Standardizing the computerized analysis and modeling of luminescence phenomena: new open-access codes in R and Python

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You can download this talk as a PDF at https://github.com/vpagonis/Python-Codes/blob/main/PagonisLED.pdf

OUTLINE OF THE TALK

- Introduction: The new R and Python initiative
  Motivation

- Why we chose R and Python

- How the codes are organized
  By type of signal: TL, OSL, IRSL, dose response etc
  By type of transition: delocalized, localized, semilocalized

- Availability of open-access codes, expected date of project completion

- Examples of currently available codes

- Conclusions

Purpose of the new R and Python initiative

Classification, organization and standardization of :

Computerized analysis of luminescence signals
Modelling of luminescence phenomena.

- Although a significant number of open access codes is already available in the literature, there is a ***lack of common standardization and homogeneity***.

- We want to develop ***new codes*** and ***include the latest modelling:***

New equations based on the Lambert W function for
TL, OSL, dose response

New equations for localized transitions in *feldspars* for
TL, CW-IRSL, LM-IRSL, Time-resolved signals

Develop codes for most available luminescence models

Why choose

R versus **Python**

R	Python
Many excellent R packages already available (e.g. *Luminescence*)	**Huge number of libraries for scientific analysis**
Various R packages are already incorporated in Analyst	**Learning curve less steep, more researchers are familiar with it**
Steeper learning curve than Python	**Structure of codes easier to read**
R is all about vectors, manipulation of large amounts of data can be very efficient	**Very large online community and websites available, that can help us find a solution quickly**
Structure of commands is not obvious to a new user.	
R is ideal for statistical analysis	

PYTHON CODES- PART I

TL

DELOCALIZED TRANSITIONS

- Kitis-Vlachos Equation with Lambert (KV-TL)
- Mixed order Kinetics (MOK)
- First order Kinetics (FOK)
- General order Kinetics (GOK)

LOCALIZED QUANTUM TUNNELING TRANSITIONS

- Kitis-Pagonis Equation for prompt TL signals (KP-TL)
- Anomalous fading analysis (g-factor)
- Transformed KP-TL equation for preconditioned samples

CW-OSL/LM-OSL

DELOCALIZED TRANSITIONS

- Kitis-Vlachos Equation with Lambert (KV-CW And KV-LM)
- First order Kinetics (exponential functions)
- General order Kinetics (GOK)

LOCALIZED QUANTUM TUNNELING TRANSITIONS

- Kitis-Pagonis Equations (KP-CW and KP-LM)

24 PYTHON CODES CURRENTLY AVAILABLE

1.1 Deconvolution of Glocanin TL with Lambert function . . . .
1.2 Deconvolution of LiF peak using the KV-TL equation . . . .
1.3 MOK deconvolution of glow curve for Al2O3:C . . . .
1.4 Deconvolution of BeO TL with transformed MOK . . . .
1.5 Deconvolution of GLOCANIN TL using the original GOK . . . .
1.6 Deconvolution of Al2O3:C glow curve (GOK) . . . .
1.7 Deconvolution LBO data using transformed KV-TL equation .
1.8 Deconvolution of TL user data (.txt file, GOK) . . . .
1.9 Deconvolution of 9-peak glow curve using the transformed KV-eqt . . . .
1.10 Deconvolution of 9-peak Glocanin TL data (GOK) . . . .

TL DELOCALIZED (quartz, most Materials)

2.1 Anomalous fading (AF) and the g-factor . . . .
2.2 Fit MBO data with KP-TL equation . . . .
2.3 Fit TL for KST4 feldspar with KP-TL equation . . . .
2.4 Deconvolution of 5-peak glow curve for BAL21 sample . . . .
2.5 Deconvolution of MBO data with transformed KP-TL equation . . . .

TL LOCALIZED (feldspars)

3.1 Isothermal analysis for LiF:Mg,Ti . . . .
3.2 Initial rise analysis for LiF:Mg,Ti . . . .
3.3 CGCD analysis of single TL peak in LiF:Mg,Ti . . . .

ITL (isothermal)

4.1 Fit dose response data with saturating exponential . . . .
4.2 Fit of experimental TL dose response data using W(x) . . . .
4.3 Fit of experimental ESR dose response data using Lambert equation . . . .
4.4 Fit of experimental OSL dose response data using W(x) . . . . . .
4.5 TL dose response of anion deficient aluminum oxide . . . .
4.6 Fit to Supralinearity index f(D) using PKC equation . . . .

DOSE RESPONSE

PYTHON CODES- PART I

TL

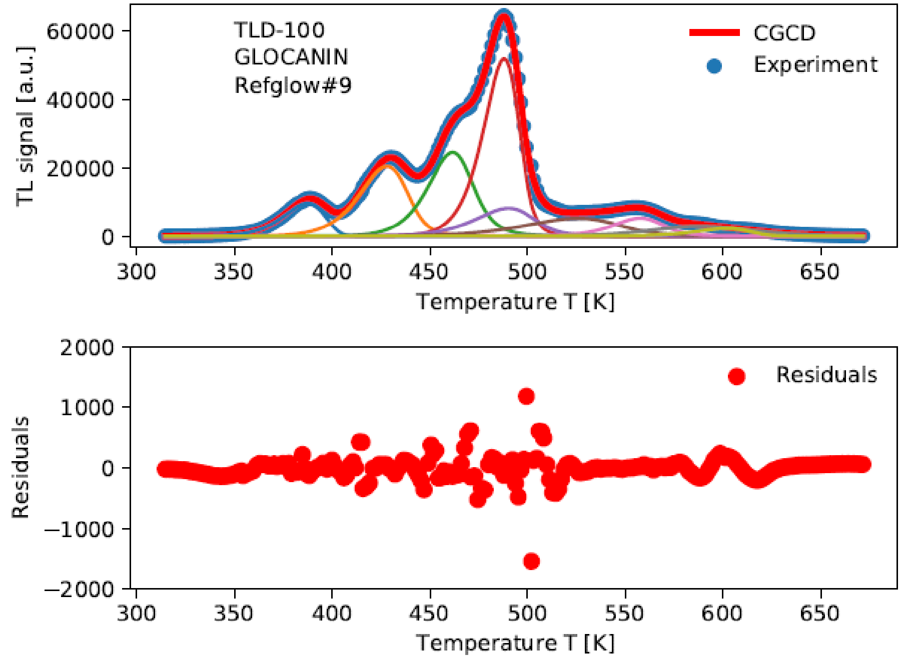
DELOCALIZED TRANSITIONS

Kitis-Vlachos Equation with Lambert (KV-TL)

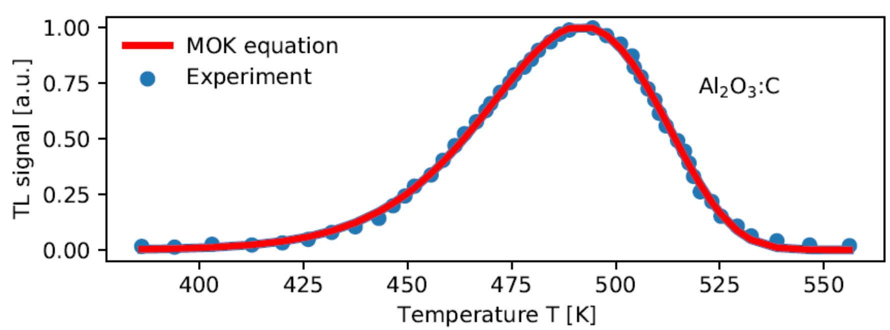
Mixed order Kinetics (MOK)

First order Kinetics (FOK)

General order Kinetics (GOK)



Deconvolution of a TLD-100 glow curve from the GLOCANIN project using 9 peaks with the transformed KV-TL equation



Deconvolution of the main dosimetric peak in Al2O3:C, using Mixed Order Kinetics (MOK).

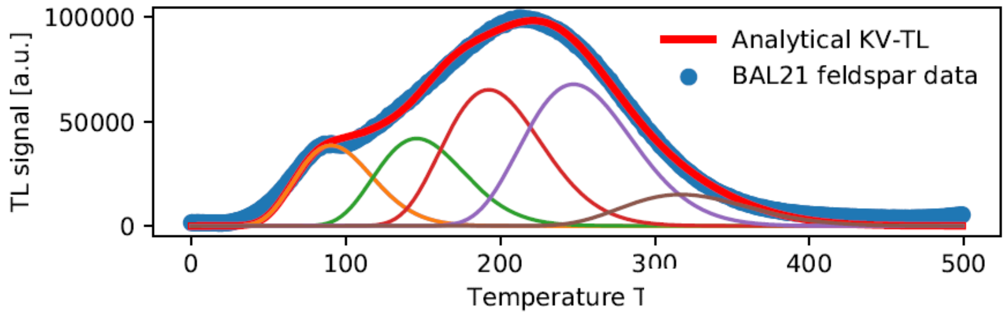
TL

LOCALIZED QUANTUM TUNNELING TRANSITIONS

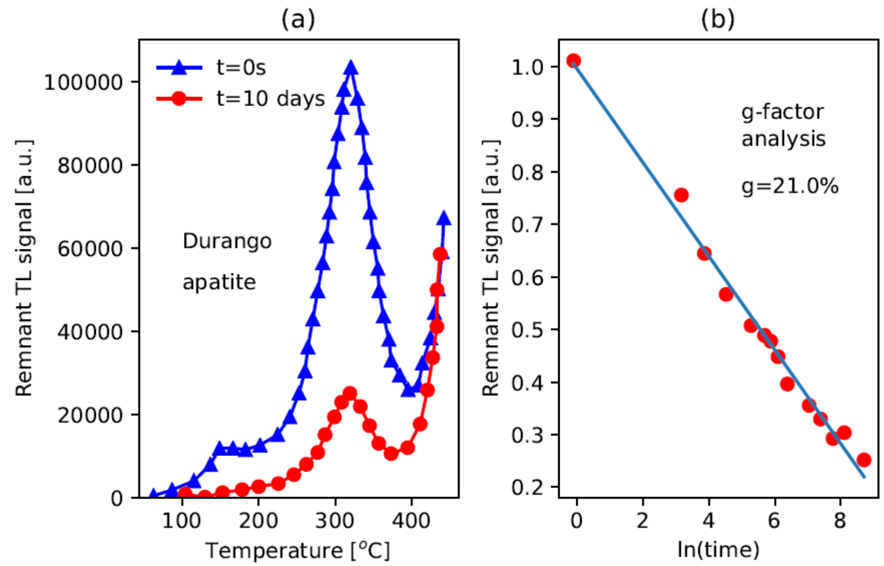
Kitis-Pagonis Equation for prompt TL signals (KP-TL)

Anomalous fading analysis (g-factor)

Transformed KP-TL equation for preconditioned samples



Experimental TL glow curve from freshly irradiated feldspar BAL21 sample, fitted using 5 peaks and the KP-TL analytical Equation.

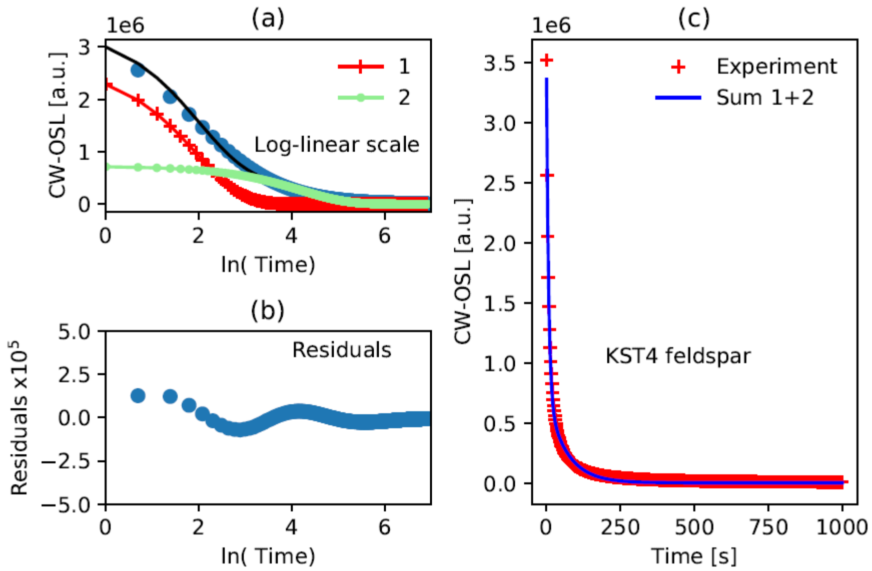


Anomalous fading effect in Durango apatite. (a) The TL signal is measured immediately after irradiation, and after 10 days have elapsed at room temperatures. (b) Analysis of (a), to obtain the g-factor for this material.

CW-OSL/LM-OSL

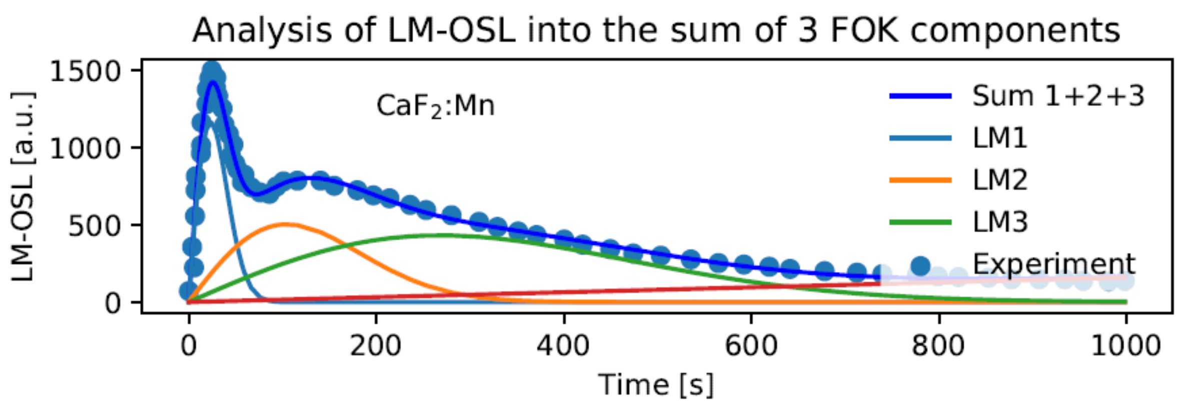
DELOCALIZED TRANSITIONS

Kitis-Vlachos Equation with Lambert (KV-CW And KV-LM)



Example of fitting 1000 s of a CW-OSL signal with two exponential components. The CW-OSL data are from a freshly irradiated aliquot of feldspar sample KST4

First order Kinetics (exponential functions)



Example of analyzing an LM-OSL signal from the dosimetric material CaF2:N with three first order components

General order Kinetics (GOK)

PYTHON CODES – PART II

ITL (isothermal)

DELOCALIZED TRANSITIONS

- Kitis-Vlachos Equation with Lambert (KV-ITL)
- Mixed order Kinetics (MOK-ITL)
- First order Kinetics (FOK-ITL exponentials)
- General order Kinetics (GOK-ITL)

LOCALIZED QUANTUM TUNNELING TRANSITIONS

- Kitis-Pagonis Equation for ITL signals (KP-ITL)

CW-IRSL/LM-IRSL

LOCALIZED QUANTUM TUNNELING TRANSITIONS

- Kitis-Pagonis Equations for IRSL (KP-CW-IRSL and KP-LM-IRSL)

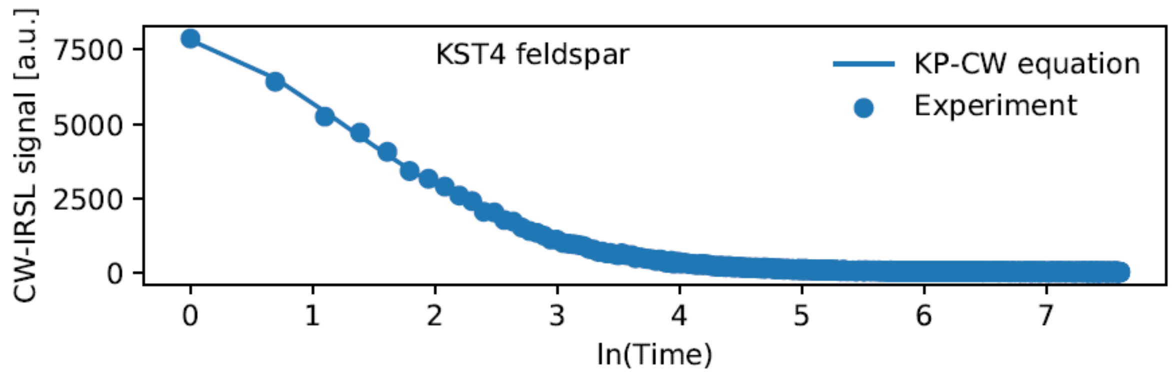
DOSE RESPONSE

- Pagonis-Kitis-Chen Equation with Lambert Function (PKC)
- Pagonis-Kitis-Chen-Superlinear response equation with Lambert (PKC-S)

CW-IRSL/LM-IRSL

LOCALIZED QUANTUM TUNNELING TRANSITIONS

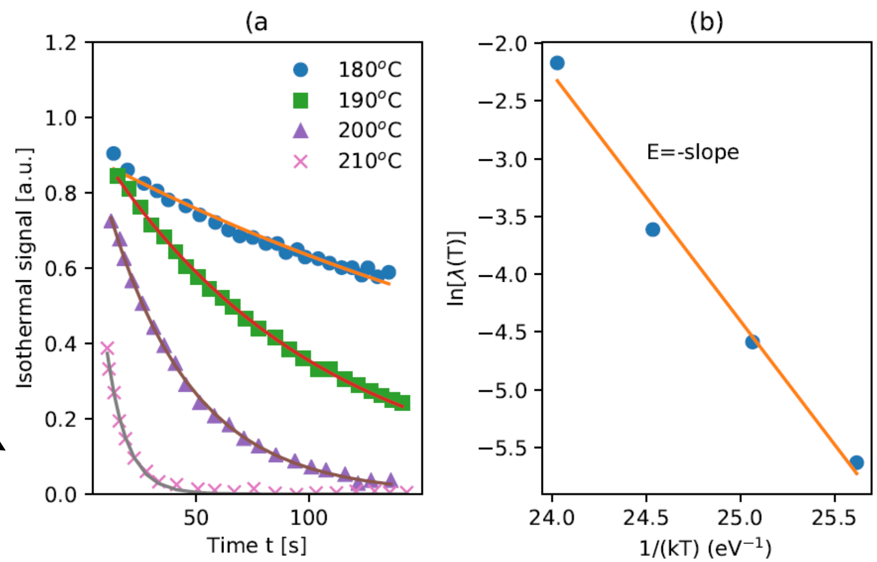
Kitis-Pagonis Equations for IRSL (KP-CWIRSL and KP-LMIRSL)



Experimental CW-IRSL curve from freshly irradiated KST4 feldspar sample, fitted using the KP-CW analytical equation.

ITL (isothermal)

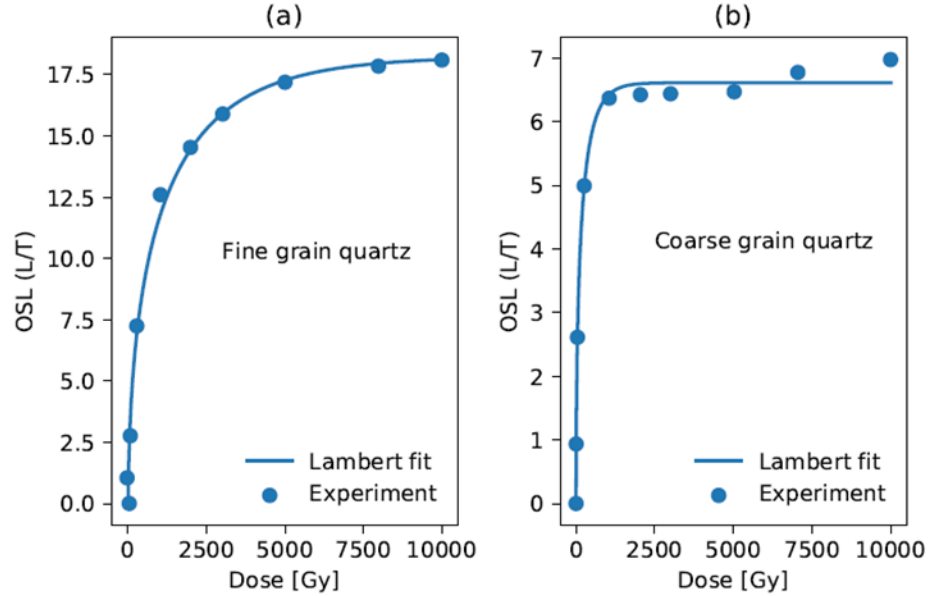
DELOCALIZED TRANSITIONS



(a) Isothermal TL decay curves for LiF: Mg,Ti (TLD-100) at temperatures of 180-210°C. The solid lines are exponential decay curves fitted to the experimental data. (b) A best line t to the Arrhenius plot yields the activation energy E

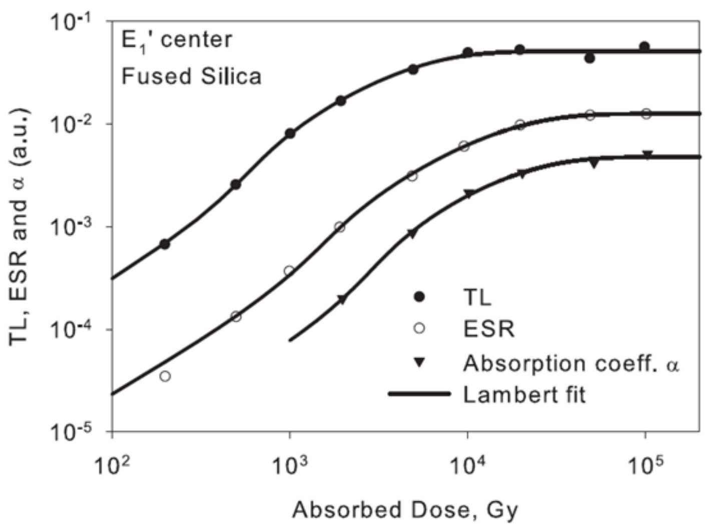
DOSE RESPONSE

Pagonis-Kitis-Chen Equation with Lambert Function (PKC)



Fit of experimental SAR-OSL experimental dose response data, for (a) fine grain and (b) coarse grain quartz samples, using the PKC equation..

Pagonis-Kitis-Chen Superlinear response equation with Lambert (PKC-S)



Superlinear dose dependence of the E_1' center concentration (ESR), TL and OA signals, from a single sample of fused silica.

PYTHON CODES – PART III

TIME-RESOLVED

DELOCALIZED TRANSITIONS

- First order Kinetics (FOK-TR exponentials)

LOCALIZED QUANTUM TUNNELING TRANSITIONS

- Pagonis-Kitis Equation for time-resolved signals (PK-TR)

GENERAL ANALYSIS CODES

- Excitation spectra analysis (Gaussians or Lorenzians)
- Initial rise analysis
- Heating rates method analysis
- Analysis of TL from a distribution of energies

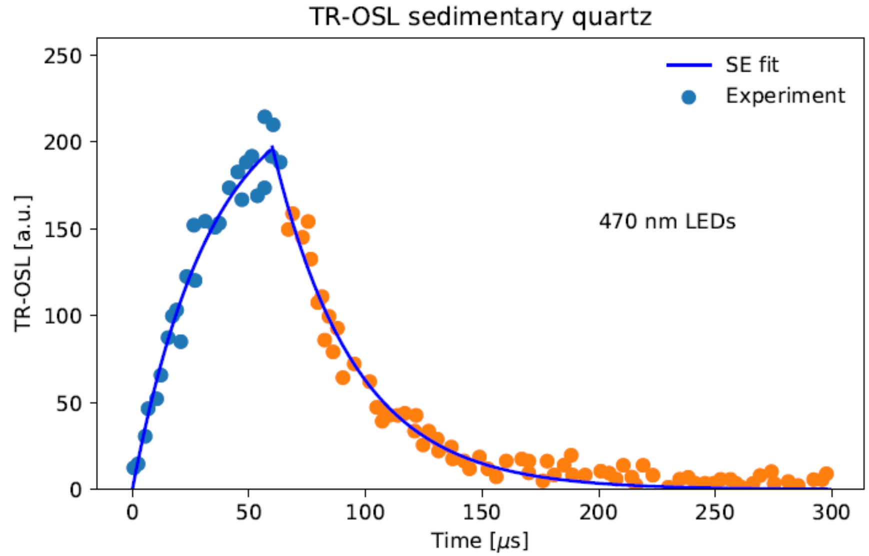
CODES FOR MODELS

- General one trap (GOT) model
- One trap one center (OTOR) model
- General one trap (GOT) model
- Localized transitions (LT) model
- Ground state tunneling (GST) model
- Excited state tunneling (EST) model

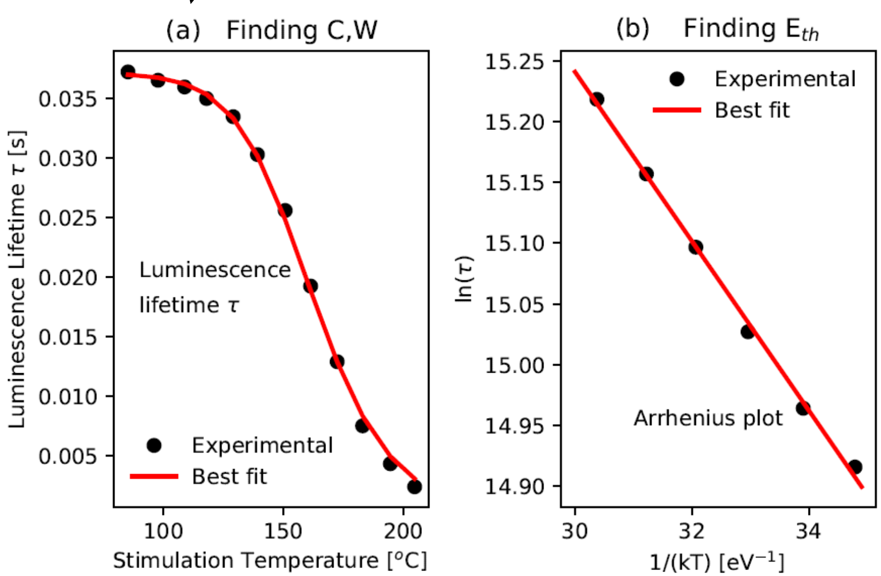
TIME-RESOLVED

DELOCALIZED TRANSITIONS

First order Kinetics (FOK-TR exponentials)



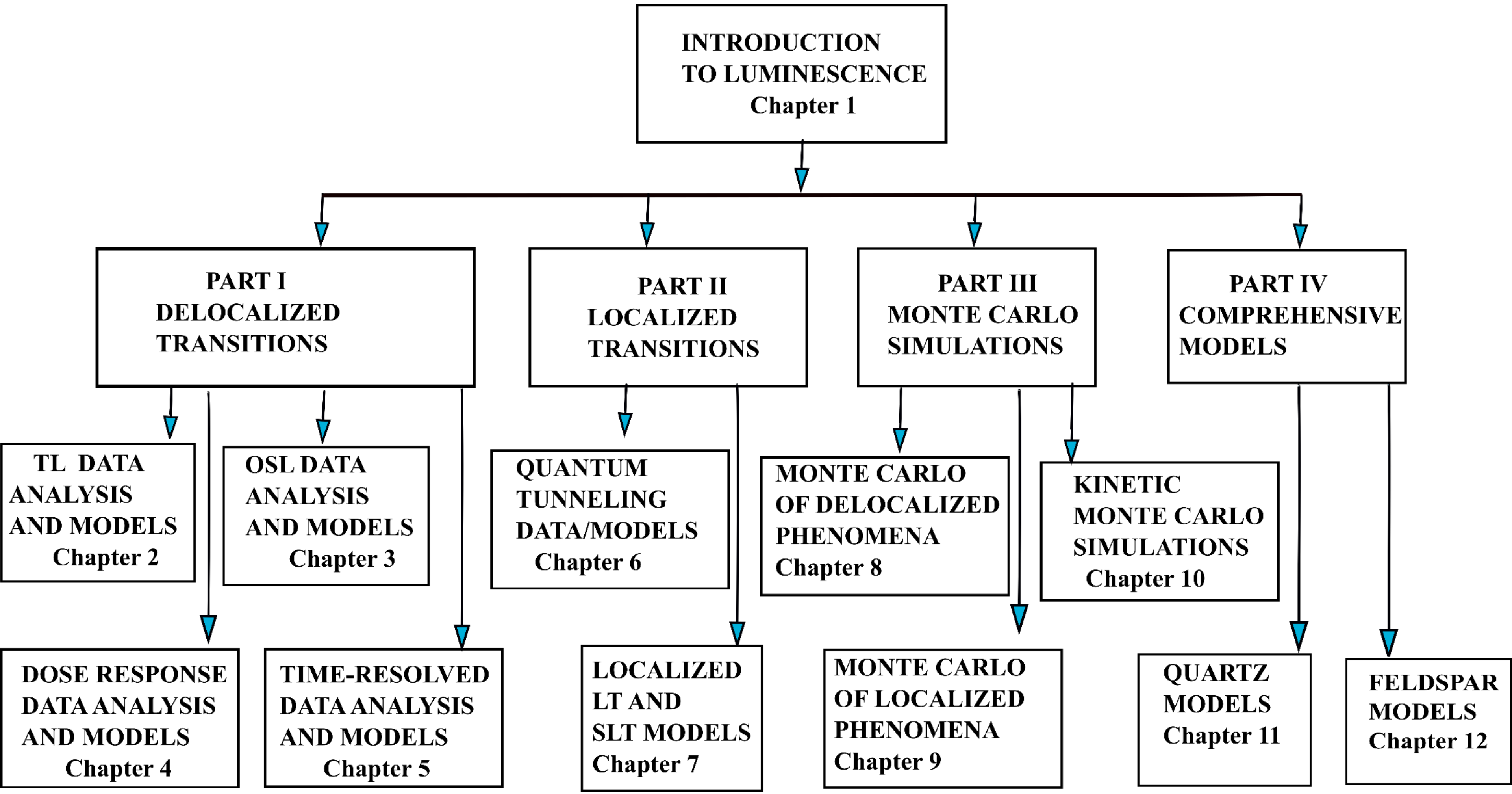
Examples of TR-OSL curves for sedimentary quarts with 60 μs pulse. For more details see Chithambo et al. [37].



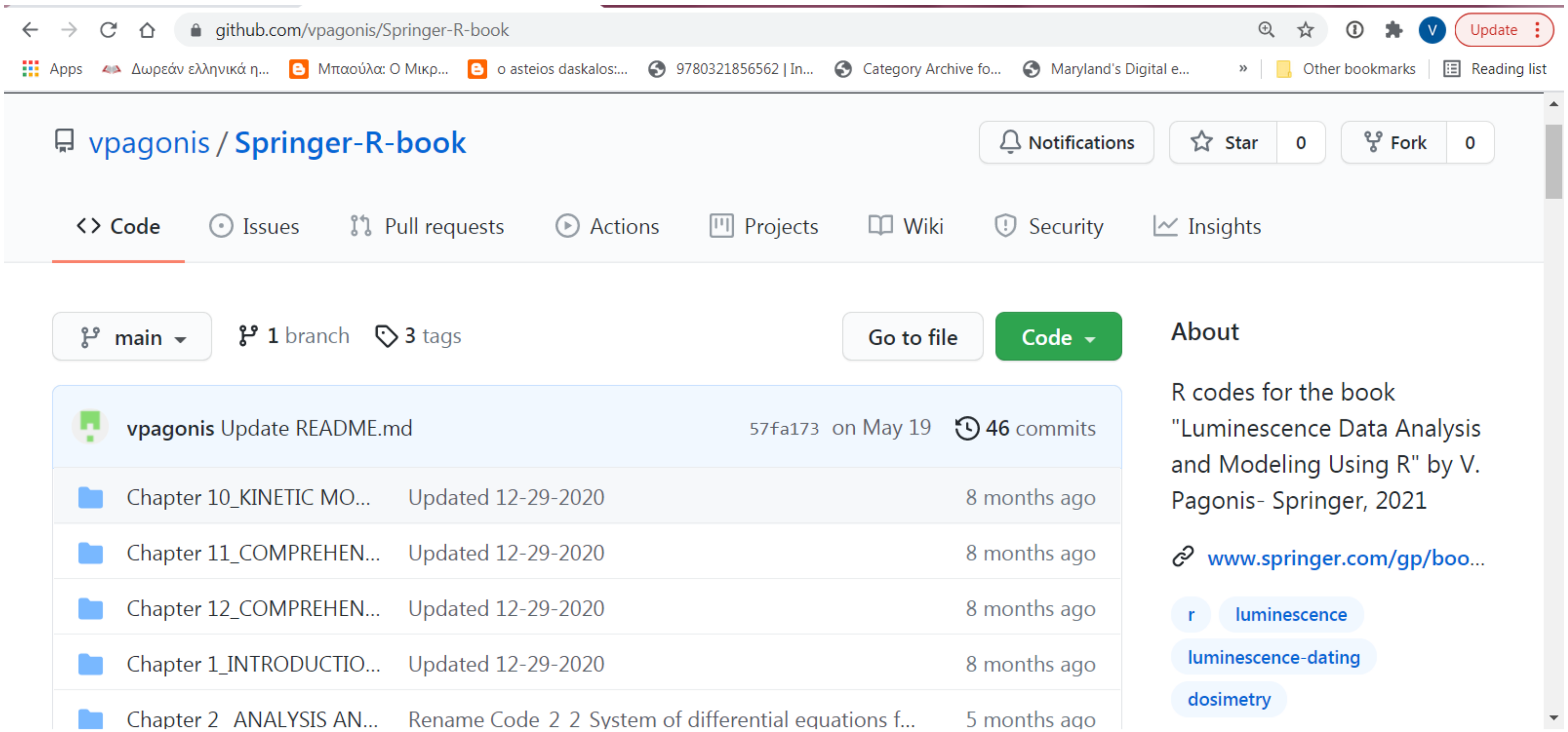
Experimental determination of the thermal quenching parameters C, W, Eth. (a) The values of C;W are obtained by fitting the decreasing part of the data. (b) The thermal activation energy Eth is obtained with an Arrhenius analysis of the increasing part of the data in (a).

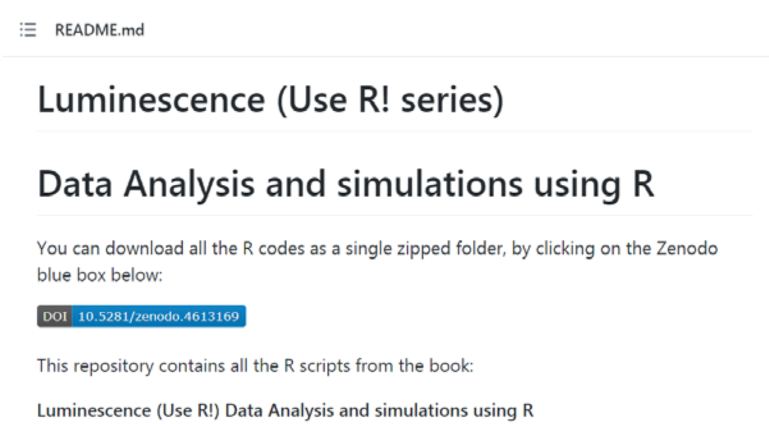
OVERALL ORGANIZATION OF PYTHON-CODES IN THE SPRINGER BOOK

ORGANIZATION OF 99 R-CODES IN THE R BOOK



The 99 R codes from the Springer Luminescence book are found at GitHub
https://github.com/vpagonis/Springer-R-book





All R codes can be downloaded as a single ZIP file from ZENODO

WHERE TO FIND THE CODES, EQUATIONS, MODELS

R codes

The complete 99 R codes from the Springer Luminescence book are found at this GitHub website:

https://github.com/vpagonis/Springer-R-book

Recently published R book

V. Pagonis. Luminescence: Data Analysis and Modeling Using R. Use R! Springer International Publishing, 2021.

(Contains all equations and models)

PYTHON

The complete 24 Python codes described here are found at this GitHub website:

https://github.com/vpagonis/Python-Codes

In the same GitHub website, this extensive 100-page PDF file describes the 24 codes:

https://github.com/vpagonis/Python-Codes/blob/main/LED2021.pdf

REVIEW PAPER: ***G. Kitis, G. S. Polymeris, V. Pagonis. Applied Radiation and Isotopes 153 (2019) 108797.***

Most PDFs of my papers are available at: https://blog.mcdaniel.edu/vasilispagonis/

CONCLUSIONS

*The initiative's goal is to **Classify, organize, standardize R and Python codes for computerized analysis and luminescence models***

Currently 99 complete R-codes and 24 Python codes are available for downloading at GitHub

The R-codes have been tested and cross-checked with Mathematica

The Python codes are still under development

Anticipated date for completion of Python codes is June 2022

*If you wish to stay updated on our progress with the codes,
please send me an email: vpagonis@mcdaniel.edu*

Thank you very much for your attention!