# R package 'OSLdecomposition'

## Easy-to-use and reliable CW-OSL component separation

Dirk Mittelstraß<sup>1,\*</sup>, Christoph Schmidt<sup>2</sup>, Sebastian Kreutzer<sup>3</sup> <sup>1</sup>Independent Researcher, Berthelsdorfer Str. 13, 09599 Freiberg, Germany <sup>2</sup>Institute of Earth Surface Dynamics, University of Lausanne, 1015 Lausanne, Switzerland <sup>3</sup>Geography & Earth Sciences, Aberystwyth University, Wales, United Kingdom \*dirk.mittelstrass@luminescence.de

## What is the package for?

Age determination via quartz CW-OSL SAR measurements is prone to systematic errors due to signal components with unequal physical behavior. The new package provides functions for mathematical component identification and separation **without fitting** to enable component resolved equivalent dose calculation in **R**.

## What were the challenges?

A large variety of approaches to separate signal components in quartz CW-OSL measurements has been proposed so far. However, all these approaches rely either on sufficiently good signal-to-noise ratios (SNR) or exact knowledge of the component decay. Alternatively, they have special requirements on the instrumentation. It was our goal to develop a new approach which fulfills the following requirements:

- 1) Identify the detectable components on a sample-to-sample basis.
- 2) Allow component-resolved dose calculation for low-SNR measurements
- 3) Allow automated data analysis, without inherent need for user interaction
- 4) Be applicable for a variety of instrumental conditions
- 5) Enable an efficient re-evaluation of existing data sets

## How did we tackle the task?

We assumed that every CW-OSL curve I(t) can be described as sum of exponential decays:

$$I(t) = \sum_{k=1}^{K} n_k \lambda_k \mathrm{e}^{-\lambda_k t}$$

Further, we assumed that the number of components K and their signal decay rates  $\lambda_k$  are constant over the whole data set, while the component intensities  $n_k$  are individual for each CW-OSL curve. We defined a three-step workflow:



The algorithm used for Step 1 is based on Bluszcz & Adamiec (2006). The algorithm used for Step 2 is novel in the field of luminescence dating and was first presented by Mittelstraß et al. (2013). For Step 3, the established function analyse\_SAR.CWOSL of the package *Luminescence* is used (newest package version 0.9.9 needed). A detailed description of the methods as well as some simulation tests and some first applications can be found in Mittelstraß (2019).

## How to use the package?

You can download the package at <u>luminescence.de</u>. It will also be available open source on <u>GitHub</u> and soon on CRAN. A typical **R** script deploying the package reads as follows:

# load libraries

library(OSLdecomposition)
library(Luminescence)

#### # wood DIN file

## Step 1: CW-OSL component identification

The signal components and their decay rates  $\lambda_k$  are identified by combining all records to one global reference CW-OSL curve. A series of multi-exponential fittings with an increasing number of components K is then applied to this global curve (Bluszcz & Adamiec 2006). As default, the CW-OSL model for K = 3 is pre-selected. However, the user can re-evaluate the best CW-OSL model by considering the photoionization cross-section values and the outcome of an F-test.



**Figure 1:** K=3 CW-OSL model of the global average curve of all CW-OSL measurements of sample BT594 (Meszner et al. 2013). *Lower right table:* Estimated type of quartz OSL component (colored), photoionization cross sections  $\sigma$ , decay rates  $\lambda$  and signal intensity n

Detailed report: luminescence.de/OSLdecomposition/report\_Step1.html

## Step 2: CW-OSL component separation

With the number of components K and their decay rates  $\lambda$  known, an **algebraic decomposition algorithm** is deployed to calculate the signal component intensities n for each CW-OSL record. This **novel algorithm** has about the same accuracy as common nonlinear regression approaches and includes an analytical estimation of the statistical error. It returns mathematically correct and reproducible values even in case of noise-dominated CW-OSL measurements.



**Figure 2:** Decomposition results of the first two CW-OSL measurements of aliquot 8 of sample BT594 with signal component intensity n, its standard deviation and share at first channel  $I_0$ .

Signal component intensities over measurement sequence



**Figure 3:** Fast and medium component intensities for all CW-OSL measurements of aliquot 8 of sample BT594. Dashed line:  $T_x$  values; Dotted line:  $L_x$  values (dose-response curve only)

# read BIN file
data <- read\_BIN2R(file.choose(), fastForward = TRUE)</pre>

# check the data for consistency (optional)
data <- RLum.OSL\_correction(data)</pre>

# identify OSL components and return an analysis report data <- RLum.OSL\_global\_fitting(data, report = TRUE)</pre>

# separate OSL components and return an analysis report data <- RLum.OSL\_decomposition(data, report = TRUE)</pre>

# the dose calculation is handled by the Luminescence package # the integration intervals are set to "NA" De\_fast <- analyse\_SAR.CWOSL(data, NA, NA, NA, NA, OSL.component = 1)</pre>

# calculate Medium component De values
De\_medium <- analyse\_SAR.CWOSL(data, NA, NA, NA, NA, OSL.component = 2)</pre>

# compare the results for example in an Abanico plot plot\_AbanicoPlot(list(De\_fast, De\_medium))

### Detailed report: luminescence.de/OSLdecomposition/report\_Step2.html

### References

Bluszcz, A., Adamiec, G., 2006. Application of differential evolution to fitting OSL decay curves. Radiation Measurements 41, 886–891. https://doi.org/10.1016/j.radmeas.2006.05.016

Meszner, S., Kreutzer, S., Fuchs, M., Faust, D., 2013. Late Pleistocene landscape dynamics in Saxony, Germany: Paleoenvironmental reconstruction using loess-paleosol sequences. Quaternary International 296, 94–107. https://doi.org/10.1016/j.quaint.2012.12.040

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