Chapter 11
COMPREHENSIVE LUMINESCENCE MODELS FOR QUARTZ AUTHOR'S NOTE:

Please note that the BOOK BIBLIOGRAPHY was updated on February 14, 2022 to include this citation to the *lamW* R-package [1]:

Avraham Adler (2015) . lamW: Lambert-W Function, 2015. URL *https://CRAN.R-project.org/package=lamW*. R package version 2.1.1.

Abstract This chapter presents several empirical comprehensive models which were developed in order to explain complex luminescence mechanisms and phenomena in quartz. We show detailed R codes for the *Baiiley2001* and the *Pagonis2008* quartz models, by using the R programs *KMS* developed by Peng and Pagonis, and also using the R package *RlumModel* by Friedrich et al. We show how to simulate the history of natural quartz samples, and how to modify the models by changing one or more of the original model parameters. R codes are provided for studying the phenomena of thermal quenching, for simulating the dose response of TL and OSL signals and also for the superlinear dose response in quartz. We show how to simulate the important phenomena of phototransfer, predose effect and thermal transfer of holes, pulse annealing and the SAR protocol in quartz. This chapter concludes with several examples from the extensive R package *RLumModel*.

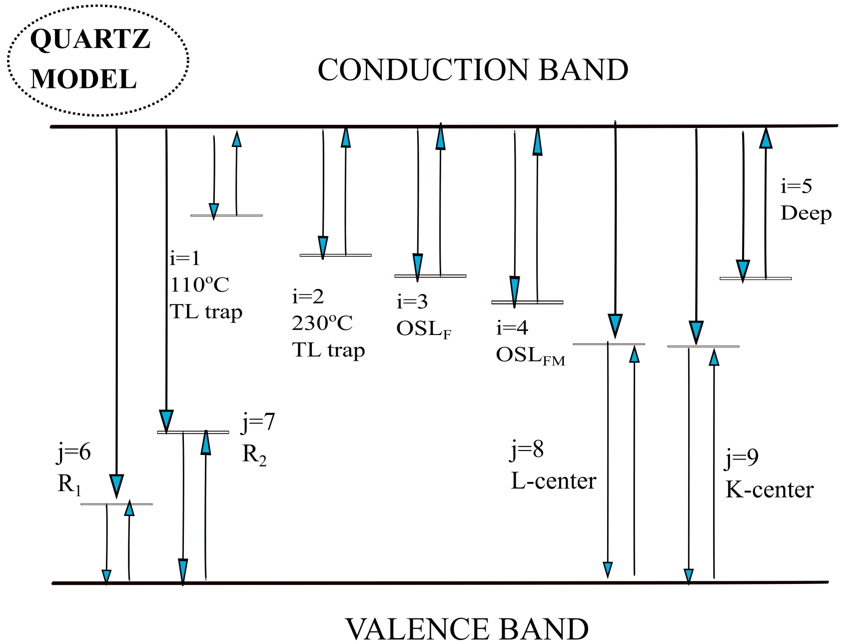

Fig. 11.1: Schematic diagram of the Bailey model, consisting of a total of nine energy levels. The arrows indicate possible transitions. (After Bailey [5]).

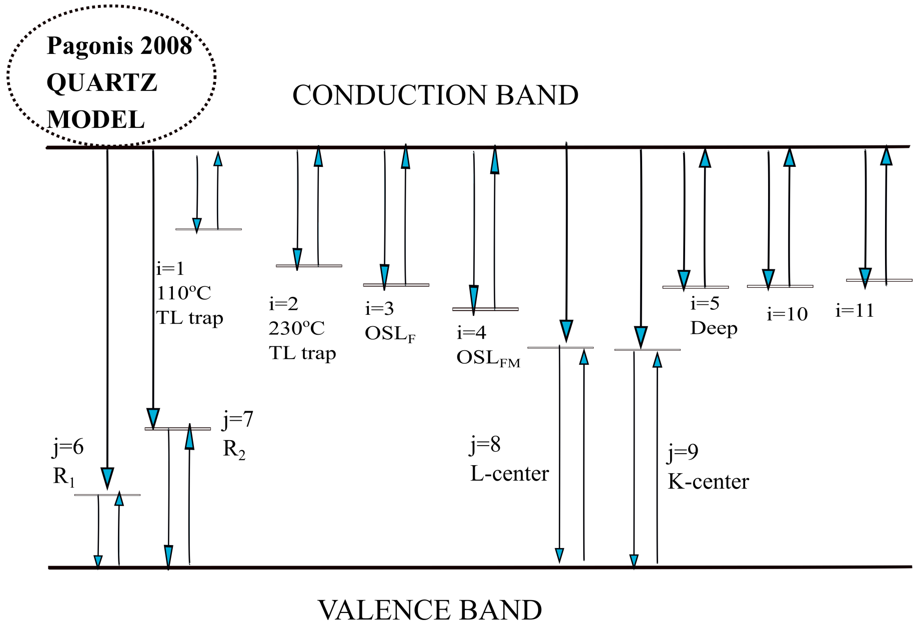

Fig. 11.2: The quartz model of Pagonis et al. [47]. Levels 10 and 11 are the additional levels introduced to the original model by Bailey [5].

Table 11.1: The various functions available in the R programs *KMS*, described in Peng and Pagonis [48].

FUNCTIONS CALLED IN KMS PROGRAMS
setInis() Set all center populations equal to zero for quartz crystallization. **setPars()** Initialize the model using appropriate kinetic parameters. **irradiate(*temp*, *tim*, *doseRate*)** Irradiate at *temp* ^{o}C for *tim* s with a dose rate of *doseRate* Gy/s. **heatAt(*temp*, *tim*)** Heat at *temp* ^{o}C for *tim* s. **heatTo(*temp1*, *temp2*, *hRate*)** Heat from *temp1* ^{o}C to *temp2* ^{o}C with a heating rate of *hRate* ^{o}C/s. **stimOSL(*temp*, *tim*, *pValue*, *nChannel*)** OSL stimulation at temp ^{o}C for *tim* s with a photon stimulation flux of *pValue* $s^{-1}cm^{-2}$ The OSL signal is evaluated at the equally spaced number of channels *nChannel*. **stimTL(*lowTemp*, *upTemp*, *hRate*, *nChannel*)** TL stimulation from *lowTemp* ^{o}C to *upTemp* ^{o}C with a heating rate of *hRate* ^{o}C/s, the number of equally spaced channels is *nChannel*

Table 11.2: The steps in simulating a *natural* sedimentary quartz sample, in the *Bailey2001* model in *KMS* [5]. Step 5a is used in the original *Bailey2001* model, step 5b is used in the *Pagonis2008* model in KMS.

	Steps in simulation of *natural* sedimentary quartz sample in the Bailey2001 model [5]
1	All electron and hole concentrations set to zero during the crystallization process.
2	Geological dose of 1000Gy with a dose rate of 1Gy/s at 20°C.
3	Heat to 350°C (simulation of geological time).
4	Illumination at 200°C for 100s, repeated exposures to sunlight over a long period.
5a	Burial dose of 20 Gy at 0.01 Gy/s at 220°C.
5b	Burial dose of 20 Gy at a very low natural dose rate of 3×10^{-11} Gy/s at 20°C.

Code 11.1: Natural history of quartz sample Pagonis2008 model

```
# Use Pagonis model to simulate quartz sample history and
# TL measured in lab after irradiating with 10 Gy at 1 Gy/s
rm(list=ls())
library("deSolve")
source("Pagonis_Model.R")
setPars()
setInis()
irradiate(temp=20, tim=1000, doseRate=1) #1000 Gy at 1 Gy/s
heatAt(temp=20, tim=60)                  #Relaxation
heatTo(temp1=20, temp2=350, hRate=5)     # Heat to 350 degC
heatTo(temp1=350, temp2=200, hRate=-5)   # Cool down to RT
stimOSL(temp=200, tim=100, pValue=2.0, nChannel=1000) #Bleach
irradiate(temp=20, tim=20/1e-11, doseRate=1e-11)# Burial dose
heatAt(20,60)
storeNat<-inis #Store concentrations for natural sample
TL<-stimTL(lowTemp=20,upTemp=500,hRate=5,nChannel=480) #TL
heatTo(temp1=500,temp2=20,hRate=-5) # Cool down
tlx<-TL[,"tlx"]
tly<-TL[,"tly"]
par(mfrow=c(1,2))
plot(tlx,tly,type="l",ylim=c(0,16000),lwd=2,
xlab=expression("Temperature "^"o"*"C]"), ylab = "TL [a.u.]")
```

```
legend("topleft",bty="n",legend=c("(a)","Pagonis model",
"Natural TL"))
# repeat irradiation and TL for lab irradiation
inis<-storeNat   # restore concentrations for natural sample
irradiate(temp=20, tim=10, doseRate=1)
heatAt(temp=20, tim=60)
TL<-stimTL(lowTemp=20,upTemp=500,hRate=5,nChannel=480)
heatTo(temp1=500,temp2=20,hRate=-5)
tlx<-TL[,"tlx"]
tly<-TL[,"tly"]
plot(tlx,tly,type="l",xlab=expression("Temperature ["^"o"*"C]"),
ylab = "TL [a.u.]",ylim=c(0,400000),lwd=2)
legend("topright",bty="n",legend=c("(b)", " ","Regenerated TL"))
```

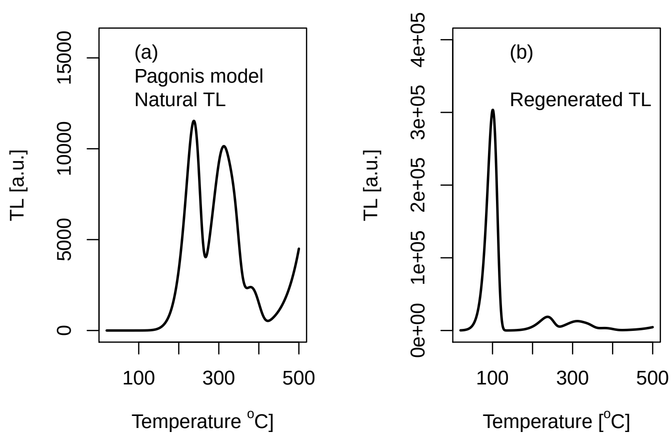

Fig. 11.3: Simulation of the natural history of a quartz sample, using the *Pagonis2008* model in *KMS* programs. (a) The TL glow curve, after the natural sample is heated in the laboratory with a heating rate of 5 K/s. Note the absence of the 110°C TL peak. (b) The TL glow curve, after the natural sample is irradiated with 10 Gy and then heated in the laboratory with a heating rate of 5 K/s. Note the restored 110°C TL peak in (b), which is missing in (a).

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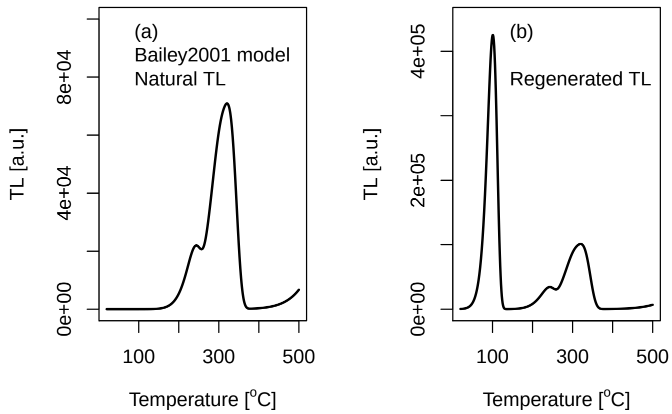


Fig. 11.4: Simulation of the natural history of a quartz sample, using the *Bailey2001* model in *KMS*. Compare these results with the similar results in Fig.11.3, which were obtained using the *Pagonis2008* model.

Code 11.2: Thermal quenching of TL signal in quartz (KMS)

```
# Use Pagonis model to simulate thermal quenching in quartz
# TL measured in laboratory with different heating rates
rm(list=ls())
library("deSolve")
source("Pagonis_Model.R")
beta<-2*seq(1:6)
tlylow<-tlyhigh<-vector(length = length(beta))
tlx<-tly<-matrix(nrow=480,ncol=length(beta))
for (i in 1:6){
  setPars()
  setInis()
  irradiate(temp=20, tim=1000, doseRate=1) #1000 Gy at 1 Gy/s
  heatAt(temp=20, tim=60)                  #Relaxation
  heatTo(temp1=20, temp2=350, hRate=5)     # Heat to 350 degC
  heatTo(temp1=350, temp2=200, hRate=-5)   # Cool down to RT
  stimOSL(temp=200, tim=100, pValue=2.0, nChannel=1000) #Bleach
  irradiate(temp=20, tim=20/1e-11, doseRate=1e-11)# Burial dose
  heatAt(20,60)
```

```
 irradiate(temp=20, tim=100, doseRate=1)
heatAt(temp=20, tim=60)
TL<-stimTL(lowTemp=20,upTemp=500,hRate=beta[i],nChannel=480)
tlx[,i]<-TL[,"tlx"]
tly[,i]<-TL[,"tly"]/i
tlyhigh[i]<-sum(tly[,i][130:400])
tlylow[i]<-sum(tly[,i][1:130])}
par(mfrow=c(1,2))
matplot(tlx,tly,typ="l",lty="solid",lwd=2,
xlab=expression("Temperature ["^"o"*"C]"), ylab = "TL [a.u.]",
ylim=c(0,350000),xlim=c(30,380))
legend("topleft",bty="n",legend=c("(a)","Heating 2-12 K/s",
"Thermal quenching"))
plot(beta,tlylow/max(tlylow),pch=1,typ="o",ylim=c(0,1.2),
xlab="Heating rate [K/s]", ylab = "Normalized TL Area")
lines(beta,colSums(tly)/max(colSums(tly)),pch=2,typ="o")
lines(beta,tlyhigh/max(tlyhigh),pch=3,typ="o")
legend("bottomleft",bty="n",legend=expression("(b)",
"Area 0-130"^"o"*"C","Area 0-500"^"o"*"C","Area
130-500"^"o"*"C"),pch=c(NA,1,2,3))
```

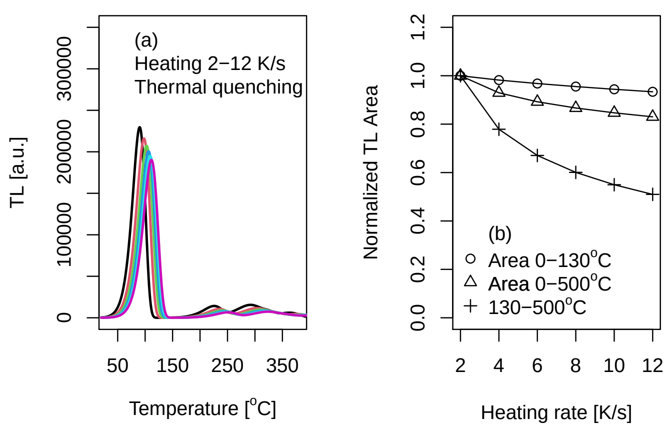


Fig. 11.5: Simulation of the thermal quenching of TL signal in quartz, demonstrated by using various heating rates in the *Pagonis2008* model of *KMS*. (a) The TL glow curves for heating rates 2-12 K/s, and (b) The areas under different parts of the TL glow curves in (a), showing the thermal quenching effects.

Code 11.3: TL dose response of quartz sample (KMS)

```
# Dose Response of 110degC TL peak in quartz
rm(list=ls())
library("deSolve")
library("minpack.lm")
library("lamW")
source("Bailey01_Model.R")
setPars()
setInis()
irradiate(temp=20, tim=1000, doseRate=1) #1000 Gy at 1 Gy/s
heatAt(temp=20, tim=60)                  #Relaxation
heatTo(temp1=20, temp2=350, hRate=5)     # Heat to 350 degC
heatTo(temp1=350, temp2=200, hRate=-5)   # Cool down to RT
stimOSL(temp=200, tim=100, pValue=2.0, nChannel=1000) #Bleach
irradiate(temp=20, tim=20/1e-11, doseRate=1e-11)# Burial dose
heatAt(20,60)    #Store concentrations for natural sample
storeNat<-inis  # in variable storeNat
reDose<-c(1,3,5,10,20,60,100,200,300,400,500,700)
tlm<-vector(length=length(reDose))
tlx<-tly<-matrix(nrow=480,ncol=length(reDose))
for (i in seq(length(reDose))) {
inis<-storeNat
irradiate(temp=20,tim=reDose[i],doseRate=1)
heatAt(temp=20,tim=60)
res<-stimTL(lowTemp=20,upTemp=500,hRate=5,nChannel=480)
heatTo(temp1=500,temp2=20,hRate=-5)
tlx[,i]<-res[,"tlx"]
tly[,i]<-res[,"tly"]
tlm[i]<-approx(x=res[,"tlx"],y=res[,"tly"],xout=330)$y }
par(mfrow=c(1,2))
matplot(tlx,tly,type="l",lty="solid",ylab = "TL [a.u.]",
xlab=expression("Temperature "^"o"*"C]"),ylim=c(0,1.4e6),
xlim=c(30,380))
legend("topright",bty="n",legend=c("(a)"," ","TL glow curves"))
plot(reDose,tlm,type="p",xlab="Dose [Gy]",ylab="TL [a.u]",
ylim=c(0,.95e6))
legend("topright",bty="n",legend=c("(b)","Dose response",
"Lambert fit"),pch=c(NA,1),lty=c(NA,NA,"solid"))
t <-reDose
y <-tlm
fit_data <-data.frame(  t ,y)
#plot(fit_data,ylim=c(0,max(y)))
```

```
fit <- minpack.lm::nlsLM(
formula=y~N*(1+lambertW0((abs(R)-1)*exp(abs(R)-1-b*t))/
(1-abs(R))),
data=fit_data,start = list(N=5* max(y),R=0.1, b = .002))
N_fit <- coef(fit)[1]
R_fit <- abs(coef(fit)[2])
b_fit <- coef(fit)[3]
## plot analytical solution
curve(
N_fit*(1+lambertW0((R_fit-1)*exp(R_fit-1-b_fit*x))/(1-R_fit)),
0,700,col = "blue",add=TRUE,lwd=2)
cat("\nfitted N: ", N_fit)
cat("\nfitted R: ", R_fit)
cat("\nfitted D0: ", 1/b_fit, " Gy")

##
## fitted N:  768904.9
## fitted R:  1.028051e-07
## fitted D0:  1045.847  Gy
```

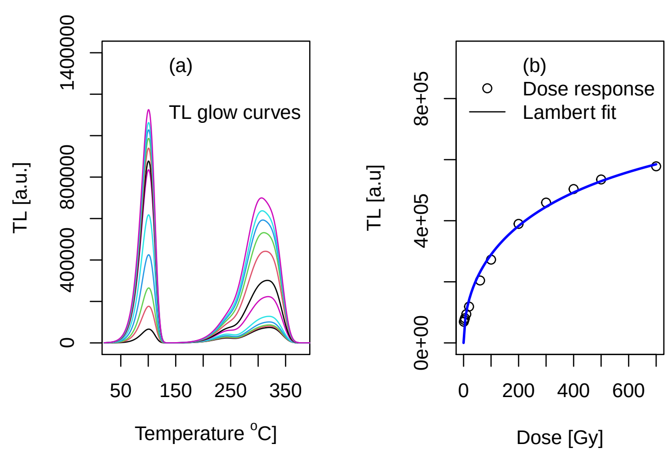


Fig. 11.6: Simulation of the dose response curve of the 330°C TL peak in a sedimentary quartz sample. (a) The TL glow curves (b) The dose response curve, fitted with the Lambert dose response equation we saw in Chapter 4.

Code 11.4: Dose Response of quartz OSL signal, Bailey2001 model

```
# Dose Response of quartz OSL signal measured at 125degC
rm(list=ls())
library("deSolve")
library("minpack.lm")
library("lamW")
source("Bailey01_Model.R")
setPars()
setInis()
irradiate(temp=20, tim=1000, doseRate=1) #1000 Gy at 1 Gy/s
heatAt(temp=20, tim=60)                  #Relaxation
heatTo(temp1=20, temp2=350, hRate=5)     # Heat to 350 degC
heatTo(temp1=350, temp2=200, hRate=-5)   # Cool down to RT
stimOSL(temp=200, tim=100, pValue=2.0, nChannel=1000) #Bleach
irradiate(temp=20, tim=20/1e-11, doseRate=1e-11)# Burial dose
heatAt(20,60)    #Store concentrations for natural sample
storeNat<-inis  # in variable storeNat
reDose<-c(1,50,100,200,300,400,500,700)
oslm<-vector(length=length(reDose))
oslx<-osly<-matrix(nrow=100,ncol=length(reDose))
for (i in seq(length(reDose))) {
  inis<-storeNat #Restore natural concentrations
  irradiate(temp=20,tim=reDose[i],doseRate=1)
  heatAt(temp=20,tim=60)
  heatTo(20,125,hRate=5)
  res<-stimOSL(temp=125, tim=100, pValue=2.0, nChannel=100)
  oslx[,i]<-res[,"oslx"]
  osly[,i]<-res[,"osly"]
  oslm[i]<-res[,"osly"][1]}
par(mfrow=c(1,2))
matplot(oslx,osly,type="l",lty="solid",xlim=c(0,20),
xlab="Time [s]",ylab = "OSL [a.u.]",ylim=c(0,1.6e8))
legend("topright",bty="n",legend=c("(a)"," ","OSL curves"))
plot(reDose,oslm,type="p",xlab="Dose [Gy]",ylab="OSL [a.u]",
ylim=c(0,2.6e8))
legend("topright",bty="n",legend=c("(b)","OSL response",
"Lambert fit"),pch=c(NA,1),lty=c(NA,NA,"solid"))
t <-reDose
y <-oslm
fit_data <-data.frame(  t ,y)
fit <- minpack.lm::nlsLM(
  formula=y~N*(1+lambertW0((abs(R)-1)*exp(abs(R)-1-b*t))/
                (1-abs(R))),  data = fit_data,
  start = list(N= max(y),R=0.1, b = .002))
N_fit <- coef(fit)[1]
```

```
R_fit <- abs(coef(fit)[2])
b_fit <- coef(fit)[3]
curve(
  N_fit*(1+lambertW0((R_fit-1)*exp(R_fit-1-b_fit*x))/(1-R_fit)),
  1,700,add=TRUE )
cat("\nfitted N: ", N_fit)
cat("\nfitted R: ", R_fit)
cat("\nfitted Dc: ", 1/b_fit, " Gy")

##
## fitted N:  200028114
## fitted R:  0.211198
## fitted Dc:  504.6785  Gy
```

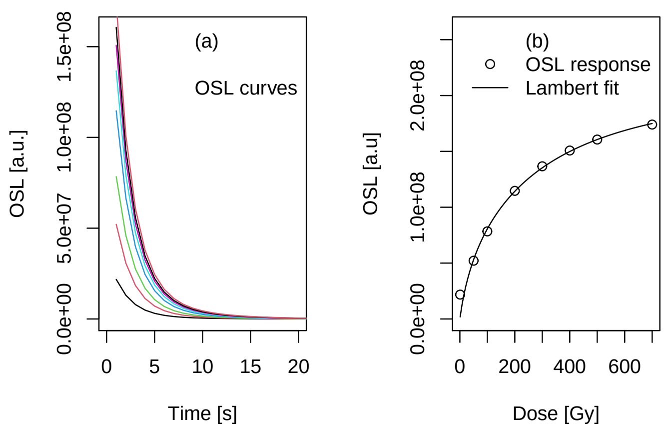


Fig. 11.7: Simulation of the dose response curve of the OSL signal measured at 125°C, in the *Bailey2001* model. (a) The CW-OSL curves and (b) The dose response curve, fitted with the Lambert function we saw in Chapter 4.

Code 11.5: Superlinearity in annealed quartz samples

```
# Superlinear TL dose response in annealed quartz
rm(list = ls(all=T))
library("deSolve")
```

```
source("Bailey01_Model.R")
reDose<-seq(0.1,2,by=1.9/7)
setInis()
setPars()
irradiate(temp=20, tim=1000, doseRate=1) #1000 Gy at 1 Gy/s
heatAt(temp=20, tim=60)                  #Relaxation
heatTo(temp1=20, temp2=350, hRate=5)     # Heat to 350 degC
heatTo(temp1=350, temp2=200, hRate=-5)   # Cool down to RT
stimOSL(temp=200, tim=100, pValue=2.0, nChannel=1000) #Bleach
irradiate(temp=20, tim=20/1e-11, doseRate=1e-11)#Burial 100 Gy
heatTo(20,700,hRate=5)
heatAt(700,3600)
heatTo(700,20,hRate=-5)
storeNat<-inis
tlm<-vector(length=8)
tlx<-tly<-matrix(nrow=480,ncol=8)
# natural dose rate =0.1 Gy
for (i in seq(8)) {
  inis<-storeNat
  irradiate(temp=20,tim=reDose[i],doseRate=1)
  heatAt(temp=20,tim=60)
  res<-stimTL(lowTemp=20,upTemp=500,hRate=5,nChannel=480)
  tlx[,i]<-res[,"tlx"]
  tly[,i]<-res[,"tly"]
  tlm[i]<-approx(x=res[,"tlx"],y=res[,"tly"],xout=330)$y }
par(mfrow=c(1,3))
matplot(tlx,tly,type="l",ylim=c(0,470),xlim=c(20,380),
lty="solid",lwd=2,xlab=expression("Temperature ["^"o"*"C]"),
ylab = "TL [a.u.]")
legend("topright",bty="n",legend=c("(a)","TL glow curves",
"Annealed quartz"))
plot(reDose,tlm,type="o",xlab = "Dose [Gy]",ylab = "TL [a.u.]",
ylim=c(0,1.4*max(tlm)),xlim=c(0,2.5))
legend("topleft",bty="n",legend=c("(b)"," ","Superlinear",
"Dose response"))
x<- log(reDose)
y<- log(tlm)
rangeData<-cbind(x,y)
lm(y~x)$coefficients
plot(x, y, xlab = "ln(Dose)",ylab = "ln(TL)",ylim=c(0,7),
xlim=c(-2,1.5))
legend("topleft",bty="n",legend=c("(c)"," ","Log-Log",
"slope=1.39"))
abline(lm(y~x))
```

```
## (Intercept)           x
##    2.481778    1.397661
```

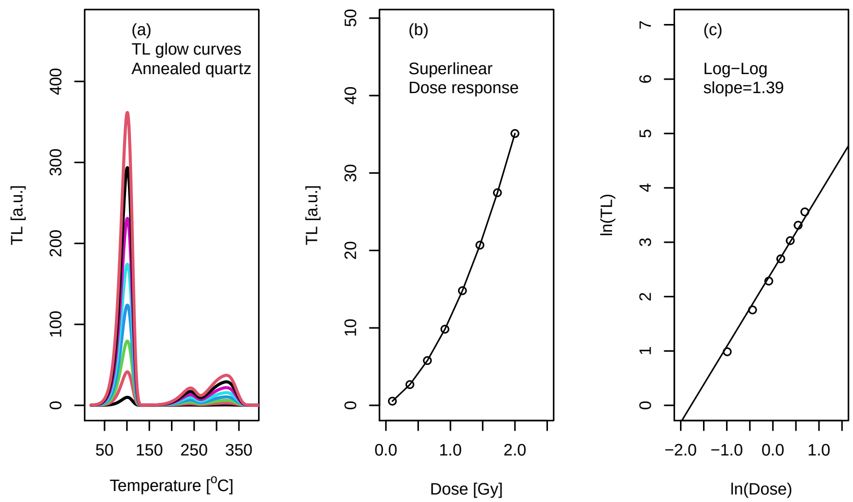


Fig. 11.8: Simulated superlinear dose response of 330°C TL peak in annealed quartz using the *Bailey2001* model. The sample was annealed for 1 h at 700°C, before measuring its TL dose response between 0.1 and 2 Gy. (a) The TL glow curves at different doses; (b) The superlinear dose dependence of the TL signal at 330°C; (c) The data in (b) is plotted on a log-log scale and fitted with a linear function, yielding a superlinearity index of $g(D)$=1.39.

Code 11.6: Phototransfer phenomenon using Bailey2001 model

```
#Phototransfer simulation using Bailey2001 model
rm(list = ls(all=T))
library("deSolve")
source("Bailey01_Model.R")
photo<-function(x,colr,ln,pchs){
  setInis()
  setPars()
  pars["N6"] <- 3e10 # change the parameter N6 in Bailey model
  # N6=total concentration of holes in hole reservoir R1
  irradiate(temp=20, tim=1000, doseRate=1) #1000 Gy at 1 Gy/s
```

```
  heatAt(temp=20, tim=60)                       #Relaxation
  heatTo(temp1=20, temp2=350, hRate=5)       # Heat to 350 degC
  heatTo(temp1=350, temp2=200, hRate=-5)     # Cool down to RT
  stimOSL(temp=200, tim=100, pValue=2.0, nChannel=1000) #Bleach
  # Large Burial dose 100 Gy
  irradiate(temp=20, tim=200/1e-11, doseRate=1e-11)
  # end natural sample simulation, store concentrations
# Next is the optical Bleach
stimOSL(temp=20, tim=x, pValue=2.0, nChannel=1000)
heatAt(temp=20, tim=60)
TL<-stimTL(lowTemp=20,upTemp=500,hRate=5,nChannel=150) #TL
heatTo(temp1=500,temp2=20,hRate=-5) # Cool down
tlx<-TL[,"tlx"]
tly<-TL[,"tly"]
par(new=TRUE)
plot(tlx,tly,type="o",xlab=expression("Temperature ["^"o"*"C]"),
 ylab = "TL [a.u.]",xlim=c(0,400),ylim=c(0,7e5),col=colr,lty=ln,
lwd=1,pch=pchs)
}   #end function photo
for (i in 1:3)
  {bleachTime<-c(1,3,6)
   colr<-c("red","blue","black")
   ln<-rep("solid",3)
   pchs<-c(1,2,4)
   photo(bleachTime[i],colr[i],ln[i],pchs[i])}
legend("topleft",bty="n","Phototransfer")
legend("topright",bty="n",lty=c(NA,ln),col=c(NA,colr),lwd=1,
 pch=c(NA,pchs), c("Bleaching times","1 s","3 s","6 s"))
```

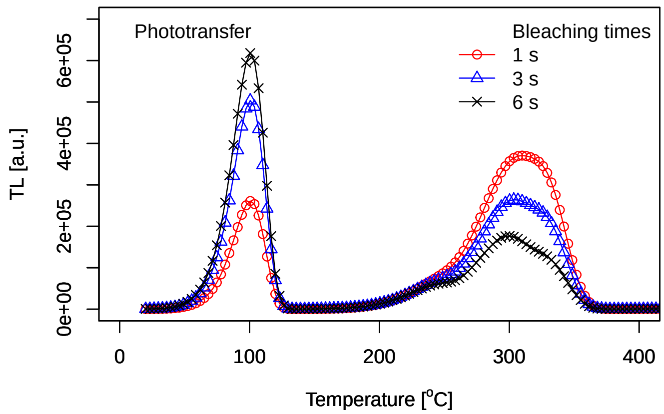
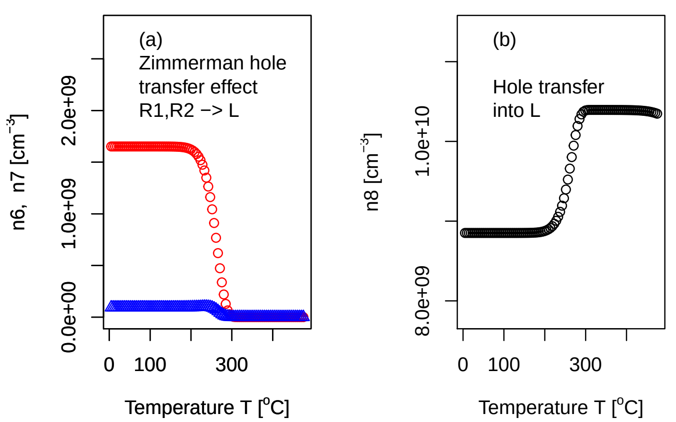


Fig. 11.9: Simulation of phototransfer process in the *Bailey2001* model. As the optical stimulation time increases, the height of the TL peak at 110°C increases, while simultaneously the 330°C TL peak decreases. For a more detailed study of this, and other quartz phenomena, see Pagonis et al. [49].

Code 11.7: The Zimmerman model: thermal transfer of holes in quartz

```
# The Zimmerman thermal transfer of holes in quartz
rm(list=ls())
library("deSolve")
source("Bailey01_Model.R")
setInis()
setPars()
pars["N6"] <- 3e10   # change the concentration of holes in R1
irradiate(temp=20, tim=1000, doseRate=1) #1000 Gy at 1 Gy/s
heatAt(temp=20, tim=60)                  #Relaxation
heatTo(temp1=20, temp2=350, hRate=5)     # Heat to 350 degC
heatTo(temp1=350, temp2=200, hRate=-5)   # Cool down to RT
stimOSL(temp=200, tim=100, pValue=2.0, nChannel=1000) #Bleach
irradiate(temp=20, tim=100/1e-11, doseRate=1e-11)#Burial 100 Gy
storeNat<-inis
# Set up parameters and vectors
testDose<-.1
```

```
nTemps<-15
initTemp<-100
finalTemp<-500
actTemp<-seq(initTemp,finalTemp,by=(finalTemp-initTemp)/
               (nTemps-1))
# Loop for activation temperatures
inis<-storeNat   # Reset concentrations for natural sample
res2<-heatTo(25,500,hRate=1)     # heat to activation temperature
par(mfrow=c(1,2))
xlabel<-expression("Temperature T ["^"o"*"C]")
ylabel<-expression("n6,  n7 [cm"^"-3"*"]")
plot(res2[,"time"],res2[,"n6"],xlab = xlabel
,ylab =ylabel,ylim=c(0,1.7*max(res2[,"n6"])),pch=1,col="red")
legend("topleft",bty="n",legend=c("(a)","Zimmerman hole",
"transfer effect","R1,R2 -> L"))
par(new = TRUE)
plot(res2[,"time"],res2[,"n7"],xlab = xlabel
,ylab =ylabel,ylim=c(0,1.7*max(res2[,"n6"])),pch=2,col="blue")
plot(res2[,"time"],res2[,"n8"],xlab = xlabel
,ylab =expression("n8 [cm"^"-3"*"]"),
ylim=c(.75*max(res2[,"n8"]),1.1*max(res2[,"n8"])))
legend("topleft",bty="n",legend=c("(b)"," ","Hole transfer",
"into L"))
```



Code 11.8: Simulation of pulse annealing experiment with Bailey2001 model

Fig. 11.10: The Zimmerman thermal transfer process for holes in quartz. (a) The concentrations of holes n_6 and n_7 in hole reservoirs R_1 and R_2, decrease as the temperature T is increased. (b) The concentration of holes n_8 in recombination center L also increases, indicating a thermal transfer of holes.

```
#Simulation of pulse annealing experiment with
# Bailey2001 model
rm(list=ls())
library("deSolve")
source("Bailey01_Model.R")
setInis()
setPars ()
pars["N6"] <- 3e9
### Start natural sample simulations
irradiate(temp=20, tim=1000, doseRate=1)
heatAt(temp=20, tim=60)
heatTo(temp1=20, temp2=350, hRate=5)
heatTo(temp1=350, temp2=200, hRate=-5)
stimOSL(temp=200, tim=100, pValue=2.0, nChannel=10)
irradiate(temp=20, tim=51/1e-11, doseRate=1e-11)  #Burial 51 Gy
## End of natural history with natural irradiation
res<- heatAt(temp=20, tim=60)
storeNat<-inis
nTemps<-20
initTemp<-100
finalTemp<-350
actTemp<-seq(initTemp,finalTemp,by=(finalTemp-initTemp)/
(nTemps-1))
tlm<-vector(length=nTemps)
tlx<-tly<-matrix(nrow=1000,ncol=nTemps)
tl<-osl<-rep(0,nTemps)
par(mfrow=c(1,2))
for (i in seq(nTemps)) {
  heatTo(20,actTemp[i],hRate=1)
  heatAt(actTemp[i],tim=10)
  heatTo(actTemp[i],20,hRate=-1)
  heatTo(20,125,hRate=1)
  resOSL<-stimOSL(temp=125, tim=0.1, pValue=2.0, nChannel=10)
  osl[i]<-sum(resOSL[,"osly"])
  heatTo(125,20,hRate=-1)
  irradiate(temp=20,tim=0.1,doseRate=1)
  heatAt(20,tim=60)
```

```
  resTL<-stimTL(20,160,hRate=1,nChannel=110)
  tl[i]<-max(resTL[,"tly"])}
xlabel<-expression("Activation T ["^"o"*"C]")
plot(actTemp,osl/tl,xlab=xlabel,
ylim=c(0,200000),ylab="Sensitivity corrected OSL/TL")
legend("topright",bty="n",legend=c("(a)"," ","Pulse annealing",
"Natural sample"))
#
inis<-storeNat  # Restore concentrations of natural sample
heatTo(20,125,hRate=1)
stimOSL(temp=125, tim=200, pValue=2.0, nChannel=10)
heatTo(125,20,hRate=-1)
irradiate(temp=20,tim=56,doseRate=1)  #56 Gy in lab
for (i in seq(nTemps)) {
  heatTo(20,actTemp[i],hRate=1)
  heatAt(actTemp[i],tim=10)
  heatTo(actTemp[i],20,hRate=-1)
  heatTo(20,125,hRate=1)
  resOSL<-stimOSL(temp=125, tim=0.1, pValue=2.0, nChannel=10)
  osl[i]<-sum(resOSL[,"osly"])
  heatTo(125,20,hRate=-1)
  irradiate(temp=20,tim=0.1,doseRate=1)
  heatAt(20,tim=60)
  resTL<-stimTL(20,160,hRate=1,nChannel=110)
  tl[i]<-max(resTL[,"tly"])}
plot(actTemp,osl/tl,xlab=xlabel,ylim=c(0,320000),
ylab="Sensitivity corrected OSL/TL")
legend("topright",bty="n",legend=c("(b)"," ",
"Irradiated sample"))
```

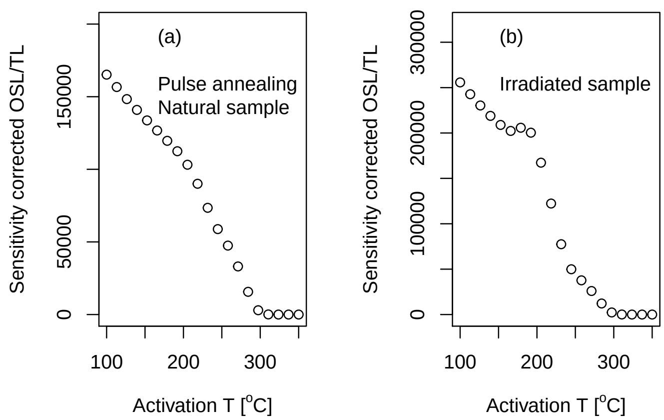


Fig. 11.11: Simulation of the experimental pulse annealing protocol of Wintle and Murray [50] for (a) A natural quartz sample, and (b) An optically bleached and irradiated sample. For details of the simulation, see Pagonis et al. [51].

Table 11.3: Steps in the simulation of the TT-OSL protocol of Wang et al. [52], based on the simulations of Pagonis et al. [47].

Step	Description
1	Geological dose - irradiation of $1000 Gy$ at $1 Gy/s$.
2	Geological time - heat to $350°C$.
3	Illuminate for $100s$ at $200°C$.
4	Burial dose - $200 Gy$ at $220°C$ at $0.01 Gy/s$.
5	Regenerative dose D_i at $20°C$ and at $1 Gy/s$.
6	Preheat to 260°C for $10s$.
7	Blue stimulation at $125°C$ for $270s$.
8	Preheat to $260°C$ for $10s$.
9	Blue stimulation at $125°C$ for $90s$ (L_{TT-OSL}).
10	Test Dose = $7.8 Gy$
11	Preheat to $220°C$ for $20s$
12	Blue stimulation at 125°C for $90s$ (T_{TT-OSL}).
13	Anneal to 300°C for $10s$
14	Blue stimulation at 125°C for $90s$.
15	Preheating at $260°C$ for $10s$.
16	Blue stimulation at $125°C$ for $90s$ (L_{BT-OSL}).
17	Test Dose = $7.8 Gy$.
18	Preheat to 220^oC for $20s$.
19	Blue stimulation at $125^0 C$ for $90s$ (T_{BT-OSL}).
20	Repeat 1-19 for different regenerative doses D_i=0-4000Gy in step 5.

Code 11.9: SAR protocol using the Pagonis model in KMS

```
### TEMPLATE1 in Peng and Pagonis (2016)
# SAR protocol using the Pagonis model in KMS
library(deSolve)
source("Pagonis_Model.R")
setPars()
setInis()
irradiate(temp=20,tim=50000/3.17e-11,doseRate=3.17e-11)
heatAt(temp=20,tim=60)
stimOSL(temp=20,tim=6000,pValue=4.73e16,nChannel=6000)
nCycle<-2
for (i in seq(nCycle)) {
irradiate(temp=20,tim=10/3.17e-11,doseRate=3.17e-11)
heatAt(temp=20,tim=60)
stimOSL(temp=20,tim=6000,pValue=4.73e16,nChannel=6000)
} #end for.
```

```
irradiate(temp=20,tim=20/3.17e-11,doseRate=3.17e-11)
heatAt(temp=20,tim=60)
### TEMPLATE4 in Peng and Pagonis (2016)
reDose<-c(1e-13,8,16,24,32,1e-13,8)
LxTx<-sLxTx<-vector(length=7)
for (i in seq(7)) {
irradiate(temp=20,tim=reDose[i]/0.1,doseRate=0.1)
heatAt(temp=20,tim=60)
heatTo(temp1=20,temp2=260,hRate=5)
heatAt(temp=260,tim=10)
heatTo(temp1=260,temp2=125,hRate=-5)
Lxdat<-stimOSL(temp=125,tim=100,pValue=4.73e16,nChannel=1000)
heatTo(temp1=125,temp2=20,hRate=-5)
irradiate(temp=20,tim=1/0.1,doseRate=0.1)
heatAt(temp=20,tim=60)
heatTo(temp1=20,temp2=220,hRate=5)
heatAt(temp=220,tim=10)
heatTo(temp1=220,temp2=125,hRate=-5)
Txdat<-stimOSL(temp=125,tim=100,pValue=4.73e16,nChannel=1000)
heatTo(temp1=125,temp2=20,hRate=-5)
LxTx[i]<-sum(Lxdat[1:5,"osly"])/sum(Txdat[1:5,"osly"])
 } #end for.
plot(reDose,LxTx,pch=c(3,2,2,2,2,1,4),col=c(1,rep(2,4),3,4),
lwd=2)
```

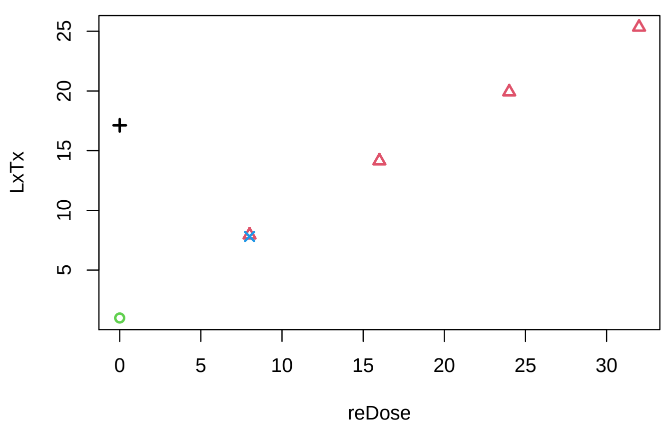


Fig. 11.12: Simulation of a sequence of thermal/optical events using the *Pagonis_Model* code in the KMS programs (Peng and Pagonis [48]).

Code 11.10: Sequence of thermal/optical events

```
# Sequence of thermal/optical events (RLumModel)
rm(list=ls())
suppressMessages(library(package = "RLumModel"))
sequence <- list(
 IRR = c(temp = 20, dose = 10, dose_rate = 1),
 TL = c(temp_begin = 20, temp_end = 400, heating_rate = 1))
model.output <- model_LuminescenceSignals(
model = "Pagonis2008",   sequence = sequence, main=" ",
verbose = FALSE)
```

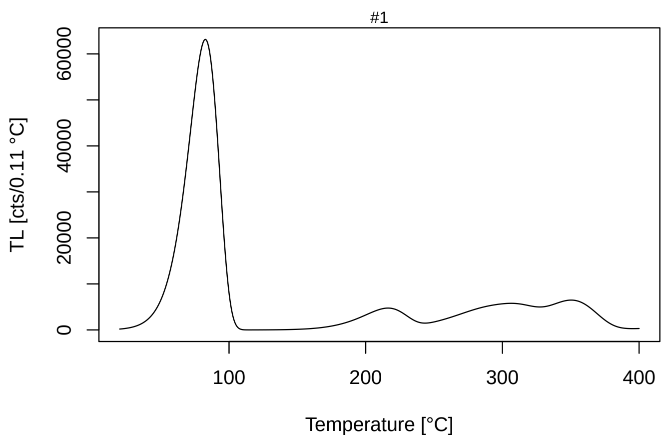


Fig. 11.13: Simulation of a sequence of thermal/optical events using the package *RLumModel*.

Code 11.11: Dose response of TL (RlumModel package)

```
#Dose response of TL (RlumModel package
rm(list=ls())
suppressMessages(library(package = "RLumModel"))
##set list with laboratory doses
```

```r
Lab.dose <- seq(from = 2, to = 8, by = 2)
model.output <- lapply(Lab.dose, function(x){
  sequence <- list(
    IRR = c(20, x, 0.1),
    TL = c(20, 400, 1))
  TL_data <- model_LuminescenceSignals(
    sequence = sequence,
    model = "Bailey2001",
    plot = FALSE,
    verbose = FALSE)
  return(Luminescence::get_RLum(TL_data, recordType = "TL$",
drop = FALSE))
})
model.output.merged <- merge_RLum(model.output)
plot_RLum(
  object = model.output.merged,
  xlab = "Temperature [\u00B0C]",
  ylab = "TL signal [a.u.]",main=" ",lwd=3,lty=1:4,
  legend.text = paste(Lab.dose, " Gy"),
  combine = TRUE)
legend("top",bty="n",legend=c("TL dose response","RLumModel"))
```

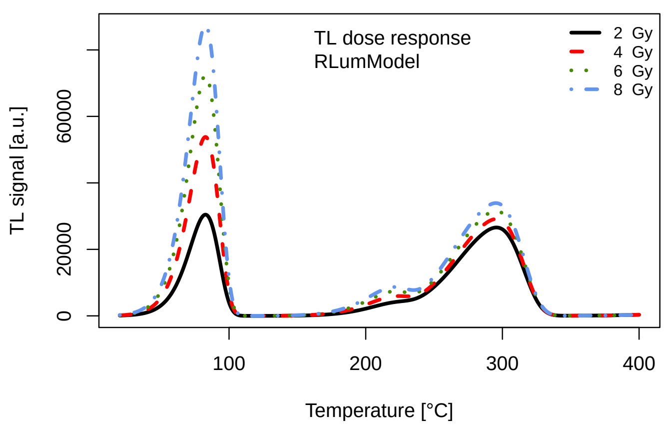


Fig. 11.14: Simulation of the dose response of the TL signal in the laboratory for doses in the range 2-8 Gy for a quartz sample, using the package *RLumModel*.

Code 11.12: Effect of burial temperature on TL of quartz (RlumModel)

```
#Effect of burial temperature on TL of quartz (RlumModel)
rm(list=ls())
suppressMessages(library(package = "RLumModel"))
##set list with burial temperatures
burial.temp <- seq(from = 0, to = 30, by = 10)
model.output <- lapply(burial.temp, function(x){
  sequence <- list(
    IRR = c(x, 20, 1e-11),
    TL = c(20, 400, 1))
  TL_data <- model_LuminescenceSignals(
    sequence = sequence,
    model = "Bailey2001",
    plot = FALSE,
    verbose = FALSE)
  return(Luminescence::get_RLum(TL_data, recordType = "TL$",
drop = FALSE))
})
model.output.merged <- merge_RLum(model.output)
plot_RLum(
  object = model.output.merged,
  xlab = "Temperature [\u00B0C]",
  ylab = "TL signal [a.u.]",main=" ",lwd=3,lty=1:4,
  legend.text = paste(burial.temp, "\u00B0C"),ylim=c(0,70000),
  combine = TRUE)
legend("top",bty="n",legend=c("Burial Temperature","RLumModel"))
```

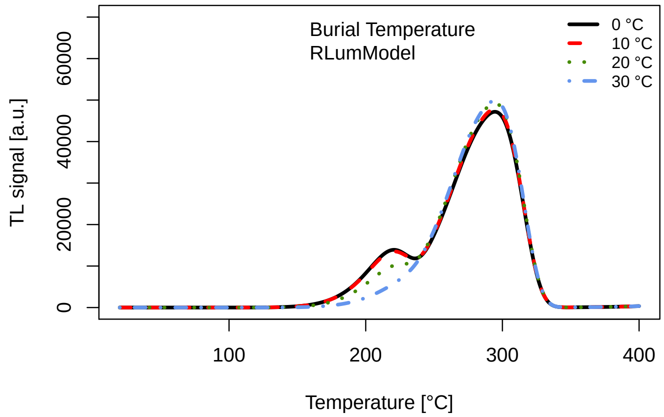


Fig. 11.15: Simulation of the effect of the burial temperature $T = 0 - 30$°C on the TL of a natural quartz sample. For a detailed study, see Koul et al. [53].

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