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Luminescence

Data Analysis and Modeling Using R

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Preface

ABOUT THIS BOOK

The past decade has seen rapid growth in the development and application of the programming language R, in the fields of radiation dosimetry, luminescence dosimetry and luminescence dating. R is now widely used in these scientific areas with new packages becoming available and used regularly by students and researchers. The present book covers applications of R to the general discipline of radiation dosimetry, and the specific areas of luminescence dosimetry, luminescence dating and radiation protection dosimetry. The book will be a useful tool for the broad scientific audience involved in luminescence dosimetry: physicists, geologists, archaeologists, solid state physicists, and scientists using radiation in their research.

The book features 99 detailed worked examples of R code fully integrated into the text, ensuring their usefulness to researchers, practitioners and students. Users can run immediately the R codes, and modify them for their experimental data and to explore the various luminescence models. In each chapter, the theory behind the subject is summarized, and appropriate references are given from the literature, so that researchers can look up the details of the theory and the relevant experiments. Each R code includes extensive comments explaining the structure and the various parts of the code. The chapters discuss how researchers can use the available R packages to analyze their own experimental data, and how to extract the various parameters describing mathematically the luminescence signals.

USING THE R CODES IN THIS BOOK

This book assumes some basic knowledge of R, however I believe that it will be useful for both newcomers to R, as well as to experienced programmers who wish to learn more about the various luminescence phenomena. The R codes for all programs in the book are available for downloading as a single R file, at the author's personal website at McDaniel College *https://blog.mcdaniel.edu/vasilispagonis.*

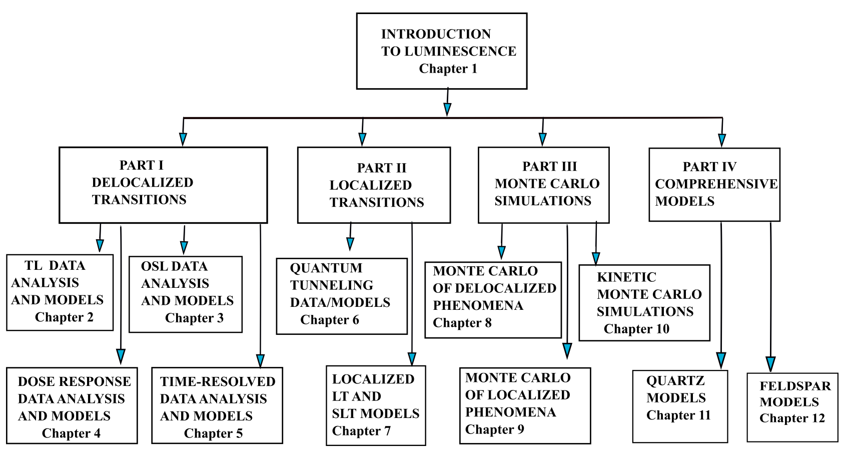
The various R codes are self contained and ready to run, and are based either on previously published R packages, or represent new codes written by the author and collaborators. In the latter case, appropriate credit is assigned to the authors of the code. Several chapters are dedicated to Monte Carlo (MC) methods, which are used to simulate the luminescence processes during the irradiation, heating and optical stimulation of solids, for a wide variety of materials. Throughout the book, both localized and delocalized transition models are simulated using the new R-package *RLumCarlo*.

Experienced programmers of R will certainly find out that they can improve the R codes given here, and it is of course possible to make the codes more compact and elegant. However, I chose to provide R codes which are simple and clear, and which can be easily modified for the purposes of the reader, rather than attempting to create compact codes which may be difficult to follow. I have kept the number of required external R packages intentionally at a minimum, so that newcomers to R can follow the R codes easily. All figures in this book were produced using the R codes in the book, so that users know immediately what to expect when they run the codes. Additional drawings for the various luminescence models in the book were drawn using *Inkscape*, and the book was produced overall using *Ly*X.

HOW THIS BOOK IS ORGANIZED

This book concerns analysis of experimental luminescence data, as well as phenomenological models used for explaining the experiments.

Overall the book is organized in four parts I-IV and 12 chapters, as shown in this diagram:



The presented models fall within two broad categories, based on delocalized and localized transitions. In delocalized transition models the conduction and/or valence band participate in the luminescence process. By contrast, in the localized type of models the luminescence process does not involve the energy bands, but rather takes place between the ground an/or excited state of the trapped electron/hole, and an energy level of the recombination center.

Chapter 1 introduces general examples of experimental luminescence data, and discusses the various experimental techniques for measuring the luminescence signals. These signals include thermoluminescence (TL), Optically stimulated luminescence (OSL), infrared stimulated luminescence (IRSL), as well as the commonly used experimental modes of continuous wave (CW-OSL or CW-IRSL), linearly modulated (LM-OSL or LM-IRSL), constant heating rate TL, isothermal TL (ITL) and time-resolved (TR). In addition, Chapter 1 provides a general overview of localized and delocalized models, which will be studied in detail later in the book.

Part I of the book is titled *LUMINESCENCE SIGNALS FROM DELOCALIZED TRANSITIONS*, and consists of Chapters 2-5, which are a practical guide for analyzing luminescence signals having their origin in delocalized transitions involving the conduction and valence band.

These four chapters provide a detailed presentation of various methods of analyzing and modeling experimental data for TL signals, OSL signals, TR-OSL signals and the Dose response of dosimetric signals. Analysis of the associated experimental data is based on a variety of available R packages *(tgcd*, *NumOSL*, *Luminescence*, *etc*), as well as on my own custom-written programs.

Part II of the book is titled *LUMINESCENCE SIGNALS FROM LOCALIZED TRANSITIONS*, and consists of Chapters 6-7, which are a practical guide for analyzing luminescence signals having their origin in localized transitions between energy states located between the conduction and valence bands. Chapter 6 contains a general introduction to quantum tunneling processes, as pertaining to dosimetric materials. Special emphasis in these chapters is on the analysis of luminescence signals from feldspars and apatites, which exhibit quantum tunneling luminescence phenomena.

Three types of models are considered in this part of the book, the localized transition model (LT), the tunneling localized transition model (TLT), and the semilocalized transition model (SLT).

Part III of the book is titled *MONTE CARLO SIMULATIONS OF LUMINESCENCE SIGNALS*, and covers chapters 8-10. Chapter 8 provides a general description of luminescence phenomena as a stochastic process, by using Monte Carlo techniques for the description of TL and OSL phenomena. Special emphasis is given in the differences between the stochastic approach which uses Monte Carlo techniques, and the deterministic approach which is based on differential equations. This chapter is of special interest to the research area of nanodosimetric materials, in which traps and centers may be spatially correlated, and the luminescence signals may be produced by a small number of these defects. A connection is also made between luminescence phenomena and the well-known *stochastic life and death phenomena,* which have been studied extensively in other areas of science. Chapters 8 and 9 are based on MC methods with fixed time intervals, while chapter 10 presents some examples of Kinetic Monte Carlo (KMC) methods.

Part IV of the book is titled *COMPREHENSIVE LUMINESCENCE MODELS.* Chapters 11 and 12 present two general classes of phenomenological models commonly used in luminescence dosimetry and dating. Specifically these chapters present several commonly used comprehensive phenomenological models for quartz and feldspars, which are two of the best studied natural luminescence materials. These two chapters also simulate several commonly used experimental protocols for luminescence dating, including the very successful single aliquot regenerative protocol (SAR). The simulations are based on the R-programs *KMS*, on the R packages *RLumModel* and on several new codes written by the author.

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LIST OF ACRONYMS

AF	Anomalous fading
CW-IRSL	Continuous-wave infrared stimulated luminescence
CW-OSL	Continuous-wave optically stimulated luminescence
EST	Excited state tunneling model
FOK	First order kinetics
GOK	General order kinetics
GST	Ground state tunneling model
GOT	General one trap model
IGST	Irradiation ground state model
IMTS	Interactive multi-trap system model
IRSL	Infrared stimulated luminescence
ITL	Isothermal luminescence
KP	Kitis-Pagonis general equation
KP-CW	Kitis-Pagonis CW-IRSL equation
KP-TL	Kitis-Pagonis TL equation
LM-IRSL	Linearly-modulated infrared stimulated luminescence
LM-OSL	Linearly-modulated optically stimulated luminescence
LT	Localized transitions model
KMC	Kinetic Monte Carlo method
MC	Monte Carlo method
MOK	Mixed order kinetics
NMTS	Non interactive multi-trap system model
OSL	Optically stimulated luminescence
OTOR	One trap one recombination center model
PKC	Pagonis-Kitis-Chen superlinearity equation
POSL	Pulsed optically stimulated luminescence
PIRSL	Pulsed infrared stimulated luminescence
SLT	Semilocalized transitions model
TA-EST	Thermally-assisted excited state tunneling model
TL	Thermoluminescence
TLT	Tunneling localized transitions model
TR-IRSL	Time resolved infrared stimulated luminescence
TR-OSL	Time resolved optically stimulated luminescence

Contents

List of Codes