

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



Vasilis Pagonis<sup>1</sup>

George Kitis<sup>2</sup>



<sup>1</sup>McDaniel College, Westminster, MD, USA

<sup>2</sup>Aristotle University of Thessaloniki, Greece

*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, IRSI, 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**

Many excellent R packages already available (e.g. *Luminescence*)

Various R packages are already incorporated in Analyst

Steeper learning curve than Python

R is all about vectors, manipulation of large amounts of data can be very efficient

Structure of commands is not obvious to a new user.

R is ideal for statistical analysis

Huge number of libraries for scientific analysis

Learning curve less steep, more researchers are familiar with it

Structure of codes easier to read

Very large online community and websites available, that can help us find a solution quickly

# PYTHON CODES- PART I

TL

DELOCALIZED  
TRANSITIONS

LOCALIZED  
QUANTUM TUNNELING  
TRANSITIONS

Kitis-Vlachos  
Equation with  
Lambert (KV-TL)

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

Mixed order  
Kinetics  
(MOK)

Anomalous fading analysis  
(g-factor)

First order  
Kinetics  
(FOK)

Transformed  
KP-TL equation for  
preconditioned  
samples

General order  
Kinetics  
(GOK)

CW-OSL/LM-OSL

DELOCALIZED  
TRANSITIONS

LOCALIZED  
QUANTUM TUNNELING  
TRANSITIONS

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

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

First order  
Kinetics  
(exponential  
functions)

General order  
Kinetics  
(GOK)

## 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 Al<sub>2</sub>O<sub>3</sub>:C .....
- 1.4 Deconvolution of BeO TL with transformed MOK .....
- 1.5 Deconvolution of GLOCANIN TL using the original GOK ....
- 1.6 Deconvolution of Al<sub>2</sub>O<sub>3</sub>: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) .....
  
- 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 .....
  
- 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 .....
  
- 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 .....

**TL  
DELOCALIZED**  
(quartz, most  
Materials)

**TL  
LOCALIZED**  
(feldspars)

**ITL (isothermal)**

**DOSE RESPONSE**

TL

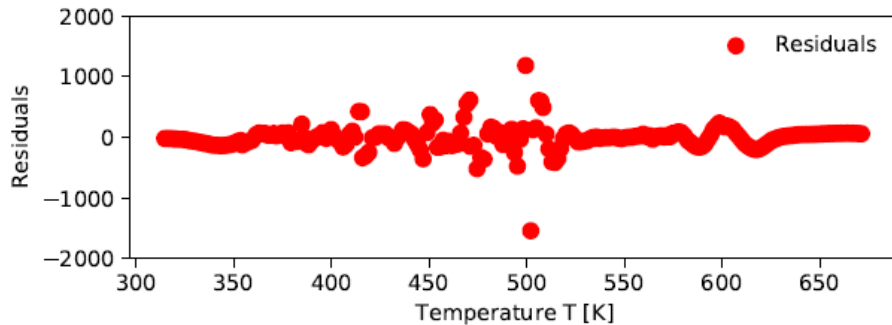
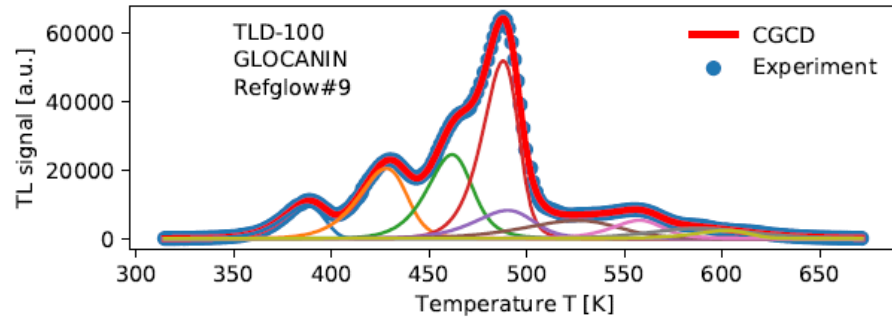
DELOCALIZED  
TRANSITIONS

Kitis-Vlachos  
Equation with  
Lambert (KV-TL)

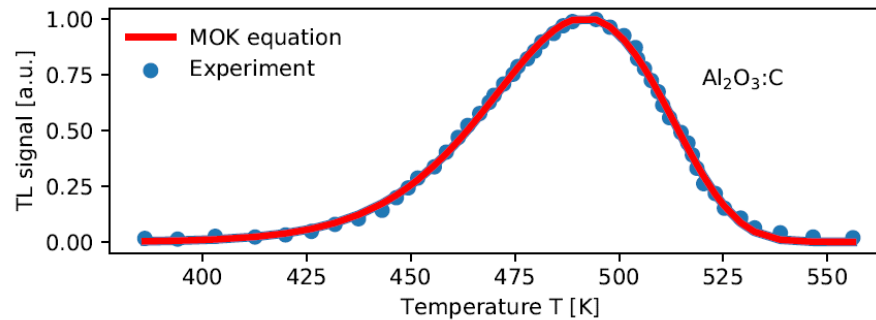
Mixed order  
Kinetics  
(MOK)

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 Al<sub>2</sub>O<sub>3</sub>:C, using Mixed Order Kinetics (MOK).

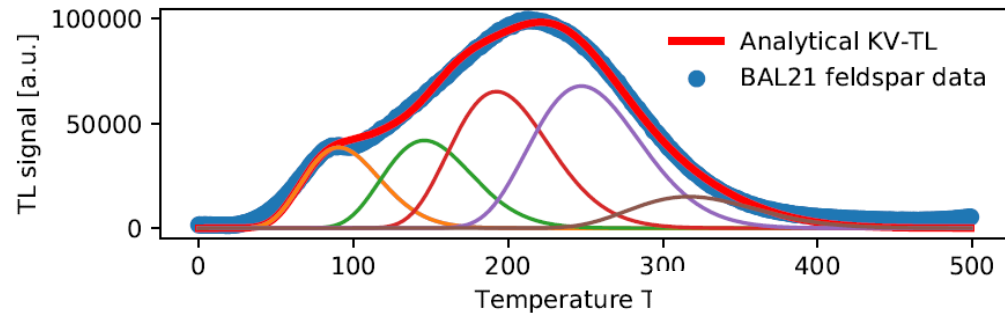
TL

LOCALIZED  
QUANTUM TUNNELING  
TRANSITIONS

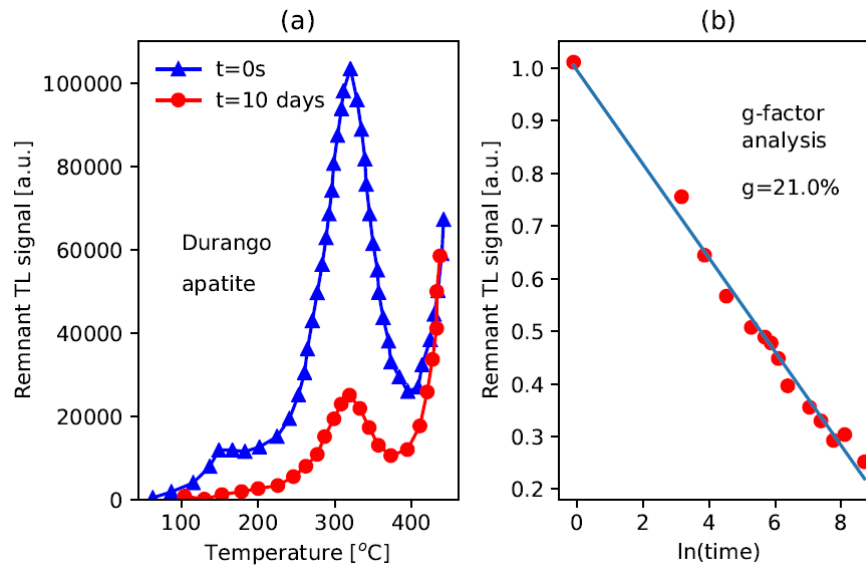
Kitis-Pagonis  
Equation for prompt  
TL signals (KP-TL)

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.



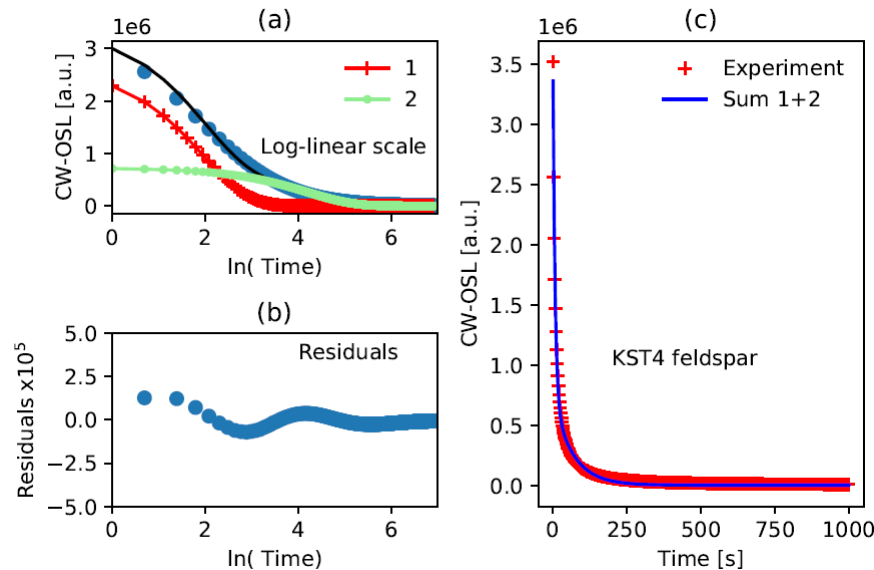
CW-OSL/LM-OSL

DELOCALIZED  
TRANSITIONS

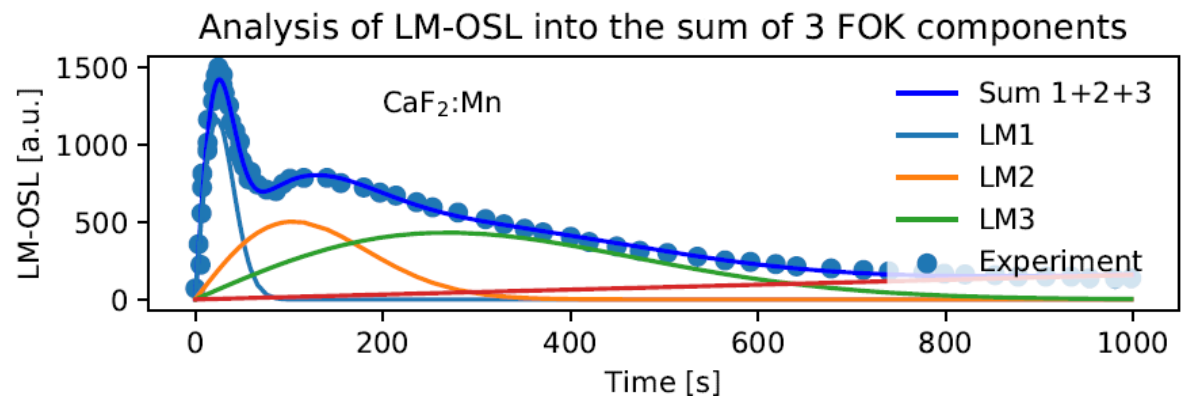
Kitis-Vlachos  
Equation with  
Lambert (KV-CW  
And KV-LM)

First order  
Kinetics  
(exponential  
functions)

General order  
Kinetics  
(GOK)



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



Example of analyzing an LM-OSL signal from the dosimetric material  $\text{CaF}_2:\text{N}$  with three first order components

## PYTHON CODES – PART II

### ITL (isothermal)

DELOCALIZED  
TRANSITIONS

LOCALIZED  
QUANTUM TUNNELING  
TRANSITIONS

Kitis-Vlachos  
Equation with  
Lambert (KV-ITL)

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

Mixed order  
Kinetics  
(MOK-ITL)

First order  
Kinetics  
(FOK-ITL  
exponentials)

General order  
Kinetics  
(GOK-ITL)

### CW-IRSL/LM-IRSL

LOCALIZED  
QUANTUM TUNNELING  
TRANSITIONS

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

### DOSE RESPONSE

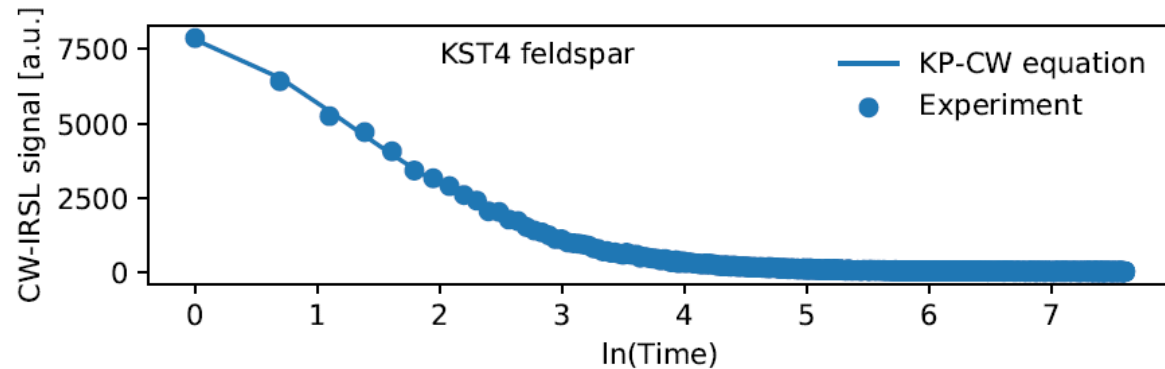
Kitis-Pagonis-Chen  
Equation with Lambert  
Function (KPC)

Kitis-Pagonis-Chen  
superlinear response  
equation with Lambert  
(KPC-S)

CW-IRSL/LM-IRSL

LOCALIZED  
QUANTUM TUNNELING  
TRANSITIONS

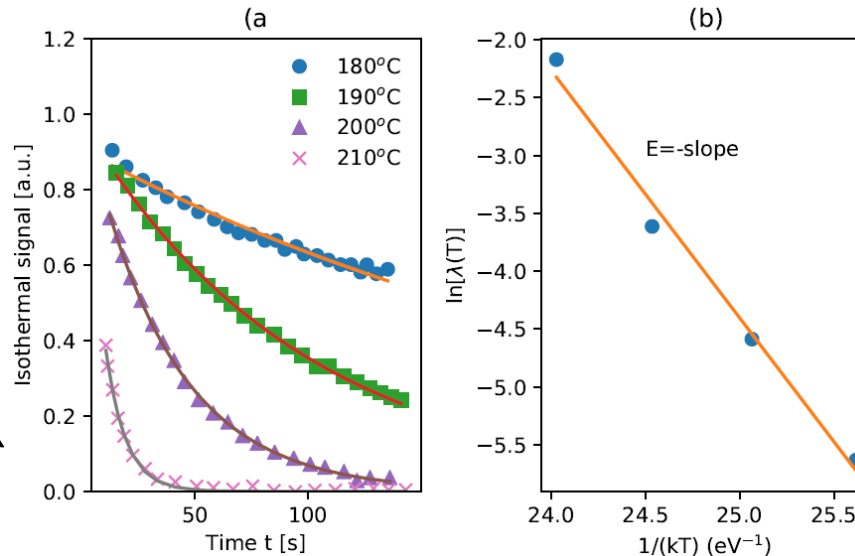
Kitis-Pagonis  
Equations for IRSL  
(KP-CWIRSL and  
KP-LMIRSL)



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

ITL (isothermal)

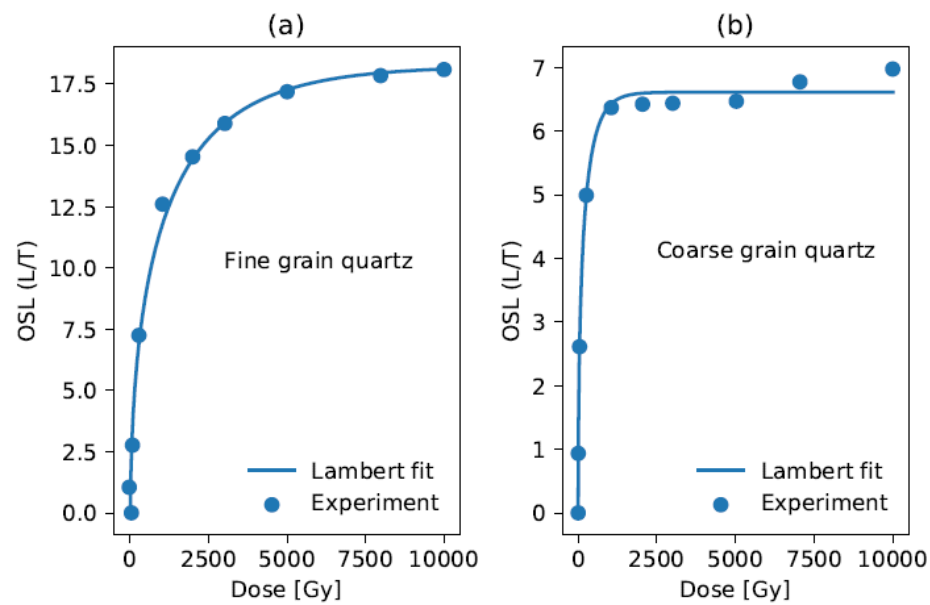
DELOCALIZED  
TRANSITIONS



(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 fit to the Arrhenius plot yields the activation energy  $E$

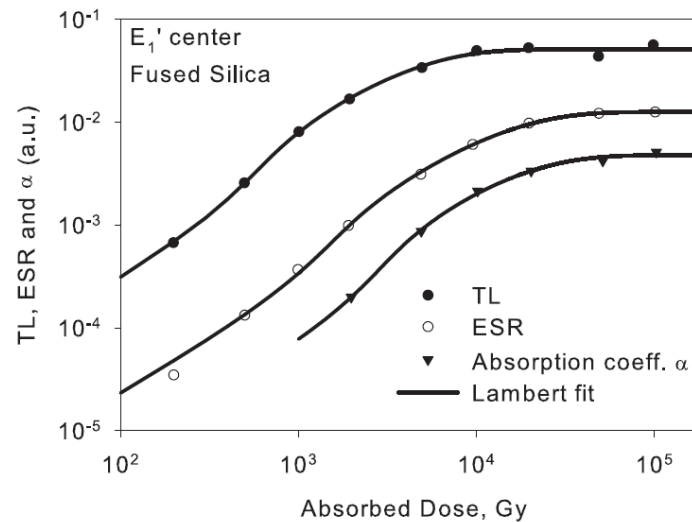
DOSE RESPONSE

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



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

Kitis-Pagonis-Chen  
superlinear response  
equation with Lambert  
(KPC-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

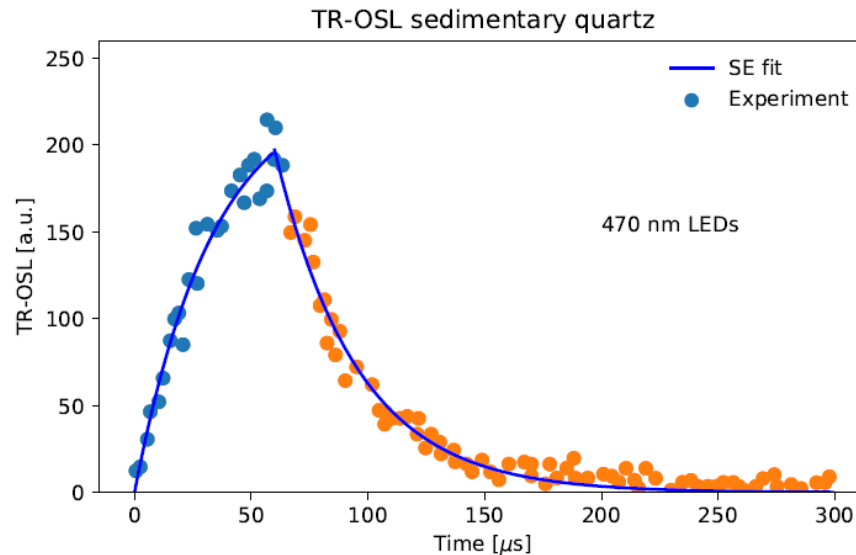
Ground state  
tunneling  
(GST) model

Excited state  
tunneling  
(EST) model

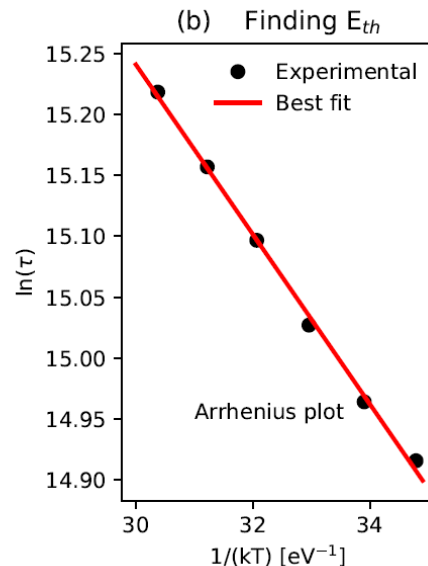
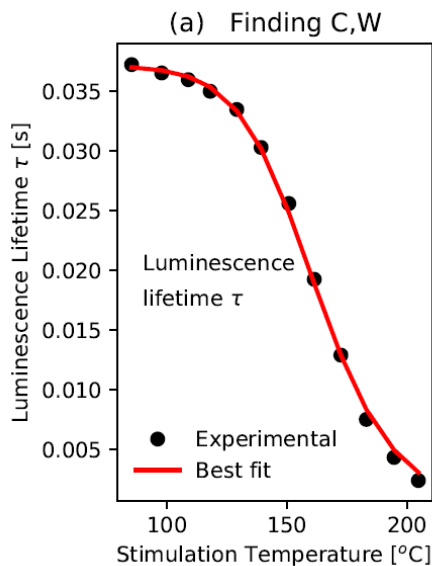
TIME-RESOLVED

DELOCALIZED  
TRANSITIONS

First order  
Kinetics  
(FOK-TR  
exponentials)



Examples of TR-OSL curves for sedimentary quartz with 60  $\mu\text{s}$  pulse. For more details see Chithambo et al. [37].

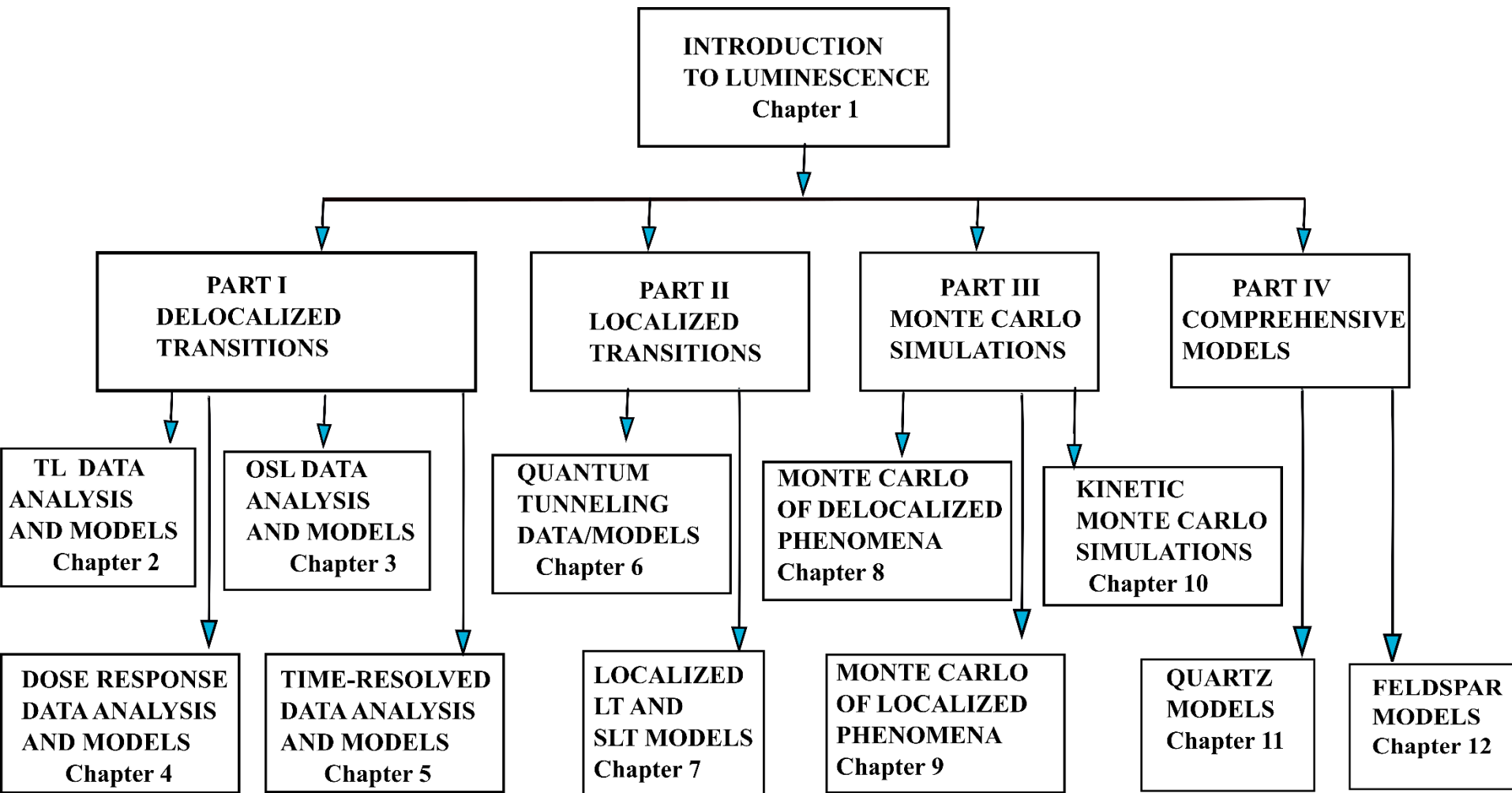


**Experimental determination of the thermal quenching parameters C, W,  $E_{th}$ .** (a) The values of C;W are obtained by fitting the decreasing part of the data. (b) The thermal activation energy  $E_{th}$  is obtained with an Arrhenius analysis of the increasing part of the data in (a).

# **OVERALL ORGANIZATION OF PYTHON-CODES IN THE SPRINGER BOOK**

- Chapter 1 \_ TL SIGNALS FROM DELOCALIZED TRANSITIONS: MODELS
- Chapter 2 \_ ANALYSIS OF TL SIGNALS FROM DELOCALIZED TRANSITIONS
- Chapter 3 \_ TL FROM QUANTUM TUNNELING PROCESSES:MODELS
- Chapter 4 \_ ANALYSIS OF TL FROM QUANTUM TUNNELING PROCESSES .
- Chapter 5 \_ ISOTHERMAL LUMINESCENCE (ITL) SIGNALS: MODELS AND ANALYSIS
- Chapter 6 \_ TL SIGNALS FROM LOCALIZED TRANSITIONS: MODELS AND ANALYSIS
- Chapter 7 \_ OSL FROM DELOCALIZED TRANSITIONS: MODELS
- Chapter 8 \_ ANALYSIS OF OSL FROM DELOCALIZED TRANSITIONS
- Chapter 9 \_ INFRARED STIMULATED LUMINESCENCE SIGNALS: MODELS
- Chapter 10 \_ ANALYSIS OF IRSL SIGNALS
- Chapter 11 \_ TIME-RESOLVED LUMINESCENCE: MODELS
- Chapter 12 \_ ANALYSIS OF TIME-RESOLVED LUMINESCENCE SIGNALS L
- Chapter 13 \_ DOSE RESPONSE OF DOSIMETRIC MATERIALS: MODELS
- Chapter 14 \_ ANALYSIS OF DOSE RESPONSE OF LUMINESCENCE SIGNALS
- Chapter 15 \_ RADIOFLUORESCENCE SIGNALS: MODELS AND ANALYSIS
- Chapter 16 \_ RADIOPHOTOLUMINESCENCE SIGNALS: MODELS AND ANALYSIS

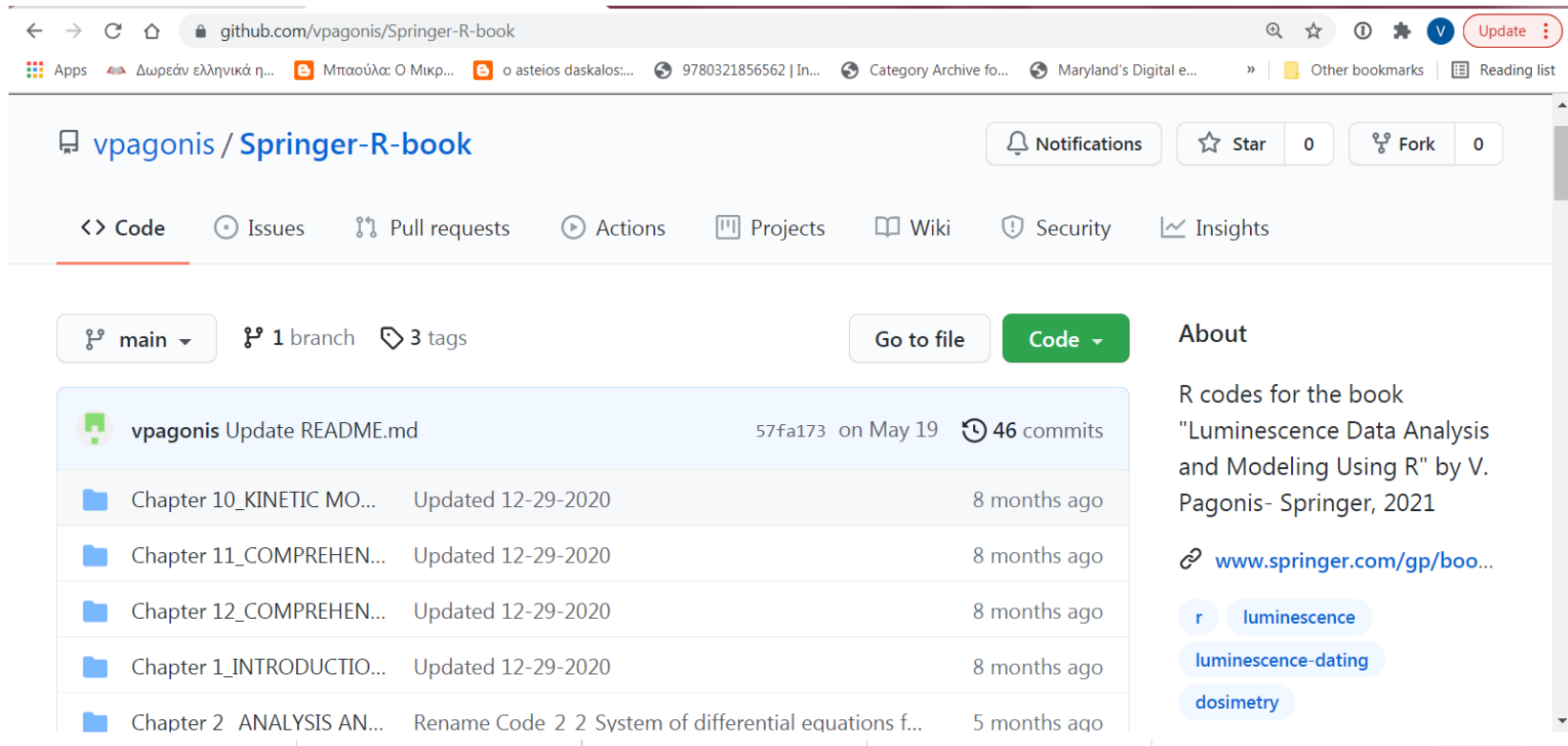
# ORGANIZATION OF 99 R-CODES IN THE R BOOK





# *The 99 R codes from the Springer Luminescence book are found at GitHub*

## *<https://github.com/vpagonis/Springer-R-book>*



vpagonis / Springer-R-book

Notifications Star 0 Fork 0

<> Code Issues Pull requests Actions Projects Wiki Security Insights

main 1 branch 3 tags Go to file Code

vpagonis Update README.md 57fa173 on May 19 46 commits

Chapter 10_KINETIC MO...	Updated 12-29-2020	8 months ago
Chapter 11_COMPREHEN...	Updated 12-29-2020	8 months ago
Chapter 12_COMPREHEN...	Updated 12-29-2020	8 months ago
Chapter 1_INTRODUCTIO...	Updated 12-29-2020	8 months ago
Chapter 2_ANALYSIS AN...	Rename Code 2 2 System of differential equations f...	5 months ago

About

R codes for the book "Luminescence Data Analysis and Modeling Using R" by V. Pagonis- Springer, 2021

[www.springer.com/gp/boo...](http://www.springer.com/gp/boo...)

r luminescence luminescence-dating dosimetry

README.md

## Luminescence (Use R! series)

### Data Analysis and simulations using R

You can download all the R codes as a single zipped folder, by clicking on the Zenodo blue box below:

DOI [10.5281/zenodo.4613169](https://doi.org/10.5281/zenodo.4613169)

This repository contains all the R scripts from the book:

Luminescence (Use R!) Data Analysis and simulations using R

*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](mailto:vpagonis@mcdaniel.edu)*

***Thank you very much for your attention!***