shown as dashed lines in the plot. Set error range to 0 to void plotting of error ranges.
preheat	numeric: optional vector of preheat temperatures to be used for grouping the De values. If specified, the temperatures are assigned to the x-axis.
boxplot	logical: optionally plot values, that are grouped by preheat temperature as boxplots. Only possible when preheat vector is specified.
mtext	character: additional text below the plot title.
summary	character (optional): adds numerical output to the plot. Can be one or more out of: "n" (number of samples), "mean" (mean De value), "mean.weighted" (error-weighted mean), "median" (median of the De values), "sdrel" (relative standard deviation in percent), "sdabs" (absolute standard deviation), "serel" (relative standard error) and "seabs" (absolute standard error).
summary.pos	numeric or character (with default): optional position coordinates or keyword (e.g. "topright") for the statistical summary. Alternatively, the keyword "sub" may be specified to place the summary below the plot header. However, this latter option in only possible if mtext is not used.
legend	character vector (optional): legend content to be added to the plot.
legend.pos	numeric or character (with default): optional position coordinates or keyword (e.g. "topright") for the legend to be plotted.
par.local	logical (with default): use local graphical parameters for plotting, e.g. the plot is shown in one column and one row. If par.local = FALSE, global parameters are inherited.
na.rm	logical: indicating wether NA values are removed before plotting from the input data set
	further arguments and graphical parameters passed to plot.

# **Details**

Procedure to test the accuracy of a measurement protocol to reliably determine the dose of a specific sample. Here, the natural signal is erased and a known laboratory dose administered which is treated as unknown. Then the De measurement is carried out and the degree of congruence between administered and recovered dose is a measure of the protocol's accuracy for this sample. In the plot the normalised De is shown on the y-axis, i.e. obtained De/Given Dose.

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#### Value

A plot is returned.

### **Function version**

```
0.1.6 (2015-08-21 14:53:14)
```

#### Note

Further data and plot arguments can be added by using the appropriate R commands.

### Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France), Michael Dietze, GFZ Potsdam (Germany) R Luminescence Package Team

#### References

Wintle, A.G., Murray, A.S., 2006. A review of quartz optically stimulated luminescence characteristics and their relevance in single-aliquot regeneration dating protocols. Radiation Measurements, 41, 369-391.

### See Also

plot

# **Examples**

```
## read example data set and misapply them for this plot type
data(ExampleData.DeValues, envir = environment())
## plot values
plot_DRTResults(values = ExampleData.DeValues$BT998[7:11,],
given.dose = 2800, mtext = "Example data")
## plot values with legend
plot_DRTResults(values = ExampleData.DeValues$BT998[7:11,],
                given.dose = 2800,
                legend = "Test data set")
## create and plot two subsets with randomised values
x.1 <- ExampleData.DeValues$BT998[7:11,]</pre>
x.2 <- ExampleData.DeValues$BT998[7:11,] * c(runif(5, 0.9, 1.1), 1)
plot_DRTResults(values = list(x.1, x.2),
                given.dose = 2800)
## some more user-defined plot parameters
plot_DRTResults(values = list(x.1, x.2),
                given.dose = 2800,
                pch = c(2, 5),
                col = c("orange", "blue"),
                xlim = c(0, 8),
                ylim = c(0.85, 1.15),
```

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```
xlab = "Sample aliquot")
## plot the data with user-defined statistical measures as legend
plot_DRTResults(values = list(x.1, x.2),
                given.dose = 2800,
                summary = c("n", "mean.weighted", "sd"))
## plot the data with user-defined statistical measures as sub-header
plot_DRTResults(values = list(x.1, x.2),
                given.dose = 2800,
                summary = c("n", "mean.weighted", "sd"),
                summary.pos = "sub")
## plot the data grouped by preheat temperatures
plot_DRTResults(values = ExampleData.DeValues$BT998[7:11,],
                given.dose = 2800,
                preheat = c(200, 200, 200, 240, 240))
## read example data set and misapply them for this plot type
data(ExampleData.DeValues, envir = environment())
## plot values
plot_DRTResults(values = ExampleData.DeValues$BT998[7:11,],
                given.dose = 2800, mtext = "Example data")
## plot two data sets grouped by preheat temperatures
plot_DRTResults(values = list(x.1, x.2),
                given.dose = 2800,
                preheat = c(200, 200, 200, 240, 240)
## plot the data grouped by preheat temperatures as boxplots
plot_DRTResults(values = ExampleData.DeValues$BT998[7:11,],
                given.dose = 2800,
                preheat = c(200, 200, 200, 240, 240),
                boxplot = TRUE)
```

plot\_GrowthCurve

Fit and plot a growth curve for luminescence data (Lx/Tx against dose)

# **Description**

A dose response curve is produced for luminescence measurements using a regenerative protocol.

### Usage

```
plot_GrowthCurve(sample, na.rm = TRUE, fit.method = "EXP",
  fit.force_through_origin = FALSE, fit.weights = TRUE,
  fit.includingRepeatedRegPoints = TRUE, fit.NumberRegPoints,
  fit.NumberRegPointsReal, fit.bounds = TRUE, NumberIterations.MC = 100,
  output.plot = TRUE, output.plotExtended = TRUE,
  output.plotExtended.single = FALSE, cex.global = 1, ...)
```

# **Arguments**

sample

data.frame (**required**): data frame with three columns for x=Dose,y=LxTx,z=LxTx.Error, y1=TnTx. The column for the test dose response is optional, but requires 'TnTx' as column name if used.

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na.rm logical (with default): excludes NA values from the data set prior to any further

operations.

fit.method character (with default): function used for fitting. Possible options are: LIN,

EXP, EXP OR LIN, EXP+LIN or EXP+EXP. See details.

fit.force\_through\_origin

logical (with default) allow to force the fitted function through the origin. For method = "EXP+EXP" the function will go to the origin in either case, so this option will have no effect

option will have no effect.

fit.weights logical (with default): option whether the fitting is done with or without weights.

See details.

fit.includingRepeatedRegPoints

logical (with default): includes repeated points for fitting (TRUE/FALSE).

fit.NumberRegPoints

integer (optional): set number of regeneration points manually. By default the number of all (!) regeneration points is used automatically.

fit.NumberRegPointsReal

integer (optional): if the number of regeneration points is provided manually, the value of the real, regeneration points = all points (repeated points) including reg 0, has to be inserted.

fit.bounds 1

logical (with default): set lower fit bounds for all fitting parameters to 0. Limited for the use with the fit methods EXP, EXP+LIN and EXP OR LIN. Argument to be inserted for experimental application only!

NumberIterations.MC

integer (with default): number of Monte Carlo simulations for error estimation. See details.

output.plot logical (with default): plot output (TRUE/FALSE).

 $\verb"output.plotExtended"$ 

logical (with default): If TRUE, 3 plots on one plot area are provided: (1) growth curve, (2) histogram from Monte Carlo error simulation and (3) a test dose response plot. If FALSE, just the growth curve will be plotted. **Requires:** output.plot = TRUE.

 $\verb"output.plotExtended.single"$ 

logical (with default): single plot output (TRUE/FALSE) to allow for plotting the results in single plot windows. Requires output.plot = TRUE and output.plotExtended = TRUE.

cex.global numeric (with default): global scaling factor.

Further arguments and graphical parameters to be passed. Note: Standard arguments will only be passed to the growth curve plot. Supported: xlim, ylim, main, xlab, ylab

# **Details**

# Fitting methods

For all options (except for the LIN and the EXP OR LIN), the nls function with the port algorithm is used.

LIN: fits a linear function to the data using lm:

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EXP: try to fit a function of the form

$$y = a * (1 - exp(-(x+c)/b))$$

Parameters b and c are approximated by a linear fit using lm. Note: b = D0

EXP OR LIN: works for some cases where an EXP fit fails. If the EXP fit fails, a LIN fit is done instead.

EXP+LIN: tries to fit an exponential plus linear function of the form:

$$y = a * (1 - exp(-(x+c)/b) + (g * x))$$

The De is calculated by iteration.

**Note:** In the context of luminescence dating, this function has no physical meaning. Therefore, no D0 value is returned.

EXP+EXP: tries to fit a double exponential function of the form

$$y = (a1 * (1 - exp(-(x)/b1))) + (a2 * (1 - exp(-(x)/b2)))$$

This fitting procedure is not robust against wrong start parameters and should be further improved.

#### Fit weighting

If the option fit.weights = TRUE is chosen, weights are calculated using provided signal errors (Lx/Tx error):

$$fit.weights = 1/error/(sum(1/error))$$

# **Error estimation using Monte Carlo simulation**

Error estimation is done using a Monte Carlo (MC) simulation approach. A set of Lx/Tx values is constructed by randomly drawing curve data from samled from normal distributions. The normal distribution is defined by the input values (mean = value, sd = value.error). Then, a growth curve fit is attempted for each dataset resulting in a new distribution of single De values. The sd of this distribution is becomes then the error of the De. With increasing iterations, the error value becomes more stable. **Note:** It may take some calculation time with increasing MC runs, especially for the composed functions (EXP+LIN and EXP+EXP).

Each error estimation is done with the function of the chosen fitting method.

# **Subtitle information**

To avoid plotting the subtitle information, provide an empty user mtext mtext = "". To plot any other subtitle text, use mtext.

#### Value

Along with a plot (so far wanted) an RLum. Results object is returned containing:

data:

- $..~\$ De: \verb"data.frame" (table of De values)$
- .. \$Fit: nls object from the fitting for EXP, EXP+LIN and EXP+EXP. In case of a resulting linear fit when using EXP OR LIN, a lm object is returned.
- .. \$Formula: expression
- .. \$call: call (the original function call)

## **Function version**

1.7.2 (2015-08-21 18:08:35)

plot\_Histogram

### Author(s)

```
Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France),
Michael Dietze, GFZ Potsdam (Germany)
R Luminescence Package Team
```

### See Also

```
nls, RLum. Results, get_RLum, nlsLM, lm
```

# **Examples**

```
##(1) plot growth curve for a dummy data.set and show De value
data(ExampleData.LxTxData, envir = environment())
temp <- plot_GrowthCurve(LxTxData)
get_RLum(temp)

##(1a) to access the fitting value try
get_RLum(temp, data.object = "Fit")

##(2) plot the growth curve only - uncomment to use
##pdf(file = "~/Desktop/Growth_Curve_Dummy.pdf", paper = "special")
plot_GrowthCurve(LxTxData)
##dev.off()

##(3) plot growth curve with pdf output - uncomment to use, single output
##pdf(file = "~/Desktop/Growth_Curve_Dummy.pdf", paper = "special")
plot_GrowthCurve(LxTxData, output.plotExtended.single = TRUE)
##dev.off()</pre>
```

plot\_Histogram

Plot a histogram with separate error plot

# Description

Function plots a predefined histogram with an accompanying error plot as suggested by Rex Galbraith at the UK LED in Oxford 2010.

# Usage

```
plot_Histogram(data, na.rm = TRUE, mtext, cex.global, se, rug, normal_curve,
    summary, summary.pos, colour, ...)
```

# **Arguments**

data	data.frame or RLum.Results object (required): for data.frame: two columns: De (data[,1]) and De error (data[,2])
na.rm	logical (with default): excludes NA values from the data set prior to any further operations.
mtext	character (optional): further sample information (mtext).
cex.global	numeric (with default): global scaling factor.

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se logical (optional): plots standard error points over the histogram, default is

FALSE.

rug logical (optional): adds rugs to the histogram, default is TRUE.

normal\_curve logical (with default): adds a normal curve to the histogram. Mean and sd are

calculated from the input data. More see details section.

summary character (optional): add statistic measures of centrality and dispersion to the

plot. Can be one or more of several keywords. See details for available key-

words.

summary.pos numeric or character (with default): optional position coordinates or key-

word (e.g. "topright") for the statistical summary. Alternatively, the keyword "sub" may be specified to place the summary below the plot header. However, this latter option in only possible if mtext is not used. In case of coordinate

specification, y-coordinate refers to the right y-axis.

colour numeric or character (with default): optional vector of length 4 which specifies

the colours of the following plot items in exactly this order: histogram bars, rug

lines, normal distribution curve and standard error points

(e.g., c("grey", "black", "red", "grey")).

... further arguments and graphical parameters passed to plot or hist. If y-axis

labels are provided, these must be specified as a vector of length 2 since the plot features two axes (e.g. ylab = c("axis label 1", "axis label 2")). Y-axes limits (ylim) must be provided as vector of length four, with the first two elements specifying the left axes limits and the latter two elements giving the

right axis limits.

## **Details**

If the normal curve is added, the y-axis in the histogram will show the probability density.

A statistic summary, i.e. a collection of statistic measures of centrality and dispersion (and further measures) can be added by specifying one or more of the following keywords: "n" (number of samples), "mean" (mean De value), "mean.weighted" (error-weighted mean), "median" (median of the De values), "sdrel" (relative standard deviation in percent), "sdrel.weighted" (error-weighted relative standard deviation in percent), "sdabs" (absolute standard deviation), "sdabs.weighted" (error-weighted absolute standard deviation), "serel" (relative standard error), "serel.weighted" (error-weighted relative standard error), "seabs" (absolute standard error), "seabs.weighted" (error-weighted absolute standard error), "kurtosis" (kurtosis) and "skewness" (skewness).

# **Function version**

0.4.4 (2015-08-21 14:53:14)

## Note

The input data is not restricted to a special type.

# Author(s)

Michael Dietze, GFZ Potsdam (Germany), Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team 118 plot\_KDE

#### See Also

```
hist, plot
```

#### **Examples**

```
## load data
data(ExampleData.DeValues, envir = environment())
ExampleData.DeValues <-</pre>
  Second2Gray(ExampleData.DeValues$BT998, dose.rate = c(0.0438,0.0019))
## plot histogram the easiest way
plot_Histogram(ExampleData.DeValues)
## plot histogram with some more modifications
plot_Histogram(ExampleData.DeValues,
                rug = TRUE,
                normal_curve = TRUE,
                cex.global = 0.9,
                pch = 2,
                colour = c("grey", "black", "blue", "green"),
summary = c("n", "mean", "sdrel"),
                summary.pos = "topleft",
                main = "Histogram of De-values",
                mtext = "Example data set",
                ylab = c(expression(paste(D[e], " distribution")),
                          "Standard error"),
                xlim = c(100, 250),
                ylim = c(0, 0.1, 5, 20))
```

plot\_KDE

Plot kernel density estimate with statistics

### **Description**

Plot a kernel density estimate of measurement values in combination with the actual values and associated error bars in ascending order. Optionally, statistical measures such as mean, median, standard deviation, standard error and quartile range can be provided visually and numerically.

### Usage

```
plot_KDE(data, na.rm = TRUE, weights = FALSE, values.cumulative = TRUE,
  centrality, dispersion, summary, summary.pos, polygon.col, order = TRUE,
  bw = "nrd0", output = FALSE, ...)
```

# **Arguments**

data data.frame or RLum.Results object (required): for data.frame: two columns:

De (values[,1]) and De error (values[,2]). For plotting multiple data sets, these must be provided as list (e.g. list(dataset1,dataset2)).

na.rm logical (with default): exclude NA values from the data set prior to any further operations.

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weights logical (with default): calculate the KDE with De-errors as weights. Attention,

using errors as weights will result in a plot similar to a a probability density plot,

with all ambiguities related to this plot type!

values.cumulative

logical (with default): show cumulative individual data.

centrality character: measure(s) of centrality, used for plotting vertical lines of the re-

spective measure. Can be one out of "mean", "median", "mean.weighted",

"median.weighted" and "kdemax".

dispersion character: measure of dispersion, used for drawing the polygon that depicts

the dose distribution. One out of "sd" (standard deviation), "2sd" (2 standard

deviations) "qr" (quartile range).

summary character (optional): add statistic measures of centrality and dispersion to the

plot. Can be one or more of several keywords. See details for available key-

words.

summary.pos numeric or character (with default): optional position coordinates or key-

word (e.g. "topright") for the statistical summary. Alternatively, the keyword "sub" may be specified to place the summary below the plot header. However, this latter option in only possible if mtext is not used. In case of coordinate

specification, y-coordinate refers to the right y-axis.

polygon.col character or numeric (with default): colour of the polygon showing the dose

dispersion around the central value. Only relevant if dispersion is specified.

order logical: Order data in ascending order.

bw character (with default): bin-width, chose a numeric value for manual setting.

output logical: Optional output of numerical plot parameters. These can be useful to

reproduce similar plots. Default is FALSE.

... further arguments and graphical parameters passed to plot.

### Details

The function allow passing several plot arguments, such as main, xlab, cex. However, as the figure is an overlay of two separate plots, ylim must be specified in the order:  $c(ymin_axis1, ymax_axis1, ymin_axis2, ymax_axis2)$  when using the cumulative values plot option. Similarly, if other than the default colours are desired, the argument col must be provided with colours in the following order: probability density function, De values, De error bars, sd or qr polygon. The line type (lty) for additional measures of centrality will cycle through the default values (1, 2, ...) by default, i.e. KDE line solid, further vertical lines dashed, dotted, dash-dotted and so on. To change this behaviour specify the desired order of line types (e.g. lty = c(1, 3, 2, 5)). See examples for some further explanations. For details on the calculation of the bin-width (parameter bw) see density.

A statistic summary, i.e. a collection of statistic measures of centrality and dispersion (and further measures) can be added by specifying one or more of the following keywords: "n" (number of samples), "mean" (mean De value), "mean.weighted" (error-weighted mean), "median" (median of the De values), "sdrel" (relative standard deviation in percent), "sdrel.weighted" (error-weighted relative standard deviation in percent), "sdabs" (absolute standard deviation), "sdabs.weighted" (error-weighted absolute standard deviation), "serel" (relative standard error), "serel.weighted" (error-weighted relative standard error), "seabs" (absolute standard error), "seabs.weighted" (error-weighted absolute standard error), "in.2s" (percent of samples in 2-sigma range), "kurtosis" (kurtosis) and "skewness" (skewness).

plot\_KDE

#### **Function version**

```
3.5 (2015-08-21 14:53:14)
```

#### Note

The plot output is no 'PD' plot (cf. the discussion of Berger and Galbraith in Ancient TL; see references)!

### Author(s)

```
Michael Dietze, GFZ Potsdam (Germany),
Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne
R Luminescence Package Team
```

### See Also

```
density, plot
```

## **Examples**

```
## read example data set
data(ExampleData.DeValues, envir = environment())
ExampleData.DeValues <-</pre>
  Second2Gray(ExampleData.DeValues$BT998, c(0.0438,0.0019))
## create plot straightforward
plot_KDE(data = ExampleData.DeValues)
## create plot with logarithmic x-axis
plot_KDE(data = ExampleData.DeValues,
         log = "x")
## create plot with user-defined labels and axes limits
plot_KDE(data = ExampleData.DeValues,
         main = "Dose distribution",
         xlab = "Dose (s)",
         ylab = c("KDE estimate", "Cumulative dose value"),
         xlim = c(100, 250),
         ylim = c(0, 0.08, 0, 30))
## create plot with centrality lines and distribution polygons
plot_KDE(data = ExampleData.DeValues,
         ylim = c(0, 0.08, 0, 35),
         centrality = c("median", "mean"),
         dispersion = "sd",
         polygon.col = "lightblue")
## create plot with statistical summary below header
plot_KDE(data = ExampleData.DeValues,
         summary = c("n", "median", "skewness", "qr"))
## create plot with statistical summary as legend
plot_KDE(data = ExampleData.DeValues,
         summary = c("n", "mean", "sdrel", "seabs"),
         summary.pos = "topleft")
```

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```
## split data set into sub-groups, one is manipulated, and merge again
data.1 <- ExampleData.DeValues[1:15,]</pre>
data.2 <- ExampleData.DeValues[16:25,] * 1.3</pre>
data.3 <- list(data.1, data.2)</pre>
## create plot with two subsets straightforward
plot_KDE(data = data.3)
## create plot with two subsets and summary legend at user coordinates
plot_KDE(data = data.3,
         summary = c("n", "median", "skewness"),
         summary.pos = c(110, 0.07),
         col = c("blue", "orange"))
## example of how to use the numerical output of the function
## return plot output to draw a thicker KDE line
KDE <- plot_KDE(data = ExampleData.DeValues,</pre>
                output = TRUE)
## read out coordinates of KDE graph
KDE.x <- KDE$De.density[[1]]$x</pre>
KDE.y <- KDE$De.density[[1]]$y</pre>
## transform y-values to right y-axis dimensions
KDE.y \leftarrow KDE.y / max(KDE.y) * (nrow(ExampleData.DeValues) - 1) + 1
## draw the KDE line
lines(x = KDE.x,
      y = KDE.y,
      1wd = 3)
```

plot\_NRt

Visualise natural/regenerated signal ratios

#### **Description**

This function creates a Natural/Regenerated signal vs. time (NR(t)) plot as shown in Steffen et al. 2009

# Usage

```
plot_NRt(data, log = FALSE, smooth = c("none", "spline", "rmean"), k = 3,
  legend = TRUE, legend.pos = "topright", ...)
```

# **Arguments**

data	a list, data.frame, matrix or RLum.Analysis object ( $\mathbf{required}$ ). X,Y data of measured values (time and counts). See details on individual data structure.
log	character (optional): logarithmic axes (c("x", "y", "xy")).
smooth	<pre>character (optional): apply data smoothing. Use "rmean" to calculate the rolling where k determines the width of the rolling window (see rollmean). "spline" applies a smoothing spline to each curve (see smooth.spline)</pre>
k	integer (with default): integer width of the rolling window.

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```
    legend logical (with default): show or hide the plot legend.
    legend.pos character (with default): keyword specifying the position of the legend (see legend).
    further parameters passed to plot (also see par).
```

#### **Details**

This function accepts the individual curve data in many different formats. If data is a list, each element of the list must contain a two column data. frame or matrix containing the XY data of the curves (time and counts). Alternatively, the elements can be objects of class RLum. Data. Curve. Input values can also be provided as a data. frame or matrix where the first column contains the time values and each following column contains the counts of each curve.

#### Value

Returns a plot and RLum. Analysis object.

# Author(s)

Christoph Burow, University of Cologne (Germany)

#### References

Steffen, D., Preusser, F., Schlunegger, F., 2009. OSL quartz underestimation due to unstable signal components. Quaternary Geochronology, 4, 353-362.

# See Also

plot

# **Examples**

```
## load example data
data("ExampleData.BINfileData")
## EXAMPLE 1
## convert Risoe.BINfileData object to RLum.Analysis object
data <- Risoe.BINfileData2RLum.Analysis(object = CWOSL.SAR.Data, pos = 8, 1type = "OSL")</pre>
## extract all OSL curves
allCurves <- get_RLum(data)</pre>
## keep only the natural and regenerated signal curves
pos < - seq(1, 9, 2)
curves <- allCurves[pos]</pre>
## plot a standard NR(t) plot
plot_NRt(curves)
## re-plot with rolling mean data smoothing
plot_NRt(curves, smooth = "rmean", k = 10)
## re-plot with a logarithmic x-axis
plot_NRt(curves, log = "x", smooth = "rmean", k = 5)
```

```
## re-plot with custom axes ranges
plot_NRt(curves, smooth = "rmean", k = 5,
         xlim = c(0.1, 5), ylim = c(0.4, 1.6),
         legend.pos = "bottomleft")
## re-plot with smoothing spline on log scale
plot_NRt(curves, smooth = "spline", log = "x",
         legend.pos = "top")
## EXAMPLE 2
# you may also use this function to check whether all
# TD curves follow the same shape (making it a TnTx(t) plot).
posTD <- seq(2, 14, 2)
curves <- allCurves[posTD]</pre>
plot_NRt(curves, main = "TnTx(t) Plot",
         smooth = "rmean", k = 20,
         ylab = "TD natural / TD regenerated",
         xlim = c(0, 20), legend = FALSE)
## EXAMPLE 3
# extract data from all positions
data <- lapply(1:24, FUN = function(pos) {</pre>
   Risoe.BINfileData2RLum.Analysis(CWOSL.SAR.Data, pos = pos, ltype = "OSL")
})
# get individual curve data from each aliquot
aliquot <- lapply(data, get_RLum)</pre>
# set graphical parameters
par(mfrow = c(2, 2))
# create NR(t) plots for all aliquots
for (i in 1:length(aliquot)) {
   plot_NRt(aliquot[[i]][pos],
            main = paste0("Aliquot #", i),
            smooth = "rmean", k = 20,
            xlim = c(0, 10),
            cex = 0.6, legend.pos = "bottomleft")
}
# reset graphical parameters
par(mfrow = c(1, 1))
```

plot\_RadialPlot

Function to create a Radial Plot

### **Description**

A Galbraith's radial plot is produced on a logarithmic or a linear scale.

### **Usage**

```
plot_RadialPlot(data, na.rm = TRUE, negatives = "remove", log.z = TRUE,
 central.value, centrality = "mean.weighted", mtext, summary, summary.pos,
 legend, legend.pos, stats, rug = FALSE, plot.ratio, bar.col,
 y.ticks = TRUE, grid.col, line, line.col, line.label, output = FALSE, ...)
```

# **Arguments**

data data.frame or RLum.Results object (required): for data.frame two columns: De (data[,1]) and De error (data[,2]). To plot several data sets in one plot, the data sets must be provided as list, e.g. list(data.1, data.2). logical (with default): excludes NA values from the data set prior to any further na.rm operations. negatives character (with default): rule for negative values. Default is "remove" (i.e. negative values are removed from the data set). logical (with default): Option to display the z-axis in logarithmic scale. Delog.z fault is TRUE. central.value numeric: User-defined central value, primarily used for horizontal centering of the z-axis. character or numeric (with default): measure of centrality, used for automatcentrality ically centering the plot and drawing the central line. Can either be one out of "mean", "median", "mean.weighted" and "median.weighted" or a numeric value used for the standardisation.

mtext character: additional text below the plot title.

character (optional): add statistic measures of centrality and dispersion to the summary plot. Can be one or more of several keywords. See details for available key-

numeric or character (with default): optional position coordinates or keyword summary.pos (e.g. "topright") for the statistical summary. Alternatively, the keyword "sub" may be specified to place the summary below the plot header. However, this

latter option is only possible if mtext is not used.

legend character vector (optional): legend content to be added to the plot.

legend.pos numeric or character (with default): optional position coordinates or keyword

(e.g. "topright") for the legend to be plotted.

stats character: additional labels of statistically important values in the plot. One

or more out of the following: "min", "max", "median".

logical: Option to add a rug to the z-scale, to indicate the location of individual rug

values

plot.ratio numeric: User-defined plot area ratio (i.e. curvature of the z-axis). If omitted,

> the default value (4.5/5.5) is used and modified automatically to optimise the zaxis curvature. The parameter should be decreased when data points are plotted

outside the z-axis or when the z-axis gets too elliptic.

bar.col character or numeric (with default): colour of the bar showing the 2-sigma

range around the central value. To disable the bar, use "none". Default is

y.ticks logical: Option to hide y-axis labels. Useful for data with small scatter.

grid.col character or numeric (with default): colour of the grid lines (originating at

[0,0] and stretching to the z-scale). To disable grid lines, use "none". Default is

"grey".

line numeric: numeric values of the additional lines to be added.

line.col character or numeric: colour of the additional lines.

line.label character: labels for the additional lines.

output logical: Optional output of numerical plot parameters. These can be useful to

reproduce similar plots. Default is FALSE.

... Further plot arguments to pass. xlab must be a vector of length 2, specifying

the upper and lower x-axes labels.

#### **Details**

Details and the theoretical background of the radial plot are given in the cited literature. This function is based on an S script of Rex Galbraith. To reduce the manual adjustments, the function has been rewritten. Thanks to Rex Galbraith for useful comments on this function.

Plotting can be disabled by adding the argument plot = "FALSE", e.g. to return only numeric plot output.

Earlier versions of the Radial Plot in this package had the 2-sigma-bar drawn onto the z-axis. However, this might have caused misunderstanding in that the 2-sigma range may also refer to the z-scale, which it does not! Rather it applies only to the x-y-coordinate system (standardised error vs. precision). A spread in doses or ages must be drawn as lines originating at zero precision (x0) and zero standardised estimate (y0). Such a range may be drawn by adding lines to the radial plot (line, line.col, line.label, cf. examples).

A statistic summary, i.e. a collection of statistic measures of centrality and dispersion (and further measures) can be added by specifying one or more of the following keywords: "n" (number of samples), "mean" (mean De value), "mean.weighted" (error-weighted mean), "median" (median of the De values), "sdrel" (relative standard deviation in percent), "sdrel.weighted" (error-weighted relative standard deviation in percent), "sdabs" (absolute standard deviation), "sdabs.weighted" (error-weighted absolute standard deviation), "serel" (relative standard error), "serel.weighted" (error-weighted relative standard error), "seabs" (absolute standard error), "seabs.weighted" (error-weighted absolute standard error), "in.2s" (percent of samples in 2-sigma range), "kurtosis" (kurtosis) and "skewness" (skewness).

# Value

Returns a plot object.

### **Function version**

0.5.3 (2015-08-21 14:53:14)

# Author(s)

Michael Dietze, GFZ Potsdam (Germany), Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) Based on a rewritten S script of Rex Galbraith, 2010 R Luminescence Package Team

#### References

Galbraith, R.F., 1988. Graphical Display of Estimates Having Differing Standard Errors. Technometrics, 30 (3), 271-281.

Galbraith, R.F., 1990. The radial plot: Graphical assessment of spread in ages. International Journal of Radiation Applications and Instrumentation. Part D. Nuclear Tracks and Radiation Measurements, 17 (3), 207-214.

Galbraith, R. & Green, P., 1990. Estimating the component ages in a finite mixture. International Journal of Radiation Applications and Instrumentation. Part D. Nuclear Tracks and Radiation Measurements, 17 (3) 197-206.

Galbraith, R.F. & Laslett, G.M., 1993. Statistical models for mixed fission track ages. Nuclear Tracks And Radiation Measurements, 21 (4), 459-470.

Galbraith, R.F., 1994. Some Applications of Radial Plots. Journal of the American Statistical Association, 89 (428), 1232-1242.

Galbraith, R.F., 2010. On plotting OSL equivalent doses. Ancient TL, 28 (1), 1-10.

Galbraith, R.F. & Roberts, R.G., 2012. Statistical aspects of equivalent dose and error calculation and display in OSL dating: An overview and some recommendations. Quaternary Geochronology, 11, 1-27.

### See Also

```
plot, plot_KDE, plot_Histogram
```

## **Examples**

```
## load example data
data(ExampleData.DeValues, envir = environment())
ExampleData.DeValues <- Second2Gray(ExampleData.DeValues$BT998, c(0.0438,0.0019))
## plot the example data straightforward
plot_RadialPlot(data = ExampleData.DeValues)
## now with linear z-scale
plot_RadialPlot(data = ExampleData.DeValues,
                log.z = FALSE)
## now with output of the plot parameters
plot1 <- plot_RadialPlot(data = ExampleData.DeValues,</pre>
                         log.z = FALSE,
                         output = TRUE)
plot1
plot1$zlim
## now with adjusted z-scale limits
plot_RadialPlot(data = ExampleData.DeValues,
               log.z = FALSE,
               zlim = c(100, 200))
## now the two plots with serious but seasonally changing fun
#plot_RadialPlot(data = data.3, fun = TRUE)
## now with user-defined central value, in log-scale again
plot_RadialPlot(data = ExampleData.DeValues,
                central.value = 150)
```

```
## now with a rug, indicating individual De values at the z-scale
plot_RadialPlot(data = ExampleData.DeValues,
                rug = TRUE)
## now with legend, colour, different points and smaller scale
plot_RadialPlot(data = ExampleData.DeValues,
                legend.text = "Sample 1",
                col = "tomato4",
                bar.col = "peachpuff",
                pch = "R",
                cex = 0.8)
## now without 2-sigma bar, y-axis, grid lines and central value line
plot_RadialPlot(data = ExampleData.DeValues,
                bar.col = "none",
                grid.col = "none",
                y.ticks = FALSE,
                lwd = 0)
## now with user-defined axes labels
plot_RadialPlot(data = ExampleData.DeValues,
                xlab = c("Data error (%)",
                         "Data precision"),
                ylab = "Scatter",
                zlab = "Equivalent dose (Gy)")
## now with minimum, maximum and median value indicated
plot_RadialPlot(data = ExampleData.DeValues,
                central.value = 150,
                stats = c("min", "max", "median"))
## now with a brief statistical summary
plot_RadialPlot(data = ExampleData.DeValues,
                summary = c("n", "in.2s"))
## now with another statistical summary as subheader
plot_RadialPlot(data = ExampleData.DeValues,
                summary = c("mean.weighted", "median"),
                summary.pos = "sub")
## now the data set is split into sub-groups, one is manipulated
data.1 <- ExampleData.DeValues[1:15,]</pre>
data.2 <- ExampleData.DeValues[16:25,] * 1.3</pre>
## now a common dataset is created from the two subgroups
data.3 <- list(data.1, data.2)</pre>
## now the two data sets are plotted in one plot
plot_RadialPlot(data = data.3)
## now with some graphical modification
plot_RadialPlot(data = data.3,
                col = c("darkblue", "darkgreen"),
                bar.col = c("lightblue", "lightgreen"),
                pch = c(2, 6),
                summary = c("n", "in.2s"),
```

```
summary.pos = "sub",
legend = c("Sample 1", "Sample 2"))
```

```
plot_Risoe.BINfileData
```

Plot single luminescence curves from a BIN file object

# Description

Plots single luminescence curves from an object returned by the read\_BIN2R function.

# Usage

```
plot_Risoe.BINfileData(BINfileData, position, run, set, sorter = "POSITION",
    ltype = c("IRSL", "OSL", "TL", "RIR", "RBR", "RL"), curve.transformation,
    dose_rate, temp.lab, cex.global = 1, ...)
```

# Arguments

BINfileData	$\label{linear} {\bf Risoe. BIN file Data-class} \ ({\bf required}): \ requires \ an \ S4 \ object \ returned \ by \ the \ {\bf read\_BIN2R} $ function.	
position	vector (optional): option to limit the plotted curves by position (e.g. position = 1, position = $c(1,3,5)$ ).	
run	vector (optional): option to limit the plotted curves by run (e.g., run = $1$ , run = $c(1,3,5)$ ).	
set	vector (optional): option to limit the plotted curves by set (e.g., set = $1$ , set = $c(1,3,5)$ ).	
sorter	character (with default): the plot output can be ordered by "POSITION", "SET" or "RUN". POSITION, SET and RUN are options defined in the Risoe Sequence Editor.	
ltype	character (with default): option to limit the plotted curves by the type of luminescence stimulation. Allowed values: "IRSL", "OSL", "TL", "RIR", "RBR" (corresponds to LM-OSL), "RL". All type of curves are plotted by default.	
curve.transformation		
	character (optional): allows transforming CW-OSL and CW-IRSL curves to pseudo-LM curves via transformation functions. Allowed values are: CW2pLM, CW2pLMi, CW2pHMi and CW2pPMi. See details.	
dose_rate	numeric (optional): dose rate of the irradition source at the measurement date. If set, the given irradiation dose will be shown in Gy. See details.	
temp.lab	character (optional): option to allow for different temperature units. If no value is set deg. C is chosen.	
cex.global	numeric (with default): global scaling factor.	
	further undocumented plot arguments.	

#### **Details**

#### **Nomenclature**

See Risoe.BINfileData-class

### curve.transformation

This argument allows transforming continuous wave (CW) curves to pseudo (linear) modulated curves. For the transformation, the functions of the package are used. Currently, it is not possible to pass further arguments to the transformation functions. The argument works only for 1type OSL and IRSL.

#### Irradiation time

Plotting the irradiation time (s) or the given dose (Gy) requires that the variable IRR\_TIME has been set within the BIN-file. This is normally done by using the 'Run Info' option within the Sequence Editor or by editing in R.

#### Value

Returns a plot.

### **Function version**

```
0.4.1 (2015-08-21 14:53:14)
```

# Note

The function has been successfully tested for the Sequence Editor file output version 3 and 4.

# Author(s)

```
Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France),
Michael Dietze, GFZ Potsdam (Germany)
R Luminescence Package Team
```

#### References

```
Duller, G., 2007. Analyst. pp. 1-45.
```

# See Also

```
Risoe.BINfileData-class,read_BIN2R, CW2pLM, CW2pLMi, CW2pPMi, CW2pHMi
```

### **Examples**

```
##load data
data(ExampleData.BINfileData, envir = environment())

##plot all curves from the first position to the desktop
#pdf(file = "~/Desktop/CurveOutput.pdf", paper = "a4", height = 11, onefile = TRUE)

##example - load from *.bin file
```

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```
#BINfile<- file.choose()
#BINfileData<-read_BIN2R(BINfile)

#par(mfrow = c(4,3), oma = c(0.5,1,0.5,1))
#plot_Risoe.BINfileData(CWOSL.SAR.Data,position = 1)
#mtext(side = 4, BINfile, outer = TRUE, col = "blue", cex = .7)
#dev.off()</pre>
```

plot\_RLum

General plot function for RLum S4 class objects

#### **Description**

Function calls object specific plot functions for RLum S4 class objects.

### Usage

```
plot_RLum(object, ...)
```

### **Arguments**

object

RLum (**required**): S4 object of class RLum. Optional a list containing objects of class RLum can be provided. In this case the function tries to plot every object in this list according to its RLum class.

. . .

further arguments and graphical parameters that will be passed to the specific plot functions. The only argument that is supported directly is main (setting the plot title). In contrast to the normal behaviour main can be here provided as list and the arguments in the list will dispatched to the plots if the object is of type list as well.

### **Details**

The function provides a generalised access point for plotting specific RLum objects. Depending on the input object, the corresponding plot function will be selected. Allowed arguments can be found in the documentations of each plot function.

objectcorresponding plot functionRLum.Data.Curve: plot\_RLum.Data.CurveRLum.Data.Spectrum: plot\_RLum.Data.SpectrumRLum.Data.Image: plot\_RLum.Data.ImageRLum.Analysis: plot\_RLum.AnalysisRLum.Results: plot\_RLum.Results

## Value

Returns a plot.

# **Function version**

```
0.4.1 (2015-08-30 15:14:19)
```

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#### Note

The provided plot output depends on the input object.

#### Author(s)

```
Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France)
R Luminescence Package Team
```

#### References

#

#### See Also

```
plot_RLum.Data.Curve, RLum.Data.Curve, plot_RLum.Data.Spectrum, RLum.Data.Spectrum,
plot_RLum.Data.Image, RLum.Data.Image, plot_RLum.Analysis, RLum.Analysis, plot_RLum.Results,
RLum.Results
```

# **Examples**

```
#load Example data
data(ExampleData.CW_OSL_Curve, envir = environment())
#transform data.frame to RLum.Data.Curve object
temp <- as(ExampleData.CW_OSL_Curve, "RLum.Data.Curve")</pre>
#plot RLum object
plot_RLum(temp)
```

plot\_RLum.Analysis

Plot function for an RLum. Analysis S4 class object

# **Description**

The function provides a standardised plot output for curve data of an RLum. Analysis S4 class object

# Usage

```
plot_RLum.Analysis(object, subset, nrows = 3, ncols = 2, abline,
  combine = FALSE, curve.transformation, plot.single = FALSE, ...)
```

# **Arguments**

ncols

```
object
                  RLum. Analysis (required): S4 object of class RLum. Analysis
                  named list (optional): subsets elements for plotting. The arguments in the
subset
                  named list will be directly passed to the function get_RLum(e.g., subset = list(curveType = "mo
                  integer (with default): sets number of rows for plot output
nrows
                  integer (with default): sets number of columns for plot output
```

abline list (optional): allows to set similar ablines in each plot. This option uses the

function do.call, meaning that every argument in the list has to be provided as list, e.g. abline = list(list(v = 120), list(v = 350)) produces two vertical ablines: One at 150 and another one at 350. Within the call all

arguments supported by abline are fully supported,

combine logical (with default): allows to combine all codeRLum.Data.Curve objects in

one single plot.

curve.transformation

character (optional): allows transforming CW-OSL and CW-IRSL curves to pseudo-LM curves via transformation functions. Allowed values are: CW2pLM,

CW2pLMi, CW2pHMi and CW2pPMi. See details.

plot.single logical (with default): global par settings are considered, normally this should

end in one plot per page

.. further arguments and graphical parameters will be passed to the plot function.

Supported arguments: main (can be provided as vector for combine = TRUE), mtext, log, lwd, lty type, pch, col, norm, ylim, xlab ... and for combine = TRUE also: xlim, ylab, sub, legend.text, legend.pos (typical plus 'outside'), legend.col

#### **Details**

The function produces a multiple plot output. A file output is recommended (e.g., pdf).

#### curve.transformation

This argument allows transforming continuous wave (CW) curves to pseudo (linear) modulated curves. For the transformation, the functions of the package are used. Currently, it is not possible to pass further arguments to the transformation functions. The argument works only for 1type OSL and IRSL.

Please note: The curve transformation within this functions works roughly, i.e. every IRSL or OSL curve is transformed, without considering whether it is measured with the PMT or not! However, for a fast look it might be helpful.

### Value

Returns multiple plots.

# **Function version**

0.2.7 (2015-08-21 14:53:14)

# Note

Not all arguments available for plot will be passed! Only plotting of RLum.Data.Curve and RLum.Data.Spectrum objects are currently supported.

# Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

plot\_RLum.Data.Curve

#### References

#

#### See Also

```
plot, plot_RLum, plot_RLum. Data. Curve
```

### **Examples**

```
###load data
data(ExampleData.BINfileData, envir = environment())

##convert values for position 1
temp <- Risoe.BINfileData2RLum.Analysis(CWOSL.SAR.Data, pos=1)

##plot all values
plot_RLum.Analysis(temp)

##plot (combine) TL curves in one plot
temp.sel <- get_RLum(temp, recordType = "TL", keep.object = TRUE)
plot_RLum.Analysis(temp.sel, combine = TRUE, norm = TRUE, main = "TL combined")</pre>
```

plot\_RLum.Data.Curve Plot function for an RLum.Data.Curve S4 class object

# Description

The function provides a standardised plot output for curve data of an RLum.Data.Curve S4 class object

### Usage

```
plot_RLum.Data.Curve(object, par.local = TRUE, norm = FALSE, ...)
```

# **Arguments**

object RLum.Data.Curve (required): S4 object of class RLum.Data.Curve

par.local logical (with default): use local graphical parameters for plotting, e.g. the plot is shown in one column and one row. If par.local = FALSE, global parameters are inherited.

norm logical (with default): allows curve normalisation to the highest count value further arguments and graphical parameters that will be passed to the plot func-

tion

### **Details**

Only single curve data can be plotted with this function. Arguments according to plot.

### Value

Returns a plot.

### **Function version**

```
0.1.5 (2015-08-21 14:53:14)
```

#### Note

Not all arguments of plot will be passed!

# Author(s)

```
Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team
```

### References

#

# See Also

```
plot, plot_RLum
```

# **Examples**

```
##plot curve data
#load Example data
data(ExampleData.CW_OSL_Curve, envir = environment())
#transform data.frame to RLum.Data.Curve object
temp <- as(ExampleData.CW_OSL_Curve, "RLum.Data.Curve")
#plot RLum.Data.Curve object
plot_RLum.Data.Curve(temp)</pre>
```

plot\_RLum.Data.Image Plot function for an RLum.Data.Image S4 class object

# **Description**

The function provides a standardised plot output for image data of an RLum.Data.ImageS4 class object, mainly using the plot functions provided by the raster package.

# Usage

```
plot_RLum.Data.Image(object, par.local = TRUE, plot.type = "plot.raster",
    ...)
```

# **Arguments**

object	RLum.Data.Image (required): S4 object of class RLum.Data.Image
par.local	<pre>logical (with default): use local graphical parameters for plotting, e.g. the plot is shown in one column and one row. If par.local = FALSE global parameters are inherited.</pre>
plot.type	$\begin{array}{c} \textbf{character} \ (with \ default) : \ plot \ types. \ Supported \ types \ are \ plot. \ raster, \ plot \ RGB \\ or \ contour \end{array}$
• • •	further arguments and graphical parameters that will be passed to the specific plot functions.

### **Details**

# **Details on the plot functions**

Image is visualised as 2D plot usinng generic plot types provided by other packages.

Supported plot types:

```
plot.type = "plot.raster"
```

Uses the standard plot function for raster data from the package raster: plot. For each raster layer in a raster brick one plot is produced.

Arguments that are passed through the function call:

```
main,axes, xlab, ylab, xlim, ylim, col
plot.type = "plotRGB"
```

Uses the function plotRGB from the raster package. Only one image plot is produced as all layers in a brick a combined. This plot type is useful to see whether any signal is recorded by the camera. Arguments that are passed through the function call:

main,axes, xlab, ylab, ext, interpolate, maxpixels, alpha, colNA, stretch

```
plot.type = "contour"
```

Uses the function contour plot function from the raster function (contour). For each raster layer one contour plot is produced. Arguments that are passed through the function call:

```
main,axes, xlab, ylab, xlim, ylim, col
```

### Value

Returns a plot.

### **Function version**

```
0.1 (2015-08-21 14:53:14)
```

#### Note

This function has been created to faciliate the plotting of image data imported by the function read\_SPE2R. However, so far the function is not optimized to handle image data > ca. 200 MByte and thus plotting of such data is extremely slow.

### Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

### References

-

### See Also

```
RLum. Data. Image, plot, plot_RLum, raster,
```

# **Examples**

```
##load data
data(ExampleData.RLum.Data.Image, envir = environment())
##plot data
plot_RLum.Data.Image(ExampleData.RLum.Data.Image)
```

```
plot_RLum.Data.Spectrum
```

Plot function for an RLum.Data.Spectrum S4 class object

# **Description**

The function provides a standardised plot output for spectrum data of an RLum.Data.Spectrum S4 class object

# Usage

```
plot_RLum.Data.Spectrum(object, par.local = TRUE, plot.type = "contour",
  optical.wavelength.colours = TRUE, bg.channels, bin.rows = 1,
  bin.cols = 1, rug = TRUE, xaxis.energy = FALSE, legend.text, ...)
```

# **Arguments**

object RLum.Data.Spectrum (required): S4 object of class RLum.Data.Spectrum

par.local logical (with default): use local graphical parameters for plotting, e.g. the plot
 is shown in one column and one row. If par.local = FALSE global parameters
 are inherited.

plot.type character (with default): plot type, for 3D-plot use persp, or persp3d, for a
 2D-plot contour, single or multiple.lines (along the time or temperature
 axis) or transect (along the wavelength axis)

Note: The use of persp3d will produce a dynamic 3D surface plot on the screen.

optical.wavelength.colours

logical (with default): use optical wavelength colour palette. Note: For this, the spectrum range is limited: c(350,750). Own colours can be set with the

argument col.

vector (optional): defines channel for background subtraction If a vector is bg.channels

provided the mean of the channels is used for subtraction. Note: Background

subtraction is applied prior to channel binning

bin.rows integer (with defaul): allow summing-up wavelength channels (horizontal bin-

ning), e.g. bin.rows = 2 two channels are summed up

integer (with default): allow summing-up channel counts (vertical binning) for bin.cols

plotting, e.g. bin.cols = 2 two channels are summed up

logical (with default): enables or disables colour rug. Currently only implerug

mented for plot type multiple. lines and single

logical (with default): enables or disables energy instead of wavelength axis. xaxis.energy

Note: This option means not only simply redrawing the axis, insteadly the

spectrum in terms of intensity is recalculated, s. details.

character (with default): possiblity to provide own legend text. This argument legend.text

is only considered for plot types providing a legend, e.g. plot.type="transect"

further arguments and graphical parameters that will be passed to the plot func-. . .

#### **Details**

#### **Matrix structure**

(cf. RLum.Data.Spectrum)

- rows (x-values): wavelengths/channels (xlim, xlab)
- columns (y-values): time/temperature (ylim, ylab)
- cells (z-values): count values (zlim, zlab)

Note: This nomenclature is valid for all plot types of this function!

# Nomenclature for value limiting

xlim: Limits values along the wavelength axis

ylim: Limits values along the time/temperature axis

zlim: Limits values along the count value axis

# **Energy axis re-calculation**

If the argument xaxis.energy = TRUE is chosen, instead intensity vs. wavelength the spectrum is plotted as intensity vs. energy. Therefore the entire spectrum is re-recaluated (e.g., Appendix 4 in Blasse and Grabmeier, 1994):

The intensity of the spectrum (z-values) is re-calcualted using the following equation:

$$\phi_E = \phi_\lambda * \lambda^2/(hc)$$

with  $\phi_E$  the intensity per interval of energy E (eV),  $\phi_{\lambda}$  the intensity per interval of wavelength  $\lambda$ (nm) and h (eV/s) the Planck constant and c (m/s) the velocity of light.

For transforming the wavelength axis (x-values) the equation

$$E = hc/\lambda$$

is used. For further details please see the cited the literature.

# **Details on the plot functions**

Spectrum is visualised as 3D or 2D plot. Both plot types are based on internal R plot functions.

```
plot.type = "persp"
```

Arguments that will be passed to persp:

shade: default is 0.4
phi: default is 30
theta: default is 30
expand: default is 1

• ticktype: default is detailed

Note: Further parameters can be adjusted via par. For example to set the background transparent and reduce the thickness of the lines use: par(bg = NA, 1wd = 0.7) previous the function call.

```
plot.type = "single"
```

Per frame a single curve is returned. Frames are time or temperature steps.

```
plot.type = "multiple.lines"
```

All frames plotted in one frame.

```
plot.type = "transect"
```

Depending on the selected wavelength/channel range a transect over the time/temperature (y-axis) will be plotted along the wavelength/channels (x-axis). If the range contains more than one channel, values (z-values) are summed up. To select a transect use the xlim argument, e.g. xlim = c(300, 310) plot along the summed up count values of channel 300 to 310.

# Further arguments that will be passed (depending on the plot type)

```
xlab, ylab, zlab, xlim, ylim, zlim, main, mtext, pch, type, col, border, box lwd, bty
```

# Value

Returns a plot.

# **Function version**

```
0.4.0 (2015-08-21 14:53:14)
```

#### Note

Not all additional arguments (...) will be passed similarly!

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#### Author(s)

```
Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team
```

## References

Blasse, G., Grabmaier, B.C., 1994. Luminescent Materials. Springer.

### See Also

```
RLum. Data. Spectrum, plot, plot_RLum, persp, persp3d, contour
```

# **Examples**

```
##load example data
data(ExampleData.XSYG, envir = environment())
##(1)plot simple spectrum (2D) - contour
plot_RLum.Data.Spectrum(TL.Spectrum,
                        plot.type="contour",
                        xlim = c(310,750),
                        ylim = c(0,300),
                        bin.rows=10,
                        bin.cols = 1)
##(2) plot simple spectrum (2D) - multiple.lines (with ylim)
plot_RLum.Data.Spectrum(TL.Spectrum,
                        plot.type="persp",
                        xlim = c(310,750),
                        ylim = c(0,100),
                        bin.rows=10,
                        bin.cols = 1)
##(3) plot 3d spectrum (uncomment for usage)
# plot_RLum.Data.Spectrum(TL.Spectrum, plot.type="persp",
\# x \lim = c(310,750), y \lim = c(0,300), bin.rows=10,
# bin.cols = 1)
```

plot\_RLum.Results

Plot function for an RLum.Results S4 class object

# Description

The function provides a standardised plot output for data of an RLum.Results S4 class object

# Usage

```
plot_RLum.Results(data, single = TRUE, ...)
```

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# Arguments

data	RLum.Results (required): S4 object of class RLum.Results
single	logical (with default): single plot output (TRUE/FALSE) to allow for plotting the results in as few plot windows as possible.
	further arguments and graphical parameters will be passed to the plot function.

### **Details**

The function produces a multiple plot output. A file output is recommended (e.g., pdf).

### Value

Returns multiple plots.

#### **Function version**

```
0.2.0 (2015-08-30 16:13:50)
```

#### Note

Not all arguments available for plot will be passed! Only plotting of RLum.Results objects are supported.

# Author(s)

Christoph Burow, University of Cologne (Germany), Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

#### References

#

# See Also

```
plot, plot_RLum,
```

### **Examples**

```
###load data
data(ExampleData.DeValues, envir = environment())

# apply the un-logged minimum age model
mam<- calc_MinDose(data = ExampleData.DeValues$CA1, sigmab = 0.2, log = TRUE, plot = FALSE)

##plot
plot_RLum.Results(mam)

# estimate the number of grains on an aliquot
grains<- calc_AliquotSize(grain.size = c(100,150), sample.diameter = 1, plot = FALSE)

##plot
plot_RLum.Results(grains)</pre>
```

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read	

Import Risoe BIN-file into R

## **Description**

Import a \*.bin or a \*.binx file produced by a Risoe DA15 and DA20 TL/OSL reader into R.

# Usage

```
read_BIN2R(file, show.raw.values = FALSE, n.records, fastForward = FALSE,
    show.record.number = FALSE, txtProgressBar = TRUE, forced.VersionNumber)
```

### Arguments

file character (required): bin-file name (including path), e.g.

[WIN]: read\_BIN2R("C:/Desktop/test.bin"),

[MAC/LINUX]: read\_BIN2R("/User/test/Desktop/test.bin")

show.raw.values

logical (with default): shows raw values from BIN file for LTYPE, DTYPE and

LIGHTSOURCE without translation in characters.

n.records raw (optional): limits the number of imported records. Can be used in com-

bination with show.record.number for debugging purposes, e.g. corrupt BIN

files.

fastForward logical (with default): if TRUE for a more efficient data processing only a list of

RLum. Analysis objects is returned instead of a Risoe.BINfileData-class object

show.record.number

logical (with default): shows record number of the imported record, for debug-

ging usage only.

txtProgressBar logical (with default): enables or disables txtProgressBar.

forced.VersionNumber

integer (optional): allows to cheat the version number check in the function by

own values for cases where the BIN-file version is not supported.

Note: The usage is at own risk, only supported BIN-file versions have been tested.

# **Details**

The binary data file is parsed byte by byte following the data structure published in the Appendices of the Analyst manual p. 42.

For the general BIN-file structure, the reader is referred to the Risoe website: http://www.nutech.dtu.dk/

# Value

Returns an S4 Risoe.BINfileData-class object containing two slots:

METADATA A data.frame containing all variables stored in the bin-file.

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DATA

A list containing a numeric vector of the measured data. The ID corresponds to the record ID in METADATA.

If fastForward = TRUE a list of RLum. Analysis object is returned. The internal coercing is done using the function Risoe.BINfileData2RLum. Analysis

#### **Function version**

```
0.9.1 (2015-08-21 14:53:14)
```

#### Note

The function works for BIN/BINX-format versions 03, 04, 06 and 07. The version number depends on the used Sequence Editor.

Potential other BIN/BINX-format versions are currently not supported. The implementation of version 07 support could not been tested so far.

# Author(s)

```
Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France), Margret C. Fuchs, TU Bergakademie Freiberg (Germany)
R Luminescence Package Team
```

#### References

```
\label{lem:condition} Duller, G., 2007. \ Analyst. \ http://www.nutech.dtu.dk/english/~/media/Andre_Universitetsenheder/Nutech/Produkter%20og%20services/Dosimetri/radiation_measurement_instruments/tl_osl_reader/Manuals/analyst_manual_v3_22b.ashx
```

# See Also

write\_R2BIN, Risoe.BINfileData, readBin, merge\_Risoe.BINfileData, RLum.Analysis txtProgressBar

### **Examples**

```
##(1) import Risoe BIN-file to R (uncomment for usage)
#FILE <- file.choose()
#temp <- read_BIN2R(FILE)
#temp</pre>
```

read\_Daybreak2R

Import Daybreak ASCII dato into R

# **Description**

Import a \*.txt (ASCII) file produced by a Daybreak reader into R.

# Usage

```
read_Daybreak2R(file, txtProgressBar = TRUE)
```

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# **Arguments**

```
file character (required): path and file name of the file to import txtProgressBar logical (with default): enables or disables txtProgressBar.
```

#### Value

A list of RLum. Analysis objects (each per position) is provided.

# **Function version**

```
0.1.0 (2015-08-21 14:53:14)
```

### Note

[BETA VERSION] This function version still needs to be properly tested.

# Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) Based on suggestion by Willian Amidon and Andrew Louis Gorin. R Luminescence Package Team

### References

-

### See Also

```
RLum.Analysis, RLum.Data.Curve
```

# **Examples**

## This function has no example yet.

read\_SPE2R

Import Princeton Intruments (TM) SPE-file into R

# **Description**

Function imports Princeton Instruments (TM) SPE-files into R environment and provides RLum objects as output.

# Usage

```
read_SPE2R(file, output.object = "RLum.Data.Image", frame.range,
    txtProgressBar = TRUE)
```

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### **Arguments**

file character (**required**): spe-file name (including path), e.g.

[WIN]: read\_SPE2R("C:/Desktop/test.spe"),

[MAC/LINUX]: readSPER("/User/test/Desktop/test.spe")

output.object character (with default): set RLum output object. Allowed types are "RLum. Data. Spectrum",

"RLum.Data.Image" or "matrix"

frame.range vector (optional): limit frame range, e.g. select first 100 frames by frame.range = c(1,100)

txtProgressBar logical (with default): enables or disables txtProgressBar.

#### **Details**

Function provides an import routine for the Princton Instruments SPE format. Import functionality is based on the file format description provided by Princton Instruments and a MatLab script written by Carl Hall (s. references).

#### Value

Depending on the chosen option the functions returns three different type of objects:

output.object.

RLum.Data.Spectrum

An object of type RLum. Data. Spectrum is returned. Row sums are used to integrate all counts over one channel.

RLum.Data.Image

An object of type RLum.Data.Image is returned. Due to performace reasons the import is aborted for files containing more than 100 frames. This limitation can be overwritten manually by using the argument frame.frange.

matrix

Returns a matrix of the form: Rows = Channels, columns = Frames. For the transformation the function get\_RLum is used, meaning that the same results can be obtained by using the function get\_RLum on an RLum.Data.Spectrum or RLum.Data.Image object.

# **Function version**

```
0.1.0 (2015-08-21 14:53:14)
```

# Note

The function does not test whether the input data are spectra or pictures for spatial resolved analysis!

The function has been successfully tested for SPE format versions 2.x.

Currently not all information provided by the SPE format are supported.

#### Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

#### References

 $\label{lem:princeton} Princeton Instruments, 2014. Princeton Instruments SPE 3.0 File Format Specification, Version 1.A, \\ ftp://ftp.princetoninstruments.com/Public/Manuals/Princeton%20Instruments/SPE%203.0%20File%20Format%20Specification.pdf$ 

 $Hall, C., 2012: \ read SPE.m.\ http://www.mathworks.com/matlabcentral/fileexchange/35940-read spe/content/read SPE.m.$ 

#### See Also

```
readBin, RLum. Data. Spectrum, raster
```

## **Examples**

```
## to run examples uncomment lines and run the code
##(1) Import data as RLum.Data.Spectrum object
#file <- file.choose()</pre>
#temp <- read_SPE2R(file)</pre>
#temp
##(2) Import data as RLum.Data.Image object
#file <- file.choose()</pre>
#temp <- read_SPE2R(file, output.object = "RLum.Data.Image")</pre>
#temp
##(3) Import data as matrix object
#file <- file.choose()</pre>
#temp <- read_SPE2R(file, output.object = "matrix")</pre>
#temp
\#\#(4) Export raw data to csv, if temp is a RLum.Data.Spectrum object
# write.table(x = get_RLum(temp),
#
               file = "[your path and filename]",
#
               sep = ";", row.names = FALSE)
```

read\_XSYG2R

Import XSYG files to R

## **Description**

Imports XSYG files produced by a Freiberg Instrument lexsyg reader into R.

# Usage

```
read_XSYG2R(file, recalculate.TL.curves = TRUE, fastForward = FALSE,
  import = TRUE, txtProgressBar = TRUE)
```

#### **Arguments**

file

character or list (**required**): path and file name of the XSYG file. If input is a list it should comprise only characters representing each valid path and xsyg-file names. Alternatively the input character can be just a directory (path), in this case the function tries to detect and import all xsyg files found in the directory.

recalculate.TL.curves

logical (with default): if set to TRUE, TL curves are returned as temperature against count values (see details for more information) Note: The option overwrites the time vs. count TL curve. Select FALSE to import the raw data delivered

by the lexsyg. Works for TL curves and spectra.

fastForward logical (with default): if TRUE for a more efficient data processing only a list

of RLum. Analysis objects is returned.

import logical (with default): if set to FALSE, only the XSYG file structure is shown.

txtProgressBar logical (with default): enables TRUE or disables FALSE the progression bar during

import

#### **Details**

#### How does the import function work?

The function uses the xml package to parse the file structure. Each sequence is subsequently translated into an RLum. Analysis object.

# General structure XSYG format

```
<?xml?
<Sample>
<Sequence>
<Record>
<Curve name="first curve" />
<Curve name="curve with data">
x0 , y0 ; x1 , y1 ; x2 , y2 ; x3 , y3
</Curve>
</Record>
</Sequence>
</Sample>
```

So far, each XSYG file can only contain one <Sample></Sample>, but multiple sequences.

Each record may comprise several curves.

## TL curve recalculation

On the FI lexsyg device TL curves are recorded as time against count values. Temperature values are monitored on the heating plate and stored in a separate curve (time vs. temperature). If the option recalculate.TL.curves = TRUE is chosen, the time values for each TL curve are replaced

by temperature values.

Practically, this means combining two matrices (Time vs. Counts and Time vs. Temperature) with different row numbers by their time values. Three cases are considered:

HE: Heating element
PMT: Photomultiplier tube
Interpolation is done using the function approx

```
CASE(1): nrow(matrix(PMT)) > nrow(matrix(HE))
```

Missing temperature values from the heating element are calculated using time values from the PMT measurement.

```
CASE(2): nrow(matrix(PMT)) < nrow(matrix(HE))</pre>
```

Missing count values from the PMT are calculated using time values from the heating element measurement.

```
CASE(3): nrow(matrix(PMT)) == nrow(matrix(HE))
```

A new matrix is produced using temperature values from the heating element and count values from the PMT.

Note: Please note that due to the recalculation of the temperature values based on values delivered by the heating element, it may happen that mutiple count values exists for each temperature value and temperature values may also decrease during heating, not only increase.

## Advanced file import

To allow for a more efficient usage of the function, instead of single path to a file just a directory can be passed as input. In this particular case the function tries to extract all XSYG-files found in the directory and import them all. Using this option internally the function constructs as list of the XSYG-files found in the directory. Please note no recursive detection is supported as this may lead to endless loops.

#### Value

```
Using the option import = FALSE
```

A list consisting of two elements is shown:

Sample data.frame with information on file.

Sequences data.frame with information on the sequences stored in the XSYG file

Using the option import = TRUE (default)

A list is provided, the list elements contain:

```
Sequence.Header

data.frame with information on the sequence.

Sequence.Object

RLum.Analysis containing the curves.
```

#### **Function version**

```
0.5.0 (2015-08-29 13:33:00)
```

#### Note

This function is a beta version as the XSYG file format is not yet fully specified. Thus, further file operations (merge, export, write) should be done using the functions provided with the package xml.

## So far, no image data import is provided!

Corresponding values in the XSXG file are skipped.

## Author(s)

```
Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team
```

#### References

Grehl, S., Kreutzer, S., Hoehne, M., 2013. Documentation of the XSYG file format. Unpublished Technical Note. Freiberg, Germany

#### **Further reading**

```
XML: http://en.wikipedia.org/wiki/XML
```

#### See Also

```
xml, RLum. Analysis, RLum. Data. Curve, approx
```

```
##(1) import XSYG file to R (uncomment for usage)

#FILE <- file.choose()
#temp <- read_XSYG2R(FILE)

##(2) additional examples for pure XML import using the package XML

## (uncomment for usage)

##import entire XML file
#FILE <- file.choose()
#temp <- XML::xmlRoot(XML::xmlTreeParse(FILE))

##search for specific subnodes with curves containing 'OSL'
#getNodeSet(temp, "//Sample/Sequence/Record[@recordType = 'OSL']/Curve")

##(2) How to extract single curves ... after import
data(ExampleData.XSYG, envir = environment())</pre>
```

```
##grep one OSL curves and plot the first curve
OSLcurve <- get_RLum(OSL.SARMeasurement$Sequence.Object, recordType="OSL")[[1]]
##(3) How to see the structure of an object?
structure_RLum(OSL.SARMeasurement$Sequence.Object)</pre>
```

```
Risoe.BINfileData-class
```

Class "Risoe.BINfileData"

#### **Description**

S4 class object for luminescence data in R. The object is produced as output of the function read\_BIN2R.

#### Usage

```
## S4 method for signature 'Risoe.BINfileData'
show(object)

## S4 method for signature 'data.frame,list'
set_Risoe.BINfileData(METADATA, DATA, .RESERVED)

## S4 method for signature 'Risoe.BINfileData'
get_Risoe.BINfileData(object)
```

# **Arguments**

object an object of class Risoe.BINfileData

METADATA Object of class "data.frame" containing the meta information for each curve.

DATA Object of class "list" containing numeric vector with count data.

. RESERVED Object of class "list" containing list of undocumented raw values for internal use

only.

# Methods (by generic)

- show: Show structure of RLum and Risoe.BINfile class objects
- set\_Risoe.BINfileData: The Risoe.BINfileData is normally produced as output of the function read\_BIN2R. This construction method is intended for internal usage only.
- get\_Risoe.BINfileData: Formal get-method for Risoe.BINfileData object. It does not allow accessing the object directly, it is just showing a terminal message.

# Slots

METADATA Object of class "data.frame" containing the meta information for each curve.

DATA Object of class "list" containing numeric vector with count data.

.RESERVED Object of class "list" containing list of undocumented raw values for internal use only.

# **Objects from the Class**

Objects can be created by calls of the form  $new("Risoe.BINfileData", \ldots)$ .

# **Function version**

0.2.0

## Note

# **Internal METADATA - object structure**

#	Name	Data Type	$\mathbf{V}$	Description
[,1]	ID	numeric	RLum	Unique record ID (same ID as in slot DATA)
[,2]	SEL	logic	RLum	Record selection, not part official BIN-format, triggered by TAG
[,3]	VERSION	raw	03-07	BIN-file version number
[,4]	LENGTH	integer	03-07	Length of this record
[,5]	PREVIOUS	integer	03-07	Length of previous record
[,6]	NPOINTS	integer	03-07	Number of data points in the record
[,7]	RUN	integer	03-07	Run number
[,8]	SET	integer	03-07	Set number
[,9]	POSITION	integer	03-07	Position number
[,10]	GRAIN	integer	03-04	Grain number
[,11]	GRAINNUMBER	integer	06-07	Grain number
[,12]	CURVENO	integer	06-07	Curve number
[,13]	XCOORD	integer	03-07	X position of a single grain
[,14]	YCOORD	integer	03-07	Y position of a single grain
[,15]	SAMPLE	factor	03-07	Sample name
[,16]	COMMENT	factor	03-07	Comment name
[,17]	SYSTEMID	integer	03-07	Risoe system id
[,18]	FNAME	factor	06-07	File name (*.bin/*.binx)
[,19]	USER	facotr	03-07	User name
[,20]	TIME	character	03-07	Data collection time (hh-mm-ss)
[,21]	DATE	factor	03-07	Data collection date (ddmmyy)
[,22]	DTYPE	character	03-07	Data type
[,23]	BL_TIME	numeric	03-07	Bleaching time
[,24]	BL_UNIT	integer	03-07	Bleaching unit (mJ, J, secs, mins, hrs)
[,25]	NORM1	numeric	03-07	Normalisation factor (1)
[,26]	NORM2	numeric	03-07	Normalisation factor (2)
[,27]	NORM3	numeric	03-07	Normalisation factor (3)
[,28]	BG	numeric	03-07	Background level
[,29]	SHIFT	integer	03-07	Number of channels to shift data
[,30]	TAG	integer	03-07	Tag, triggers SEL
[,31]	LTYPE	character	03-07	Luminescence type
[,32]	LIGHTSOURCE	character	03-07	Light source
[,33]	LPOWER	numeric	03-07	Optical stimulation power
[,34]	LIGHTPOWER	numeric	06-07	Optical stimulation power
[,35]	LOW	numeric	03-07	Low (temperature, time, wavelength)
[,36]	HIGH	numeric	03-07	High (temperature, time, wavelength)
[,37]	RATE	numeric	03-07	Rate (heating rate, scan rate)
[,38]	TEMPERATURE	integer	03-07	Sample temperature
[,39]	MEASTEMP	integer	06-07	Measured temperature
[,40]	AN_TEMP	numeric	03-07	Annealing temperature
[,41]	AN_TIME	numeric	03-07	Annealing time

[,42]	TOLDELAY	integer	03-07	TOL 'delay' channels
[,43]	TOLON	integer	03-07	TOL 'on' channels
[,44]	TOLOFF	integer	03-07	TOL 'off' channels
[,45]	IRR_TIME	numeric	03-07	Irradiation time
[,46]	IRR_TYPE	integer	03-07	Irradiation type (alpha, beta or gamma)
[,47]	IRR_UNIT	integer	03-04	Irradiation unit (Gy, Rads, secs, mins, hrs)
[,48]	IRR_DOSERATE	numeric	06-07	Irradiation dose rate (Gy/s)
[,49]	IRR_DOSERATEERR	numeric	06-07	Irradiation dose rate error (Gy/s)
[,50]	TIMESINCEIRR	integer	06-07	Time since irradiation (s)
[,51]	TIMETICK	numeric	06-07	Time tick for pulsing (s)
[,52]	ONTIME	integer	06-07	On-time for pulsing (in time ticks)
[,53]	STIMPERIOD	integer	06-07	Stimulation period (on+off in time ticks)
[,54]	GATE_ENABLED	raw	06-07	PMT signal gating enabled
[,55]	ENABLE_FLAGS	raw	06-07	PMT signal gating enabled
[,56]	GATE_START	integer	06-07	Start gating (in time ticks)
[,57]	GATE_STOP	ingeter	06-07	Stop gating (in time ticks), 'Gateend' for version 04, here only G
[,58]	PTENABLED	raw	06-07	Photon time enabled
[,59]	DTENABLED	raw	06-07	PMT dead time correction enabled
[,60]	DEADTIME	numeric	06-07	PMT dead time (s)
[,61]	MAXLPOWER	numeric	06-07	Stimulation power to 100 percent (mW/cm^2)
[,62]	XRF_ACQTIME	numeric	06-07	XRF acquisition time (s)
[,63]	XRF_HV	numeric	06-07	XRF X-ray high voltage (V)
[,64]	XRF_CURR	integer	06-07	XRF X-ray current (uA)
[,65]	XRF_DEADTIMEF	numeric	06-07	XRF dead time fraction
[,66]	SEQUENCE	character	03-04	Sequence name
[,67]	DETECTOR_ID	raw	07	Detector ID
[,68]	LOWERFILTER_ID	integer	07	Lower filter ID in reader
[,69]	UPPERFILTER_ID	integer	07	Uper filter ID in reader
[,70]	ENOISEFACTOR	numeric	07	Excess noise filter, usage unknown

V = BIN-file version (RLum means that it does not depend on a specific BIN version)

Note that the Risoe.BINfileData object combines all values from different versions from the BIN-file, reserved bits are skipped, however, the function write\_R2BIN reset arbitrary reserved bits. Invalid values for a specific version are set to NA. Furthermore, the internal R data types do not necessarily match the required data types for the BIN-file data import! Data types are converted during data import.

# LTYPE values

[,0]	TL	: Thermoluminescence
[,1]	OSL	: Optically stimulated luminescence
[,2]	IRSL	: Infrared stimulated luminescence
[,3]	M-IR	: Infrared monochromator scan
[,4]	M-VIS	: Visible monochromator scan
[,5]	TOL	: Thermo-optical luminescence
[,6]	TRPOSL	: Time Resolved Pulsed OSL
[,7]	RIR	: Ramped IRSL
[,8]	RBR	: Ramped (Blue) LEDs
[,9]	USER	: User defined
,10]	POSL	: Pulsed OSL
,11]	SGOSL	: Single Grain OSL

[,12] RL : Radio Luminescence [,13] XRF : X-ray Fluorescence

#### **DTYPE** values

- [,0] 0 Natural
- [,1] 1 N+dose
- [,2] 2 Bleach
- [,3] 3 Bleach+dose
- [,4] 4 Natural (Bleach)
- [,5] 5 N+dose (Bleach)
- [,6] 6 Dose
- [,7] 7 Background

## **LIGHTSOURCE** values

- [,0] 0 Non
- [,1] 1 Lamp
- [,2] 2 IR diodes/IR Laser
- [,3] 3 Calibration LED
- [,4] 4 Blue Diodes
- [,5] 5 White lite
- [,6] 6 Green laser (single grain)
- [,7] 7 IR laser (single grain)

(information on the BIN/BINX file format are kindly provided by Risoe, DTU Nutech)

## Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

## References

Risoe DTU, 2013. The Sequence Editor User Manual - Feb 2013 and Risoe DTU, 2015. The Sequence Editor User Manual - March 2015

http://www.nutech.dtu.dk/

#### See Also

plot\_Risoe.BINfileData, read\_BIN2R, write\_R2BIN, merge\_Risoe.BINfileData, Risoe.BINfileData2RLum. AnaRisoe.BINfileData2RLum. Data.Curve

# Examples

 $\verb|showClass("Risoe.BINfileData")| \\$ 

Risoe.BINfileData2RLum.Analysis

Convert Risoe.BINfileData object to an RLum.Analysis object

# Description

Converts values from one specific position of a Risoe.BINfileData S4-class object to an RLum.Analysis object.

# Usage

```
Risoe.BINfileData2RLum.Analysis(object, pos, grain, run, set, ltype,
    protocol = "unknown", txtProgressBar = FALSE)
```

## **Arguments**

object	Risoe.BINfileData (required): Risoe.BINfileData object
pos	numeric (optional): position number of the Risoe.BINfileData object for which the curves are stored in the RLum. Analysis object. If length(position)>1 a list of RLum. Analysis objects is returned. If nothing is provided every position will be converted. If the position is not valid NA is returned.
grain	vector, numeric (optional): grain number from the measurement to limit the converted data set (e.g., grain = $c(1:48)$ ). Please be aware that this option may lead to unwanted effects, as the output is strictly limited to the choosen grain number for all position numbers
run	vector, numeric (optional): run number from the measurement to limit the converted data set (e.g., run = $c(1:48)$ ).
set	vector, numeric (optional): set number from the measurement to limit the converted data set (e.g., set = $c(1:48)$ ).
ltype	vector, character (optional): curve type to limit the converted data. Allowed values are: IRSL, OSL, TL, RIR, RBR and USER
protocol	character (optional): sets protocol type for analysis object. Value may be used by subsequent analysis functions.
txtProgressBar	logical (with default): enables or disables txtProgressBar.

## **Details**

The RLum. Analysis object requires a set of curves for specific further protocol analyses. However, the Risoe.BINfileData usually contains a set of curves for different aliquots and different protocol types that may be mixed up. Therefore, a conversion is needed.

## Value

Returns an RLum. Analysis object.

## **Function version**

0.2.0 (2015-08-21 14:53:14)

#### Note

The protocol argument of the RLum. Analysis object is set to 'unknown' if not stated otherwise.

#### Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

#### References

#

#### See Also

```
Risoe.BINfileData, RLum.Analysis, read_BIN2R
```

# **Examples**

```
##load data
data(ExampleData.BINfileData, envir = environment())
##convert values for position 1
Risoe.BINfileData2RLum.Analysis(CWOSL.SAR.Data, pos = 1)
```

Risoe.BINfileData2RLum.Data.Curve

Convert an element from a Risoe.BINfileData object to an RLum.Data.Curve object

# Description

The function converts one specified single record from a Risoe.BINfileData object to an RLum.Data.Curve object.

## Usage

```
Risoe.BINfileData2RLum.Data.Curve(object, id, pos, run, set)
```

## **Arguments**

object	Risoe.BINfileData (required): Risoe.BINfileData object
id	<pre>integer (required): record id in the Risoe.BINfileData object of the curve that is to be stored in the RLum.Data.Curve object. If no value for id is provided, the record has to be specified by pos, set and run.</pre>
pos	<pre>integer (optional): record position number in the Risoe.BINfileData object of the curve that is to be stored in the RLum.Data.Curve object. If a value for id is provided, this argument is ignored.</pre>
run	<pre>integer (optional): record run number in the Risoe.BINfileData object of the curve that is to be stored in the RLum.Data.Curve object. If a value for id is provided, this argument is ignored.</pre>

set

integer (optional): record set number in the Risoe.BINfileData object of the curve that is to be stored in the RLum.Data.Curve object. If a value for id is provided, this argument is ignored.

#### **Details**

The function extracts all METADATA from the Risoe.BINfileData object and stores them in the RLum.Data.Curve object.

#### Value

Returns an RLum. Data. Curve object.

#### **Function version**

```
0.1.1 (2015-08-21 14:53:14)
```

#### Note

The function is intended for experimental usage. Normally, the function Risoe.BINfileData2RLum.Analysis should be used for the conversion.

# Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

#### References

#

# See Also

 $Risoe. BINfile Data 2 RLum. Analysis, set\_RLum, RLum. Data. Curve, RLum. Analysis, Risoe. BINfile Data, plot\_RLum$ 

```
##get package example data
data(ExampleData.BINfileData, envir = environment())

##convert one record
Risoe.BINfileData2RLum.Data.Curve(CWOSL.SAR.Data, id = 1)
```

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RLum-class

Class "RLum"

# Description

Abstract class for data in the package Luminescence

#### **Slots**

originator Object of class "character" containing the name of the producing function for the object

.uid Object of class "character" containing a unified object identifier

# **Objects from the Class**

A virtual Class: No objects can be created from it.

## **Class version**

0.3.0

#### Note

RLum is a virtual class.

# Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France)

## See Also

```
RLum.Data, RLum.Analysis
```

## **Examples**

```
showClass("RLum")
```

RLum.Analysis-class

Class "RLum. Analysis"

# Description

Object class containing analysis data for protocol analysis.

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## Usage

```
## S4 method for signature 'RLum.Analysis'
show(object)

## S4 method for signature 'RLum.Analysis'
structure_RLum(object)

## S4 method for signature 'RLum.Analysis'
set_RLum(class, records, protocol)

## S4 method for signature 'RLum.Analysis'
get_RLum(object, record.id, recordType, curveType,
    RLum.type, protocol = "UNKNOWN", subset, get.index, keep.object = FALSE,
    recursive = TRUE)

## S4 method for signature 'RLum.Analysis'
length_RLum(object)
```

## **Arguments**

object	[structure_RLum] an object of class RLum. Analysis (required)
class	[set_RLum] character (required): name of the RLum class to be created
records	[set_RLum] list (required): list of RLum. Analysis objects
protocol	[set_RLum] character (optional): sets protocol type for analysis object. Value may be used by subsequent analysis functions. UNKNOWN by default.
record.id	[get_RLum] numeric (optional): IDs of specific records
recordType	[get_RLum] character (optional): record type (e.g. "OSL")
curveType	[get_RLum] character (optional): curve type (e.g. "predefined" or "measured")
RLum.type	$\label{lem:character} \begin{tabular}{ll} [\tt get\_RLum] character (optional): RLum object type. Defaults to "RLum.Data.Curve" and "RLum.Data.Spectrum". \end{tabular}$
subset	[get_RLum] list: currently not used.
get.index	[get_RLum] logical (optional): return a numeric vector with the index of each element in the RLum.Analysis object.
keep.object	[get_RLum] logical (with default): return an RLum.Analysis object instead of the single elements.
recursive	[get_RLum] logical (with default): if TRUE (the default) and the result of the 'get_RLum' request is a single object this object will be unlisted, means only the object itself and no list containing exactly one object is returned. Mostly this makes things easier, however, if this method in a loop this might become annoying

# Methods (by generic)

- show: Show structure of RLum and Risoe.BINfile class objects
- structure\_RLum: Method to show the structure of an RLum. Analysis object.
- set\_RLum: Construction method for RLum. Analysis objects.

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• get\_RLum: Accessor method for RLum. Analysis object.

The slots record.id, recordType, curveType and RLum.type are optional to allow for records limited by their id (list index number), their record type (e.g. recordType = "OSL") or object type.

Example: curve type (e.g. curveType = "predefined" or curveType = "measured")

The selection of a specific RLum.type object superimposes the default selection. Currently supported objects are: RLum.Data.Curve and RLum.Data.Spectrum

• length\_RLum: Returns the length of the object, i.e., number of stored records.

#### **Slots**

```
records Object of class "list" containing objects of class RLum.Data protocol Object of class "character" describing the applied measurement protocol
```

# **Objects from the Class**

Objects can be created by calls of the form new("RLum.Analysis", ...).

#### **Class version**

0.2.0

#### Note

The method get\_structure is currently just avaiblable for objects containing RLum. Data. Curve.

## Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France)

# See Also

```
Risoe.BINfileData2RLum.Analysis, Risoe.BINfileData, RLum
```

## **Examples**

```
showClass("RLum.Analysis")
## usage of get_RLum() with returning an RLum.Analysis object
# get_RLum(object, keep.object = TRUE)
```

RLum.Data-class

Class "RLum.Data"

## **Description**

Generalized virtual data class for luminescence data.

## **Objects from the Class**

A virtual Class: No objects can be created from it.

RLum.Data.Curve-class 159

#### **Class version**

0.2.1

#### Note

Just a virtual class.

#### Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France)

#### See Also

```
RLum, RLum. Data. Curve, RLum. Data. Spectrum
```

# **Examples**

```
showClass("RLum.Data")
```

```
RLum.Data.Curve-class Class "RLum.Data.Curve"
```

# Description

Class for luminescence curve data.

## Usage

```
## S4 method for signature 'RLum.Data.Curve'
show(object)

## S4 method for signature 'RLum.Data.Curve'
set_RLum(class, recordType, curveType, data, info)

## S4 method for signature 'RLum.Data.Curve'
get_RLum(object, info.object)
```

## **Arguments**

```
object [get_RLum] an object of class RLum.Data.Curve (required)

class [set_RLum] character (required): name of the RLum class to create

recordType [set_RLum] character (optional): record type (e.g., "OSL")

curveType [set_RLum] character (optional): curve type (e.g., "predefined" or "measured")

data [set_RLum] matrix (required): raw curve data

info [set_RLum] list (optional): info elements

info.object [get_RLum] character (optional): name of the wanted info element
```

160 RLum.Data.Curve-class

## Methods (by generic)

- show: Show structure of RLum and Risoe.BINfile class objects
- set\_RLum: Construction method for RLum.Data.Curve object. The slot info is optional and predefined as empty list by default.
- get\_RLum: Accessor method for RLum.Data.Curve object. The argument info.object is optional to directly access the info elements. If no info element name is provided, the raw curve data (matrix) will be returned.

#### **Slots**

```
recordType Object of class "character" containing the type of the curve (e.g. "TL" or "OSL")

curveType Object of class "character" containing curve type, allowed values are measured or predefined

data Object of class "matrix" containing curve x and y data

info Object of class "list" containing further meta information objects
```

# **Objects from the Class**

Objects can be created by calls of the form new("RLum.Data.Curve", ...).

## **Class version**

0.2.0

## Note

The class should only contain data for a single curve. For additional elements the slot info can be used (e.g. providing additional heating ramp curve).

# Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France)

#### See Also

```
RLum, RLum. Data, plot_RLum
```

```
showClass("RLum.Data.Curve")
```

```
RLum.Data.Image-class Class "RLum.Data.Image"
```

# Description

Class for luminescence image data (TL/OSL/RF).

## Usage

```
## S4 method for signature 'RLum.Data.Image'
show(object)

## S4 method for signature 'RLum.Data.Image'
set_RLum(class, recordType, curveType, data, info)

## S4 method for signature 'RLum.Data.Image'
get_RLum(object, info.object)
```

## **Arguments**

```
object an object of class RLum.Data.Image
class character: name of the RLum class to create
recordType character: record type (e.g. "OSL")
curveType character: curve type (e.g. "predefined" or "measured")
data matrix: raw curve data
```

info list: info elements

info.object of class "list" containing further meta information objects

## Methods (by generic)

- show: Show structure of RLum and Risoe.BINfile class objects
- set\_RLum: Construction method for RLum.Data.Image object. The slot info is optional and predefined as empty list by default..
- get\_RLum: Accessor method for RLum.Data.Image object. The argument info.object is optional to directly access the info elements. If no info element name is provided, the raw image data (RasterBrick) will be returned.

#### **Slots**

```
recordType Object of class "character" containing the type of the curve (e.g. "OSL image", "TL image")

curveType Object of class "character" containing curve type, allowed values are measured or predefined

data Object of class "RasterBrick" containing images (raster data).

info Object of class "list" containing further meta information objects
```

## **Objects from the Class**

```
Objects can be created by calls of the form new("RLum.Data.Image", ...).
```

#### **Class version**

0.2.0

#### Note

The class should only contain data for a set of images. For additional elements the slot info can be used.

#### Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France)

#### See Also

```
RLum, RLum. Data, plot_RLum
```

#### **Examples**

```
showClass("RLum.Data.Image")
##so far no further example available
```

```
RLum.Data.Spectrum-class
```

Class "RLum.Data.Spectrum"

# **Description**

Class for luminescence spectra data (TL/OSL/RF).

## Usage

```
## S4 method for signature 'RLum.Data.Spectrum'
show(object)

## S4 method for signature 'RLum.Data.Spectrum'
set_RLum(class, recordType, curveType, data,
    info)

## S4 method for signature 'RLum.Data.Spectrum'
get_RLum(object, info.object)
```

## **Arguments**

object an object of class RLum. Data. Image

class character: name of the RLum class to create

recordType character: record type (e.g. "OSL")

curveType character: curve type (e.g. "predefined" or "measured")

data matrix: raw curve data info list: info elements

info.object object of class "list" containing further meta information objects

# Methods (by generic)

- show: Show structure of RLum and Risoe.BINfile class objects
- set\_RLum: Construction method for RLum.Data.Spectrum object. The slot info is optional and predefined as empty list by default
- get\_RLum: Accessor method for RLum.Data.Spectrum object. The argument info.object is optional to directly access the info elements. If no info element name is provided, the raw curve data (matrix) will be returned

#### **Slots**

```
recordType Object of class "character" containing the type of the curve (e.g. "TL" or "OSL")
```

curveType Object of class "character" containing curve type, allowed values are measured or predefined

data Object of class "matrix" containing spectrum (count) values. Row labels indicate wavelength/pixel values, column labels are temperature or time values.

info Object of class "list" containing further meta information objects

## **Objects from the Class**

Objects can be created by calls of the form new("RLum.Data.Spectrum", ...).

#### **Class version**

0.2.1

## Note

The class should only contain data for a single spectra data set. For additional elements the slot info can be used.

## Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France)

## See Also

```
RLum, RLum. Data, plot_RLum
```

```
showClass("RLum.Data.Spectrum")
##show example data (uncomment for usage)
# data(ExampleData.XSYG, envir = environment())
# TL.Spectrum
```

164 RLum.Results-class

RLum.Results-class Class "RLum.Results"

## **Description**

Object class contains results data from functions.

## Usage

```
## S4 method for signature 'RLum.Results'
show(object)

## S4 method for signature 'RLum.Results'
set_RLum(class, originator, data)

## S4 method for signature 'RLum.Results'
get_RLum(object, data.object)

## S4 method for signature 'list'
merge_RLum.Results(object.list)
```

#### **Arguments**

object	[get_RLum] RLum.Results (required): an object of class RLum.Results to be evaluated
class	[set_RLum] character (required): name of the RLum class to create
originator	[set_RLum] character (optional): argument to manually set the originator.
data	[set_RLum] list (optional): a list containing the data to be stored in the object
data.object	[get_RLum] character: name of the data slot to be returned
object.list	[merge_RLum.Results] list (required): a list of RLum.Results objects

## Methods (by generic)

- show: Show structure of RLum and Risoe.BINfile class objects
- set\_RLum: Construction method for RLum.Results object. The slot originator is optional and predefined as the function that calls the function set RLum.
- get\_RLum: Accessor method for RLum.Results object. The argument data.object allows directly accessing objects delivered within the slot data. If no data.object is specified, a preselected object is returned. The default return object depends on the object originator (e.g., fit\_LMCurve).
- merge\_RLum.Results: merge method for RLum.Results objects. The argument object.list requires a list of RLum.Results objects. Merging is done by appending similar elements to the first object of the input list.

#### **Slots**

```
originator Object of class "character" containing name of the producing function data Object of class "list" containing output data
```

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# **Objects from the Class**

Objects can be created by calls of the form new("RLum.Results", ...).

#### **Class version**

0.2.0

## Note

The class is intended to store results from functions to be used by other functions. The data in the object should always be accessed by the method get\_RLum.

## Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France)

## See Also

**RLum** 

# **Examples**

```
showClass("RLum.Results")
```

Second2Gray

Converting values from seconds (s) to gray (Gy)

# Description

Conversion of absorbed radiation dose in seconds (s) to the SI unit gray (Gy) including error propagation. Normally used for equivalent dose data.

# Usage

```
Second2Gray(data, dose.rate, method = "gaussian")
```

## **Arguments**

data	<pre>data.frame (required): input values, structure: data (values[,1]) and data error (values [,2]) are required</pre>
dose.rate	RLum.Results or data.frame or numeric ( <b>required</b> ): RLum.Results needs to be orginated from the function calc_SourceDoseRate, for vector dose rate in Gy/s and dose rate error in Gy/s
method	character (with default): method used for error calculation (gaussian or absolute),

see details for further information

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#### **Details**

Calculation of De values from seconds (s) to gray (Gy)

$$De[Gy] = De[s] * DoseRate[Gy/s])$$

Provided calculation methods for error calculation: gaussian error propagation

```
De.error.gray = \sqrt{(dose.rate*De.error.seconds)^2 + (De.seconds*dose.rate.error)^2))} 
 absolute error propagation
```

```
De.error.gray = abs(dose.rate*De.error.seconds) + abs(De.seconds*dose.rate.error)
```

#### Value

Returns a data.frame with converted values.

#### **Function version**

```
0.5.0 (2015-08-29 13:33:00)
```

#### Note

If no or a wrong method is given, the execution of the function is stopped. Furthermore, if a data.frame is provided for the dose rate values is has to be of the same length as the data frame provided with the argument data

# Author(s)

```
Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France),
Michael Dietze, GFZ Potsdam (Germany),
Margret C. Fuchs, HZDR, Helmholtz-Institute Freiberg for Resource Technology (Germany)
R Luminescence Package Team
```

#### References

#

#### See Also

#

```
##(A) for known source dose rate at date of measurement
## - load De data from the example data help file
data(ExampleData.DeValues, envir = environment())
## - convert De(s) to De(Gy)
Second2Gray(ExampleData.DeValues$BT998, c(0.0438,0.0019))
```

set\_Risoe.BINfileData 167

set\_Risoe.BINfileData General accessor function for RLum S4 class objects

## **Description**

Function calls object-specific get functions for RisoeBINfileData S4 class objects.

## Usage

```
set_Risoe.BINfileData(METADATA, DATA, .RESERVED)
```

## **Arguments**

METADATA x
DATA x
.RESERVED x

#### **Details**

The function provides a generalised access point for specific Risoe.BINfileData objects. Depending on the input object, the corresponding get function will be selected. Allowed arguments can be found in the documentations of the corresponding Risoe.BINfileData class.

#### Value

Return is the same as input objects as provided in the list.

#### **Function version**

```
0.1 (2015-08-21 14:53:14)
```

## Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

## See Also

```
Risoe.BINfileData
```

set\_RLum

set\_RLum

General accessor function for RLum S4 class objects

# Description

Function calls object-specific set functions for RLum S4 class objects.

# Usage

```
set_RLum(class, ...)
```

## **Arguments**

class RLum (required): name of the S4 class to create

... further arguments that one might want to pass to the specific get function

#### **Details**

The function provides a generalised access point for specific RLum objects.

Depending on the input object, the corresponding set function will be selected. Allowed arguments can be found in the documentations of the corresponding RLum class.

#### Value

Return is the same as input objects as provided in the list.

#### **Function version**

```
0.1 (2015-08-21 14:53:14)
```

#### Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

## See Also

RLum.Data.Curve, RLum.Data.Image, RLum.Data.Spectrum, RLum.Analysis, RLum.Results

sTeve 169

sTeve

sTeve - sophisticated tool for efficient data validation and evaluation

# Description

This function provides a sophisticated routine for comprehensive luminescence dating data analysis.

# Usage

```
sTeve(n_frames = 10, t_animation = 2, n.tree = 7, type)
```

## **Arguments**

```
n_frames integer (with default): n frames
t_animation integer (with default): t animation
```

n. tree integer (with default): How many trees do you want to cut?

type integer (optional): Make a decision: 1, 2 or 3

#### **Details**

This amazing sophisticated function validates your data seriously.

## Value

Validates your data.

# Note

This function should not be taken too seriously.

# Author(s)

R Luminescence Team, 2012-2013

#### References

#

## See Also

```
plot_KDE
```

# **Examples**

##no example available

170 template\_DRAC

structure\_RLum

General accessor function for RLum S4 class objects

# **Description**

Function calls object-specific get functions for RLum S4 class objects.

## Usage

```
structure_RLum(object)
```

# **Arguments**

object

RLum (required): S4 object of class RLum

#### **Details**

The function provides a generalised access point for specific RLum objects.

Depending on the input object, the corresponding get function will be selected. Allowed arguments can be found in the documentations of the corresponding RLum class.

#### Value

Return is the same as input objects as provided in the list.

## **Function version**

```
0.1 (2015-08-21 14:53:14)
```

#### Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

## See Also

RLum.Data.Curve, RLum.Data.Image, RLum.Data.Spectrum, RLum.Analysis, RLum.Results

template\_DRAC

Create a DRAC input data template (v1.1)

# Description

This function returns a DRAC input template (v1.1) to be used in conjunction with the use\_DRAC() function

# Usage

```
template_DRAC(nrow = 1, notification = TRUE)
```

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#### **Arguments**

nrow integer (with default): specifies the number of rows of the template (i.e., the

number of data sets you want to submit)

notification logical (with default): show or hide the notification

#### Value

A list.

#### Author(s)

Christoph Burow, University of Cologne (Germany)

#### References

Durcan, J.A., King, G.E., Duller, G.A.T., 2015. DRAC: Dose Rate and Age Calculator for trapped charge dating. Quaternary Geochronology 28, 54-61. doi:10.1016/j.quageo.2015.03.012

#### See Also

```
as.data.frame list
```

```
# create a new DRAC input input
input <- template_DRAC()</pre>
# show content of the input
print(input)
print(input$`Project ID`)
print(input[[4]])
## Example: DRAC Quartz example
# note that you only have to assign new values where they
# are different to the default values
input$`Project ID` <- "DRAC-Example"</pre>
input$`Sample ID` <- "Quartz"</pre>
input

$`Conversion factors` <- "AdamiecAitken1998"
input$`ExternalU (ppm)` <- 3.4</pre>
input$`errExternal U (ppm)` <- 0.51</pre>
input$`External Th (ppm)` <- 14.47</pre>
input$`errExternal Th (ppm)` <- 1.69</pre>
input\External K (%) <- 1.2
input
$`errExternal K (%)` <- 0.14
input$`Calculate external Rb from K conc?` <- "N"</pre>
input
$`Calculate internal Rb from K conc?` <- "N"  
input
$`Scale gammadoserate at shallow depths?` <- "N"  
input$`Grain size min (microns)` <- 90</pre>
input\Grain size max (microns) <- 125
input$`Water content ((wet weight - dry weight)/dry weight) %` <- 5</pre>
input$`errWater content %` <- 2</pre>
input^Depth (m) < -2.2
input$`errDepth (m)` <- 0.22</pre>
input$`Overburden density (g cm-3)` <- 1.8
```

use\_DRAC

```
input$`errOverburden density (g cm-3)` <- 0.1
input$`Latitude (decimal degrees)` <- 30.0000
input$`Longitude (decimal degrees)` <- 70.0000
input$`Altitude (m)` <- 150
input$`De (Gy)` <- 20
input$`errDe (Gy)` <- 0.2

# use DRAC
## Not run:
output <- use_DRAC(input)

## End(Not run)</pre>
```

use\_DRAC

Use DRAC to calculate dose rate data

#### **Description**

The function provides an interface from R to DRAC. An R-object or a pre-formatted XLS/XLSX file is passed to the DRAC website and the results are re-imported into R.

## Usage

```
use_DRAC(file, name, ...)
```

## **Arguments**

file	character: spreadsheet to be passed to the DRAC website for calculation. Can also be a DRAC template object obtained from template_DRAC().
name	character: Optional user name submitted to DRAC. If omitted, a random name will be generated
	Further arguments.

#### Value

Returns an RLum. Results object containing the following elements:

DRAC list: a named list containing the following elements in slot @data:

```
$highlights data.frame summary of 25 most important input/output fields
$header character HTTP header from the DRAC server response
$labels data.frame descriptive headers of all input/output fields
$content data.frame complete DRAC input/output table
$input data.frame DRAC input table
```

\$input data.frame DRAC input table boutput data.frame DRAC output table

data character or list path to the input spreadsheet or a DRAC template

call call the function call args list used arguments

The output should be accessed using the function get\_RLum.

 $use\_DRAC$  173

#### **Function version**

```
0.1.0 (2015-08-21 14:53:14)
```

#### Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France), Michael Dietze, GFZ Potsdam (Germany), Christoph Burow, University of Cologne (Germany)

R Luminescence Package Team

#### References

Durcan, J.A., King, G.E., Duller, G.A.T., 2015. DRAC: Dose Rate and Age Calculator for trapped charge dating. Quaternary Geochronology 28, 54-61. doi:10.1016/j.quageo.2015.03.012

```
## (1) Method using the DRAC spreadsheet
file <- "/PATH/TO/DRAC_Input_and_Output_Template.xlsx"</pre>
# send the actual IO template spreadsheet to DRAC
## Not run:
use_DRAC(file = file)
## End(Not run)
## (2) Method using an R template object
# Create a template
input <- template_DRAC()</pre>
# Fill the template with values
input$`Project ID` <- "DRAC-Example"</pre>
input$`Sample ID` <- "Quartz"</pre>
input$`Conversion factors` <- "AdamiecAitken1998"</pre>
input$`ExternalU (ppm)` <- 3.4</pre>
input$`errExternal U (ppm)` <- 0.51</pre>
input$`External Th (ppm)` <- 14.47</pre>
input$`errExternal Th (ppm)` <- 1.69</pre>
input$`External K (%)` <- 1.2</pre>
input$`errExternal K (%)` <- 0.14</pre>
input$`Calculate external Rb from K conc?` <- "N"</pre>
input
$`Calculate internal Rb from K conc?` <- "N"  
input$`Scale gammadoserate at shallow depths?` <- "N"</pre>
input$`Grain size min (microns)` <- 90</pre>
input$`Grain size max (microns)` <- 125</pre>
input$`Water content ((wet weight - dry weight)/dry weight) %' <- 5</pre>
input\ensuremath{\text{`errWater}} content \ensuremath{\text{``}} <- 2
input^Depth (m) < -2.2
input$`errDepth (m)` <- 0.22</pre>
input\olimits'Overburden density (g cm-3)' <- 1.8
input$`errOverburden density (g cm-3)` <- 0.1
input$`Latitude (decimal degrees)` <- 30.0000</pre>
```

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```
input$`Longitude (decimal degrees)` <- 70.0000
input$`Altitude (m)` <- 150
input$`De (Gy)` <- 20
input$`errDe (Gy)` <- 0.2

# use DRAC
## Not run:
output <- use_DRAC(input)

## End(Not run)</pre>
```

write\_R2BIN

Export Risoe.BINfileData into Risoe BIN-file

## **Description**

Exports a Risoe.BINfileData object in a \*.bin or \*.binx file that can be opened by the Analyst software or other Risoe software.

## Usage

```
write_R2BIN(object, file, version, compatibility.mode = FALSE,
    txtProgressBar = TRUE)
```

#### **Arguments**

object Risoe.BINfileData (**required**): input object to be stored in a bin file.

file character (**required**): file name and path of the output file

[WIN]: write\_R2BIN(object, "C:/Desktop/test.bin"),

[MAC/LINUX]: write\_R2BIN("/User/test/Desktop/test.bin")

version character (optional): version number for the output file. If no value is pro-

vided the highest version number from the Risoe.BINfileData is taken auto-

matically.

Note: This argument can be used to convert BIN-file versions.

compatibility.mode

logical (with default): this option recalculates the position values if necessary and set the max. value to 48. The old position number is appended as comment (e.g., 'OP: 70). This option accounts for potential compatibility problems with the Application of the problems.

the Analyst software.

txtProgressBar logical (with default): enables or disables txtProgressBar.

## **Details**

The structure of the exported binary data follows the data structure published in the Appendices of the Analyst manual p. 42.

If LTYPE, DTYPE and LIGHTSOURCE are not of type character, no transformation into numeric values is done.

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#### Value

Write a binary file.

#### **Function version**

```
0.3.2 (2015-08-21 14:53:14)
```

#### Note

The function just roughly checks the data structures. The validity of the output data depends on the user.

The validity of the file path is not further checked.

BIN-file conversions using the argument version may be a lossy conversion, depending on the chosen input and output data (e.g., conversion from version 07 to 06 to 04 or 03).

#### Warning

Although the coding was done carefully it seems that the BIN/BINX-files produced by Risoe DA 15/20 TL/OSL readers slightly differ on the byte level. No obvious differences are observed in the METADATA, however, the BIN/BINX-file may not fully compatible, at least not similar to the once directly produced by the Risoe readers!

Implementation of support for version 07 could so far not properly tested.

## Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France) R Luminescence Package Team

#### References

Duller, G., 2007. Analyst.

## See Also

```
read_BIN2R, Risoe.BINfileData, writeBin
```

```
##uncomment for usage

##data(ExampleData.BINfileData, envir = environment())
##write_R2BIN(CWOSL.SAR.Data, file="[your path]/output.bin")
```

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