Signal component analysis of IR-RF decay curves of K-feldspars

Multi-exponential fitting for enabling exploratory data science

Dirk Mittelstraß[1]*, Mariana Sontag-González[2], Christoph Schmidt[3], Tobias Lauer[4], Margret Fuchs[5] and Markus Fuchs[2]

[1] Independent Researcher, Dresden, Germany
[2] Department of Geography, Justus Liebig University Giessen, Giessen, Germany
[3] Institute of Earth Surface Dynamics, Université de Lausanne, Lausanne, Switzerland
[4] Terrestrial Sedimentology, Department of Geosciences, University of Tübingen, Tübingen, Germany
[5] Helmholtz-Zentrum Dresden-Rossendorf, Helmholtz Institute Freiberg for Resource Technology, Freiberg, Germany

*Corresponding author: dirk.mittelstrass@luminescence.de

Scope

Infrared-radiofluorescence (IR-RF) dating of K-feldspars has the potential to increase the knowledge about sedimentation processes through its extended age range, low liability for anomalous fading and good suitability for single grain measurements [1][2]. However, the composition and the underlying physics of the IR-RF signal are still only partly understood. In our approach to improve the knowledge about IR-RF, we use multi-exponential curve fitting as a tool to determine curve attributes, e.g. signal components. The statistics of these signal components can then be investigated further by data science methods. We hypothesize that trends and correlations found in these investigations will give evidence about underlying physical processes and their dependence on protocol parameters and sample history.

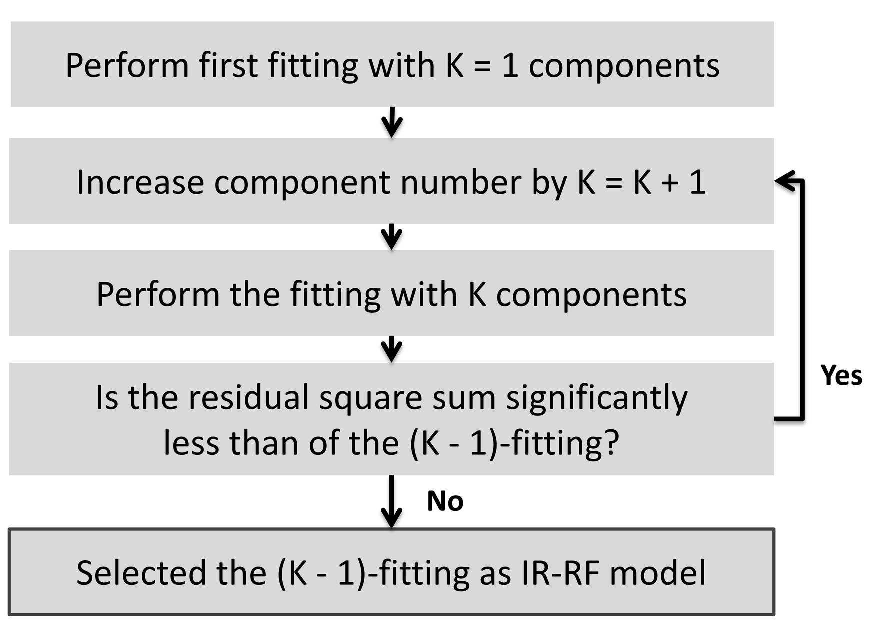
Signal curve fitting

As a working hypothesis we assume that each signal curve can be described by the sum of several exponential decay curves.

$$I_{RF}(d) = \sum_{k=1}^{K} \frac{n_k}{D_k} e^{-\frac{d}{D_k}}$$

- I_{RF} IR-RF signal
- d Accumulated dose during measurement, given by measurement time t and laboratory dose rate $\dot{D}_{lab}$, thus $d = t\dot{D}_{lab}$
- K Number of signal components
- k Signal component index
- n_k Signal component intensity, equals area below component curve
- D_k Half-decay dose of the signal component, related to the half-life τ by $D_k = \tau\dot{D}_{lab}$

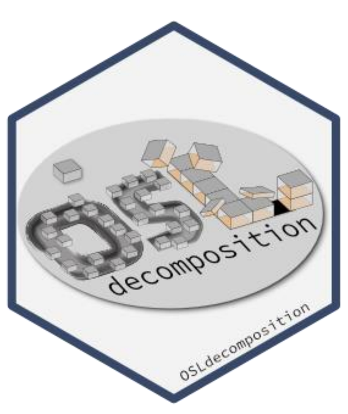
The decay constants D_k are optimized iteratively by a genetic algorithm [3] until the minimum of the residual square sum (RSS) is reached.
The number of exponential terms K is determined iteratively. A statistical test, e.g. an *F*-test, proves whether a new model with one component leads to significantly lower residual signals.



This approach has already proven itself useful for CW-OSL component analyses of quartz [4][5]. However, compared to older publications we used a novel determinant-based algorithm for the calculation of the pre-factors n_k to improve robustness and reproducibility of the approach. Also, we deduced the *F*-value threshold not from *p*-value considerations but from simulations focused on minimizing curve over- and under-fitting [6].

Used software

All data processing and plotting was performed using statistical programming language **R** and mulitple R packages, especially the package `Luminescence` [7]. The fitting algorithm is an adapted version of the `fit_OSLcurve()` function of the R package `OSLdecomposition` [8] and will be publicly available with a future update.



R package OSLdecomposition

Function library for the identification and separation of exponentially decaying signal components in CW-OSL.
Learn more at **luminescence.de**

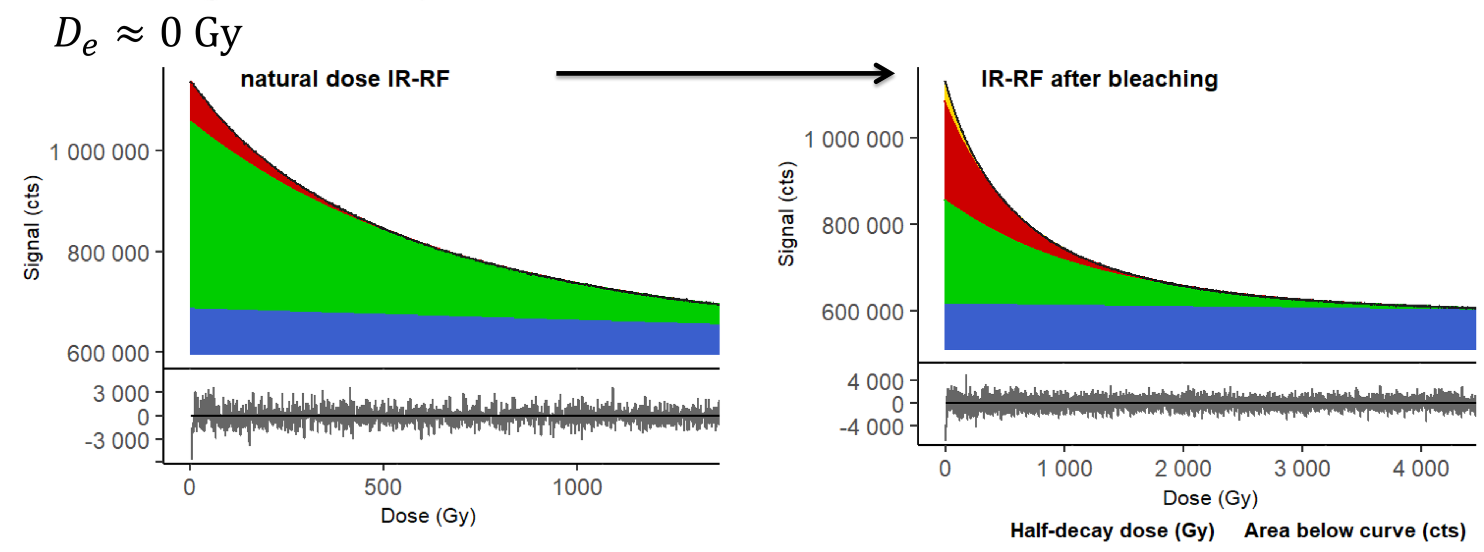
OSLdecomposition is part of the RLum.Network
Learn more at **r-luminescence.org**

References

[1] Mittelstraß, D. & Kreutzer, S. Spatially resolved infrared radiofluorescence: single-grain K-feldspar dating using CCD imaging. Geochronology 3, 299–319 (2021).
[2] Murari, M. K. et al. Infrared radiofluorescence (IR-RF) dating: A review. Quaternary Geochronology 64, 101155 (2021).
[3] Mullen, K., Ardia, D., Gil, D., Windover, D. & Cline, J. DEoptim: An R Package for Global Optimization by Differential Evolution. Journal of Statistical Software 40, 1–26 (2011).
[4] Bluszcz, A. & Adamiec, G. Application of differential evolution to fitting OSL decay curves. Radiation Measurements 41, 886–891 (2006).
[5] Peng, J., Dong, Z., Han, F., Long, H. & Liu, X. R package numOSL: numeric routines for optically stimulated luminescence dating. Ancient TL 31, (2013).
[6] Mittelstraß, D. Master thesis: Decomposition of weak optically stimulated luminescence signals and its application in retrospective dosimetry at quartz. (TU Dresden, 2019).
[7] Kreutzer, S. et al. Introducing an R package for luminescence dating analysis. Ancient TL 30, 1–8 (2012).
[8] Mittelstraß, D., Schmidt, C. & Kreutzer, S. R package 'OSLdecomposition' - Easy-to-use and reliable CW-OSL component separation. (2020).
[9] Richter, D., Richter, A. & Dornich, K. Lexsyg — A new system for luminescence research. Geochronometria 40, (2013).
[10] Frouin, M. et al. An improved radiofluorescence single-aliquot regenerative dose protocol for K-feldspars. Quaternary Geochronology 38, 13–24 (2017).
[11] Murton, J. B. et al. A multimethod dating study of ancient permafrost, Batagay megaslump, east Siberia. Quat. res. 105, 1–22 (2022).
[12] Kunz, A., Frechen, M., Ramesh, R. & Urban, B. Periods of recent dune sand mobilisation in Cuddalore, Southeast India. zdgg 161, 353–368 (2010).
[13] Key, A. et al. On the earliest Acheulean in Britain: first dates and in-situ artefacts from the MIS 15 site of Fordwich (Kent, UK). R. Soc. open sci. 9, 211904 (2022).

Fitting examples

$D_e \approx 0$ Gy



natural dose IR-RF:

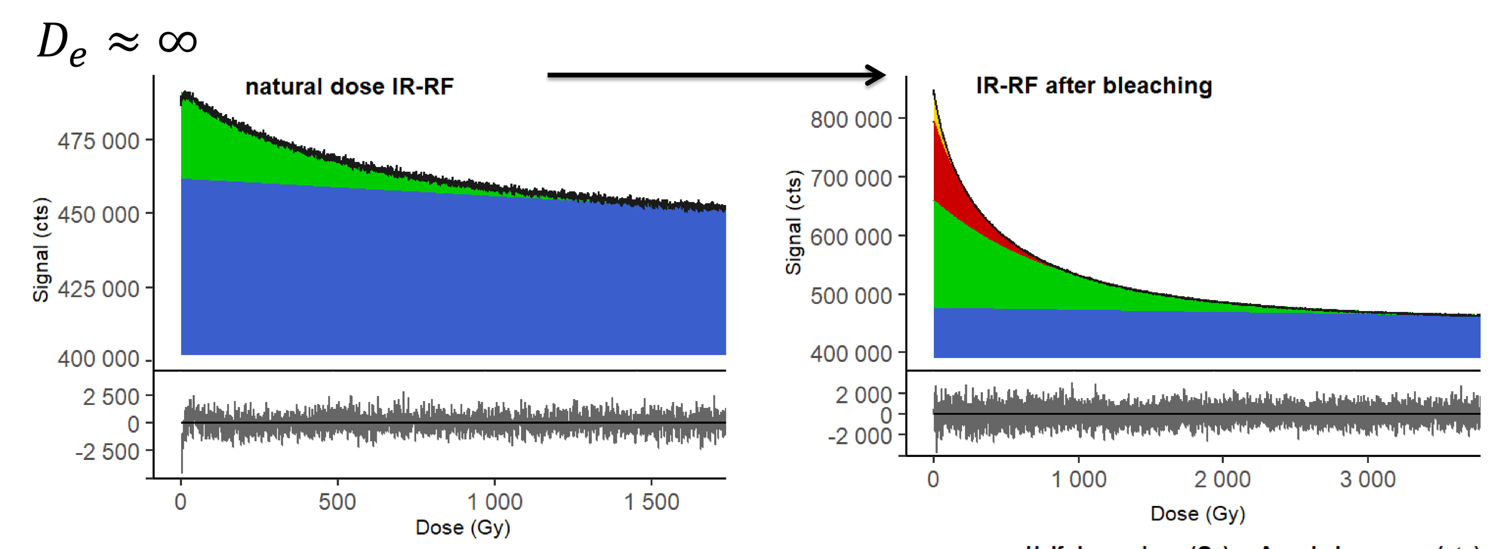
	Half-decay dose (Gy)	Area below curve (cts)
Component 1	175.1	2.09e+07 ± 9.57e+04
Component 2	622.5	3.38e+08 ± 2.63e+05
Component 3	2.855e+04	2.85e+10 ± 3.29e+06

IR-RF after bleaching:

	Half-decay dose (Gy)	Area below curve (cts)
Component 1	165.6	1.24e+07 ± 1.07e+05
Component 2	471.4	1.57e+08 ± 3.19e+05
Component 3	1209	4.26e+08 ± 3.95e+05
Component 4	1.982e+05	1.77e+11 ± 8.46e+06

Figure 1a,b: IR-RF signal components of aliquot 78 of modern age sample Gi361, measured on a lexsyg research device [9] using the RF_{70} protocol [10], thus IR-RF was measured at 70°C with a 850/40 filter. The sample was solar simulator bleached for 7 h before the second measurement (b). The sample consists of ca. 96 % K-feldspar (QEM).

$D_e \approx \infty$



natural dose IR-RF:

	Half-decay dose (Gy)	Area below curve (cts)
Component 1	460.9	2.27e+07 ± 5.78e+04
Component 2	7.951e+04	6.11e+10 ± 3.06e+06

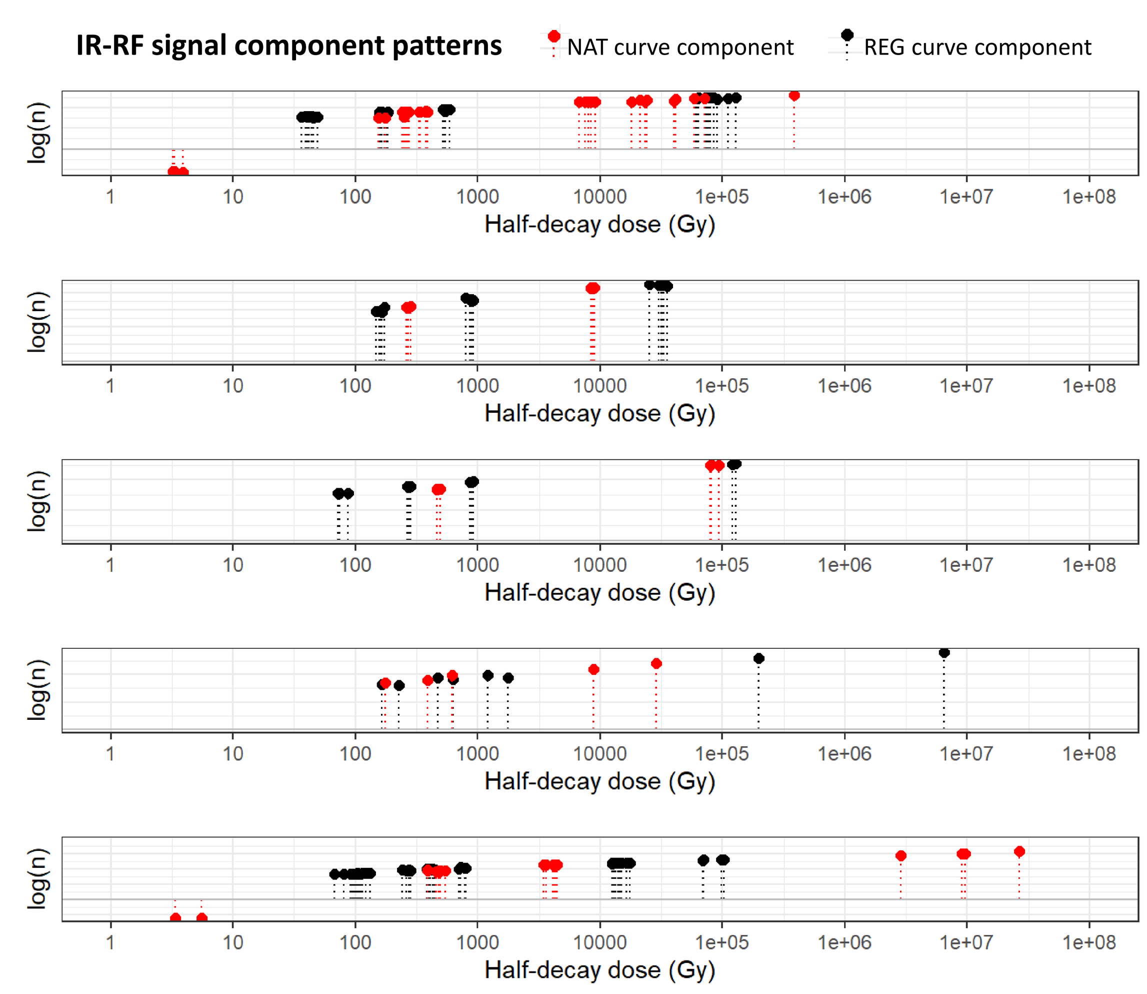
IR-RF after bleaching:

	Half-decay dose (Gy)	Area below curve (cts)
Component 1	71.41	6.37e+06 ± 4.62e+04
Component 2	264.8	6.01e+07 ± 1.48e+05
Component 3	894.9	2.76e+08 ± 2.30e+05
Component 4	1.279e+05	1.01e+11 ± 4.68e+06

Figure 2a,b: IR-RF signal components of aliquot 34 of dose saturated sample 326. Protocol and measurement settings are equal to figure 1. The sample consists of ca. 89 % K-feldspar (QEM).

Sample statistics

We tested multiple K-feldspar samples of different provenance, all measured with the RF_{70} protocol [10]:



B19-LU: Batagay mega-slump, Sibiria [11]
Multiple layers of a permafrost sediment
Grain size 63–100 µm, age 100–500 ka

BT1657: Persani mountains, Romania
Baked paleosol below lava flow
Grain size 90–200 µm, age ~ 1 Ma

Gi361: Cuddalore, India [12]
Recently formed coastal dune
Grain size 150–200 µm, modern age

Gi326: Bayreuth, Germany
Crushed from Triassic sandstone
Grain size 90–200 µm, in dose saturation

L-Eva-2275 & **2277**: Fordwich, UK [13]
Fluvial sands from stone age excavation site
Grain size 90–250 µm, age ~ 500 ka

Figure 3a-e: Intensity n_k over decay constant D_k of all components of multiple aliquots of multiple samples on double-logarithmic scale. **Red dots**: Natural dose IR-RF signal component, **black dots**: After bleaching IR-RF signal component.

Observations

- In most cases, natural dose curves (NAT curves) can be sufficiently described with two signal components
- Long IR-RF curves after bleaching (REG curves) can be sufficiently described with four signal components
- Multiple specimen of signal components can be identified, where the NAT curve component with D_k's between 200 and 600 Gy dominates the curvature and therefore the equivalent dose results.
- That part of the REG curve which matches the NAT curve in the sliding technique can also be sufficiently described by just two components. However, the dominating component is usually shifted toward higher D_k.

Luminescence data analysis as a service

https://luminescence.de/author.html

The algorithms and analyses presented here are an unfunded hobbyist project of the main author. Dirk can be booked to perform advanced analyses of OSL, IRSL and IR-RF data sets. He is also experienced in setting up and analyzing spectrally resolved and spatially resolved luminescence measurements.
Dirk has also a cooperation with the newly founded **LUNA lab** in Freiberg, Germany. The LUNA lab is a joint project of HZDR, TU Freiberg and Freiberg Instruments and is led by Dr. Margret Fuchs. The lab provides commercial services for sample preparation, luminescence dating and drill core sample mapping.