Chapter 7
LOCALIZED TRANSITIONS: THE LT AND SLT MODEL

Abstract In this chapter we study two localized models found in the luminescence literature, the localized transition model (LT), and the semilocalized transitions model (SLT). We provide R codes for numerically solving the differential equations for the LT model, and compare the solution with the analytical equations involving the Lambert W function. Several examples are presented using the R package *RLumCarlo* to simulate these types of localized transition phenomena. We present R codes for the important hybrid SLT model developed by Mandowski, which can be used to explain the anomalous heating rate effect observed in several dosimetric materials. Finally, the chapter concludes with the presentation of a simplified form of the SLT model, developed by Pagonis et al.

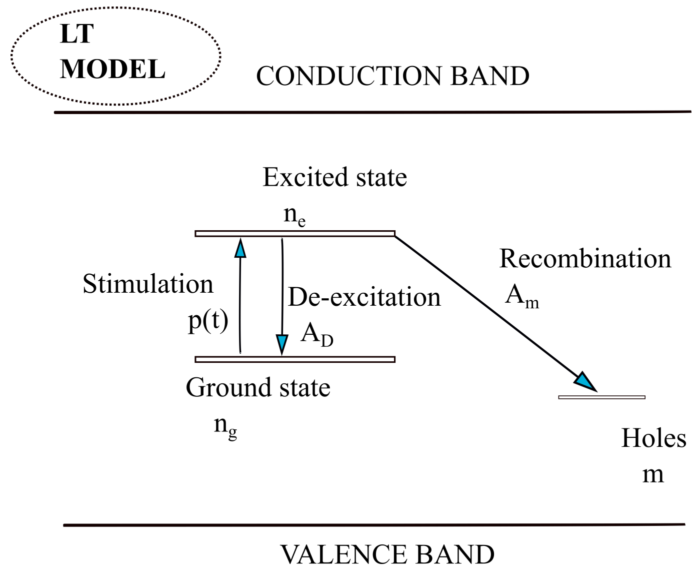

Fig. 7.1: Energy band diagram for the localized transition LT model.

Code 7.1: Plot W(x) solution of LT model

```
rm(list=ls())
library(lamW)
## Plot the analytical solution of LT, using Lambert W-function
x1<-300:450
kB<-8.617E-5
no<-1E8
r<-1e4
En<-1
s<-1E13
beta<-1
k<-function(u) {integrate(function(p){exp(-En/(kB*p))},
300,u)[[1]]}
y1<-lapply(x1,k)
x<-unlist(x1)
y<-unlist(y1)
zTL<-(r/no)-log(no/r)+(s*y)
plot(x,r*s*exp(-En/(kB*x))/(lambertW0(exp(zTL))
      +lambertW0(exp(zTL))^2),type="l",col="red",
```

```
lwd=3,lty=1,xlab="Temperature, K",ylab="TL in LT model [a.u.]")
zTL<-(r/no)-log(no/r)+(s*y)
r<-1e8
zTL<-(r/no)-log(no/r)+(s*y)
lines(x,r*s*exp(-En/(kB*x))/(lambertW0(exp(zTL))
      +lambertW0(exp(zTL))^2),col="green",
      lwd=3,  lty=2,   xlab="Temperature, K",ylab="TL")
r<-1e9
zTL<-(r/no)-log(no/r)+(s*y)
lines(x,r*s*exp(-En/(kB*x))/(lambertW0(exp(zTL))
      +lambertW0(exp(zTL))^2),col="blue",
      lwd=3,  lty=3,    xlab="Temperature, K",ylab="TL")
legend("topright",bty="n",lwd=2, lty=c(NA,NA,1,2,3),
legend = c("Retrapping ratio r", expression("(cm"^"-3"*")"),
expression("10"^"4"*""),expression("10"^"8"*""),
expression("10"^"9"*"")),
       col=c(NA,NA,"red","green","blue"))
```

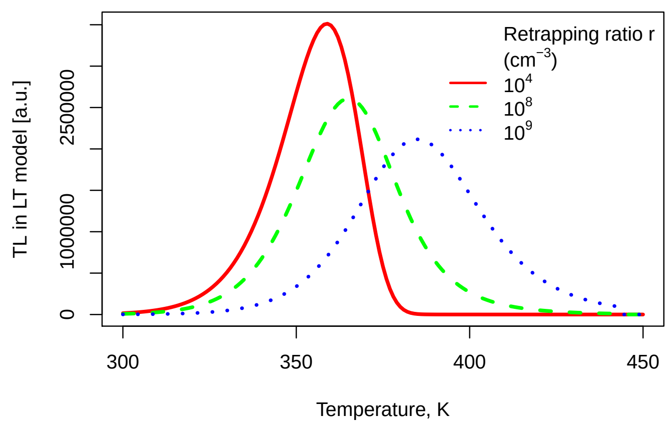

Fig. 7.2: Plots of the analytical solution of the LT model, using the Lambert W function, for three values of the retrapping ratio $r = 10^4,\ 10^8,\ 10^9$ cm^{-3} and $n_0 = 10^8$ cm^{-3}. As r increases, the shape of the TL glow curve changes from an asymmetric peak for first order kinetics, to a symmetric shape for second order kinetics. For details, see Kitis and Pagonis [14].

Process	**Symbol**	**Parameter in RLumCarlo function**	**Unit**	**Typical values**
Localized TL	E	Thermal activation energy of the trap	eV	0.5-3
	s	Frequency factor of the trap	1/s	1E8-1E16
	times	Sequence of time steps for simulation (heating rate 1 K/s)	s	0-700
	clusters	Number of MC runs	1	1E1-1E4
	n_filled	Number of filled electron traps at the beginning of the simulation	1	1-1E5
	r	Localized retrapping ratio	1	0-1E5
Localized CW-IRSL	A	Optical excitation rate from ground state of the trap to the excited state	1/s	1E-3-1
	times	Sequence of time steps for simulation	s	0-500
	clusters	Number of MC runs	1	1E1-1E4
	n_filled	Number of filled electron traps at the beginning of the simulation	1	1-1E5
	r	Localized retrapping ratio	1	0-1E5
Localized ISO	E	Thermal activation energy of the trap	eV	0.5-3
	s	Frequency factor of the trap	1/s	1E8-1E16
	T	Temperature of the isothermal process	°C	20-300
	times	Sequence of time steps for simulation	s	0-1000
	clusters	Number of MC runs	1	1E1-1E4
	n_filled	Number of filled electron traps at the beginning of the simulation	1	1-1E5
	r	Localized retrapping ratio	1	0-1E5
Localized LM-OSL	A	Optical excitation rate from ground state of the trap to the excited state	1/s	1E-3-1
	times	Sequence of time steps for simulation	s	0-3000
	clusters	Number of MC runs	1	1E1-1E4
	n_filled	Number of filled electron traps at the beginning of the simulation	1	1-1E5
	r	Localized retrapping ratio	1	0-1E5

Table 7.1: Table of input parameters for LOC functions in *RLumCarlo.*

Function Name	Description
plot_RLumCarlo	Plots 'RLumCarlo' modeling results (the averaged signal or the number of remaining electrons), with modeling uncertainties.
run_MC_CW_IRSL_LOC	Simulation of CW-IRSL signals in the LT model, due to tunneling transitions from the excited state of the trap, into a recombination center (RC).
run_MC_ISO_LOC	Simulation of ITL signals in the LT model, due to tunneling from the excited state into the RC.
run_MC_LM_OSL_LOC	Simulation of LM-IRSL signals in the LT model, due to tunneling from the excited state into the RC.
run_MC_TL_LOC	Simulation of TL signals in the LT model, due to tunneling from the excited state into the RC.

Table 7.2: Table of LOCalized transition functions available in the package *RLumCarlo*.

Code 7.2: Single plot MC simulations for localized CW-IRSL (LT model)

```
##============================================================##
## Example: MC simulations for localized CW_IRSL (LT model)
##============================================================##
rm(list = ls(all=T))
library(RLumCarlo)
run_MC_CW_IRSL_LOC(
A = 0.12,
times = 0:100,
clusters = 10,
n_filled = 100,
r = 1e-7,
method = "seq",
output = "signal"
) %>%
#Plot results of the MC simulation
plot_RLumCarlo(legend = T)
 legend("top",bty="n",c("CW-IRSL signal","LOC function",
"LT model"))
```

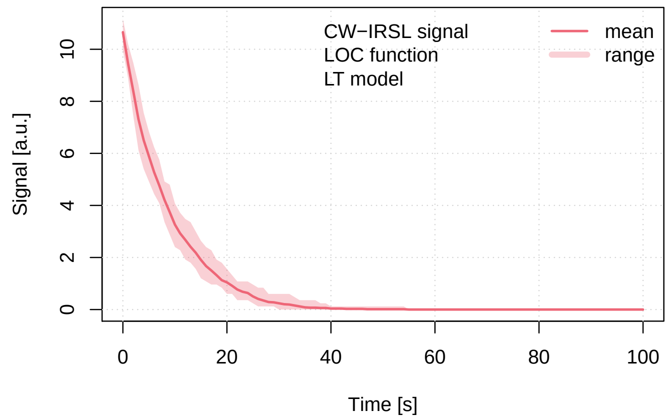

Fig. 7.3: Simulation of CW-IRSL signal in the LT model, using the function *run_MC_LM_IRSL_LOC* in the package *RLumCarlo*.

Code 7.3: Single plot MC simulations for localized LM-OSL

```
##============================================================##
##============================================================##
## MC simulations for localized LM-OSL
##============================================================##
rm(list = ls(all=T))
library(RLumCarlo)
run_MC_LM_OSL_LOC(
A = 0.1,
times = 0:250,
clusters = 100,
n_filled = 50,
r = 1e-7,
method = "seq",
output = "signal"
) %>%
#Plot results of the MC simulation
plot_RLumCarlo(legend = T)
legend("top",bty="n",c("LM-IRSL signal","LOC function",
"LT model"))
```

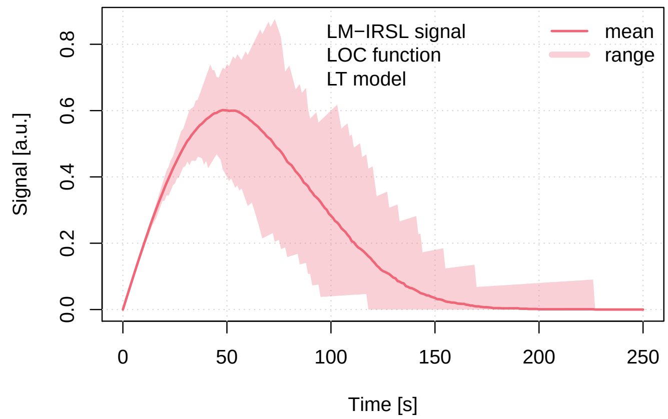

Fig. 7.4: Simulation of LM-IRSL signal in the LT model, using the function *run_MC_LM_IRSL_LOC* in the package *RLumCarlo*.

Code 7.4: Localized TL with variable retrapping ratio r

```
##=======================================================##
## Localized TL with variable retrapping ratio r (LT model)
##=======================================================##
rm(list = ls(all=T))
library(RLumCarlo)
f<-function(rvar,vars,addTF){
  run_MC_TL_LOC(
    s = 1e12,
    E = 1,
    times = 0:300,
    r = rvar
  ) %>%
    #Plot results of the MC simulation
    plot_RLumCarlo(legend = F,plot_uncertainty=NULL,type="o",
  pch=vars,col=vars,add=addTF, xlim=c(50,275))}
f(1,1,FALSE)
f(1e3,2,TRUE)
f(1e4,3,TRUE)
```

```
legend("topright",bty="n",pch=c(NA,NA,NA,1:3),
col=c(NA,NA,NA,1:3),legend = c("Retrapping"  ,"Ratio r ",
 " ","1",  expression("10"^"3"*""),expression("10"^"4"*"")) )
```

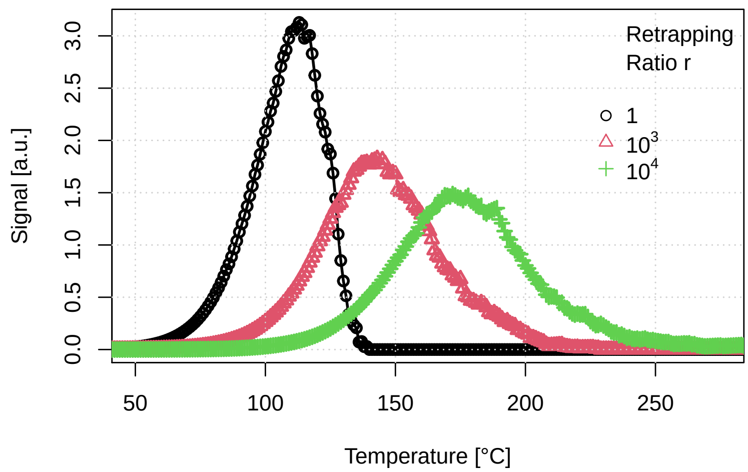

Fig. 7.5: Simulation of TL signal in the LT model, by using the function *run_MC_TL_LOC* in the package *RLumCarlo*, for three different values of the retrapping ratio r.

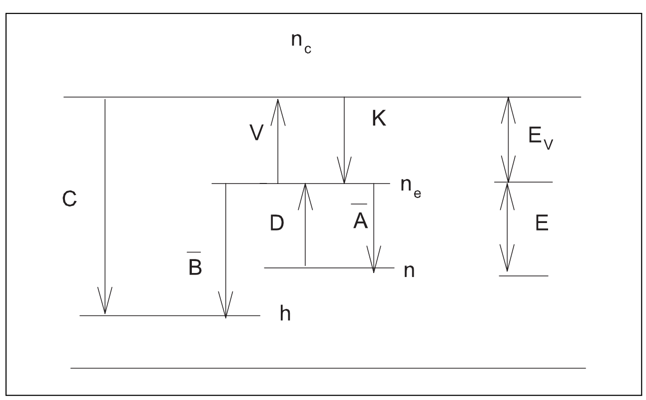

Fig. 7.6: The SLT model proposed by Mandowski [24].

$$
\begin{array}{ccccc}
H_1^0 & \underset{\bar{A}}{\overset{D}{\rightleftarrows}} & H_0^1 & \xrightarrow{V} & H_0^0 \\
C\downarrow & & C\downarrow & \overset{\bar{B}}{\searrow} & C\downarrow \\
E_1^0 & \underset{\bar{A}}{\overset{D}{\rightleftarrows}} & E_0^1 & \xrightarrow{V} & E_0^0.
\end{array}
$$

Fig. 7.7: Schematic representation of the possible transitions in the SLT model by Mandowski [24].

Code 7.5: Mandowski SLT model: simulation of TL experiment

```
# Mandowski SLT model: simulation of TL experiment
rm(list=ls())
library("deSolve")
TLMandowski <- function(t, x, parms) {
  with(as.list(c(parms, x)), {
 dH01<- -(s*exp(-E/(kb*(273+hr*t)))+C*(H00-E01-E10))*H01+A*H10
 dH10 <- s*exp(-E/(kb*(273+hr*t)))*H01-(A+B+sv*exp(-Ev/(kb*
    (273+hr*t)))+C*(H00-E01-E10))*H10
 dH00<-sv*exp(-Ev/(kb*(273+hr*t)))*H10-C*(H00-E01-E10)*H00
 dE01<-C*(H00-E01-E10)*H01-s*exp(-E/(kb*(273+hr*t)))*E01+A*E10
 dE10<-C*(H00-E01-E10)*H10+s*exp(-E/(kb*(273+hr*t)))*E01-
      (A+sv*exp(-Ev/(kb*(273+hr*t))))*E10
 dE00<-B*H10+C*(H00-E01-E10)*H00+sv*exp(-Ev/(kb*(273+hr*t)))*E10
     res <- c(dH01,dH10,dH00,dE01,dE10,dE00)
    list(res)  })}
enVar<-function(en){
parms  <- c(E =en, s=1e10, sv=1e10, kb=8.617*10^-5,
hr=1, C=C,B=B,Ev=0.7,A=2*10^4)
y <- xstart <- c(H01 = 10^17,   H10=0,H00=0,E10=0,E01=0,E00=0)
out <-  ode(xstart, times, TLMandowski, parms, method = "lsoda",
 atol = 1,rtol=1) }
C<-1e-10
B<-1e4
temps<-times  <- seq(0, 360,by=.5)
```

```
Lc<-Lb<-matrix(NA,nrow=length(times),ncol=4)
areaLb<-areaLc<-vector(length=4)
  en<-.95
  a<-enVar(en)
  Lc<-(C*(a[,"H00"]-a[,"E01"]-a[,"E10"])*
          (a[,"H10"]+a[,"H01"]+a[,"H00"]))
  Lb<-B*a[,"H10"]
  areaLc<-sum(Lc)*0.5
  areaLb<-sum(Lb)*0.5
par(mfrow=c(2,3))
xlabs=expression("Temperature ["^"o"*"C]")
plot(temps,Lb,typ="l",xlim=c(100,270),ylim=c(0,4e15),col="blue",
pch=1,xlab=expression("Temperature ["^"o"*"C]"),lwd=5,
ylab="LB [a.u.])")
legend("topleft",bty="n",col="red",
legend=c("(a)","Mandowski","SLT model","LB TL peak"))
plot(temps,Lc,typ="o",xlim=c(100,270),ylim=c(0,.7e14),col="red",
xlab=xlabs,ylab="LC [a.u.])")
legend("topleft",bty="n",col="red",
legend=c("(b)"," ","LC TL peak"))
plot(temps,a[,"H00"],typ="o",xlim=c(100,270),ylim=c(0,2e15),
xlab=xlabs,ylab=expression("H00 [cm"^-3*"]"),col="red",pch=1)
legend("top",bty="n",c("(c)"," ","H00"))
plot(temps,a[,"H01"],typ="o",xlim=c(100,270),ylim=c(0,2e17),
xlab=xlabs,ylab=expression("H01 [cm"^-3*"]"),col="green")
lines(temps,a[,"E00"],typ="o",col="gray",pch=3)
legend("topleft",bty="n",c("(d)"," ","H01"))
text(200,1.2e17,"E00")
plot(temps,a[,"E01"],typ="o",xlim=c(100,270),ylim=c(0,2e15),
xlab=xlabs,ylab=expression("E01 [cm"^-3*"]"),col="magenta")
legend("top",bty="n",c("(e)"," ","E01"))
plot(temps,a[,"H10"],typ="o",xlim=c(100,270),ylim=c(0,4e11),
col="black",xlab=xlabs,ylab=expression("H10,  E10 [cm"^-3*"]"))
lines(temps,a[,"E10"],typ="o",col="green",)
legend("top",bty="n",c("(f)"," ","H10"))
text(220,1e11, "E10")
```

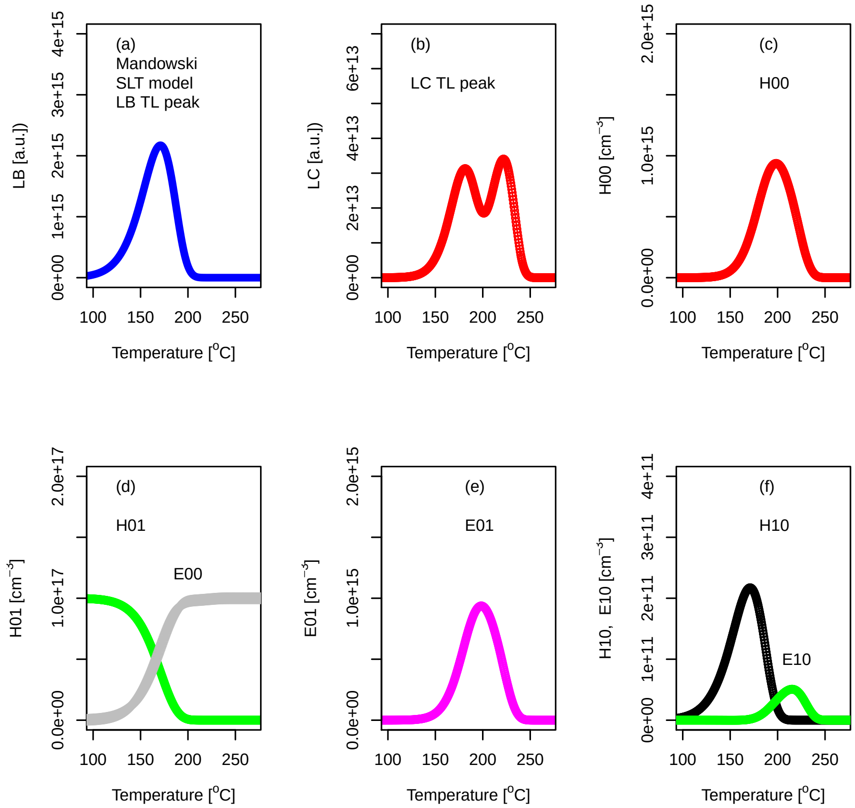

Fig. 7.8: Simulations of a TL process in the Mandowski SLT model, using the parameters given in the text, showing plots of the various concentrations H_m^n and E_m^n. (a) The L_B peak due to localized transitions in the model; (b) The double L_C peak from delocalized transitions; (c)-(f) The concentrations H_m^n and E_m^n as a function of temperature. *Caution:* Note that the numerical integration used in the *deSolve* package can often become numerically unstable for this type of model, see the discussion in the text.

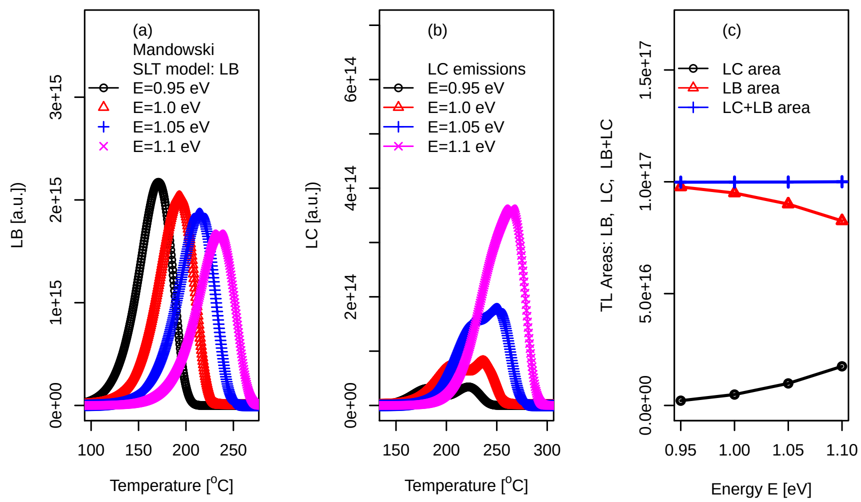

Fig. 7.9: Simulations of the Mandowski SLT model, using the parameters given in the text, and four different values of the parameter $E = 0.95,\ 1.0,\ 1.05,\ 1.1$ eV. (a) The L_B peaks due to localized transitions in the model; (b) The double L_C peaks from delocalized transitions; (c) The areas under the L_C and L_B peaks, and their sum $L_C + L_B$ as a function of the activation energy E.

Code 7.6: Mandowski model: the anomalous heating rate effect

```
#Mandowski model: the anomalous heating rate effect
rm(list=ls())
library("deSolve")
TLMandowski <- function(t, x, parms) {
  with(as.list(c(parms, x)), {
  dH01<- -(s*exp(-E/(kb*(273+hr*t)))+C*(H00-E01-E10))*H01+A*H10
    dH10 <- s*exp(-E/(kb*(273+hr*t)))*H01-(A+B+sv*exp(-Ev/(kb*
  (273+hr*t)))+C*(H00-E01-E10))*H10
    dH00<-sv*exp(-Ev/(kb*(273+hr*t)))*H10-C*(H00-E01-E10)*H00
  dE01<-C*(H00-E01-E10)*H01-s*exp(-E/(kb*(273+hr*t)))*E01+A*E10
    dE10<-C*(H00-E01-E10)*H10+s*exp(-E/(kb*(273+hr*t)))*E01-
```

```
      (A+sv*exp(-Ev/(kb*(273+hr*t))))*E10
dE00<-B*H10+C*(H00-E01-E10)*H00+sv*exp(-Ev/(kb*(273+hr*t)))*E10
    res <- c(dH01,dH10,dH00,dE01,dE10,dE00)
    list(res)  })}
hrVar<-function(hr){
  parms  <- c(E =1.05, s=1e10, sv=1e10, kb=8.617*10^-5,
              hr=hr, C=C,B=B,Ev=0.7,A=2*10^4)
  y <- xstart <- c(H01 = 10^17,   H10=0,H00=0,E10=0,E01=0,E00=0)
  out <-ode(xstart,times, TLMandowski, parms, method = "lsoda",
              atol = 1,rtol=1) }
C<-1e-10
B<-1e4
times  <- seq(0, 300,by=.5)
Lc<-Lb<-temps<-matrix(NA,nrow=length(times),ncol=4)
areaLb<-areaLc<-vector(length=4)
for (i in 1:4){
  hr<-i
  a<-hrVar(hr)
  Lc[,i]<-(C*(a[,"H00"]-a[,"E01"]-a[,"E10"])*
             (a[,"H10"]+a[,"H01"]+a[,"H00"]))/hr
  Lb[,i]<-B*a[,"H10"]/hr
  temps[,i]<-hr*times
  areaLc[i]<-sum(Lc[,i])*hr*0.5
  areaLb[i]<-sum(Lb[,i])*hr*0.5
}
par(mfrow=c(1,3))
var<-c(NA,NA,NA,1:4)
matplot(cbind(temps),cbind(Lb),lty="solid",typ="o",pch=1:4,
xlim=c(150,270),ylim=c(0,3e15),lwd=2, col=1:4 ,
xlab=expression("Temperature ["^"o"*"C]"), ylab="LB [a.u.])")
legend("topleft",bty="n",pch=var,lty="solid",col=var,
legend=c("(a)",
"Mandowski","SLT model: LB","1 K/s","2 K/s","3 K/s","4 K/s"))
matplot(cbind(temps),cbind(Lc),lty="solid",typ="o",pch=1:4,
xlim=c(170,300),ylim=c(0,7e14),lwd=2,col=1:4,
xlab=expression("Temperature ["^"o"*"C]"), ylab="LC [a.u.])")
legend("topleft",bty="n",pch=var,lty="solid",col=var,
legend=c("(b)"," ","LC peaks","1 K/s","2 K/s","3 K/s","4 K/s"))
matplot(1:4,cbind(areaLc,areaLb,areaLb+areaLc),lty="solid",
typ="o",lwd=3, pch=1:3,col=1:3,ylim=c(0,1.7e17),
xlab="Heating rate [K/s]",ylab="TL Areas: LB,  LC,  LB+LC")
legend("topleft",bty="n",pch=c(NA,NA,1:3),lty="solid",col=c(NA,
NA,1:3),legend= c("(c)"," ","LC area","LB area","LC+LB area"))
```

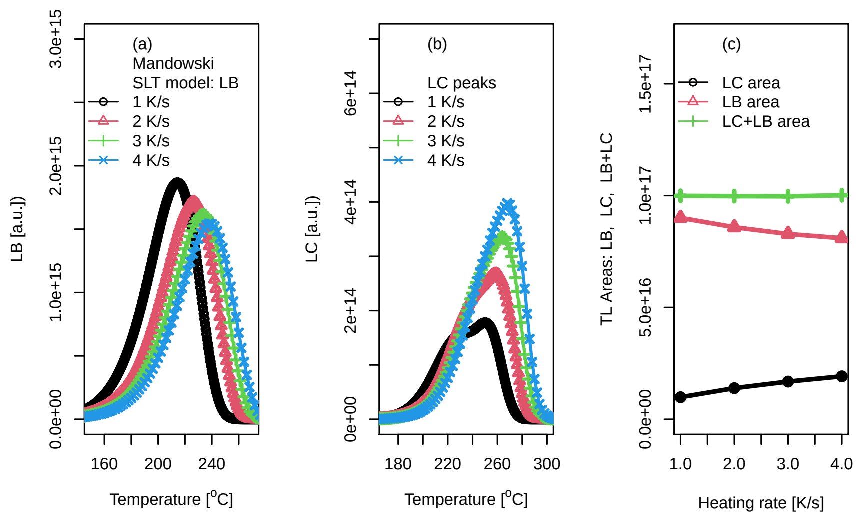

Fig. 7.10: Simulations of the anomalous heating rate effect using the Mandowski model, with the parameters given in the text, and for four different values of the heating rate $\beta = 1-4$ K/s. (a) The L_B peaks due to localized transitions in the model; (b) The L_C peaks from delocalized transitions. (c) The areas under the TL glow curves in (a),(b) and their sum $L_C + L_B$, as a function of the heating rate.

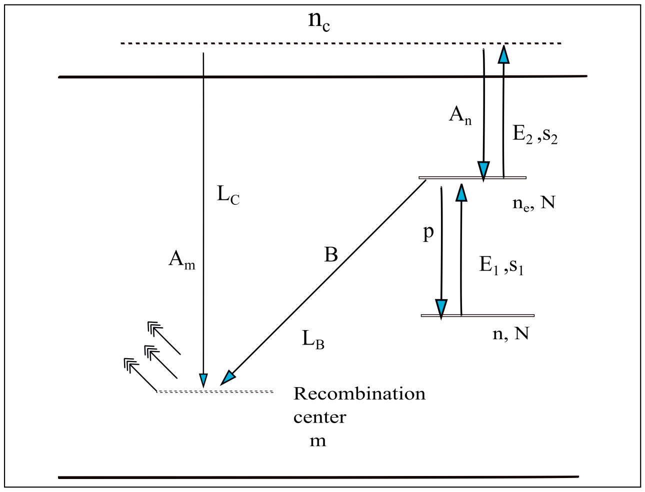

Fig. 7.11: The simplified SLT model proposed by Pagonis et al. [31].

Code 7.7: Pagonis SLT model: the anomalous heating rate effect

```
#Pagonis SLT model: the anomalous heating rate effect
rm(list=ls())
library("deSolve")
PagonisHR <- function(t, x, parms) {
  with(as.list(c(parms, x)), {
    dn<- -s1*n*exp(-E1/(kb*(273+hr*t)))+p*
      (An*(N-n)*(m-n)+s1*n*exp(-E1/(kb*(273+hr*t))))/
( s2*exp(-E2/(kb*(273+hr*t)))+p+B)
      dm<- -Am*m*(m-n)-B*
        (An*(N-n)*(m-n)+s1*n*exp(-E1/(kb*(273+hr*t))))/(
          s2*exp(-E2/(kb*(273+hr*t)))+p+B)
      res <- c(dn,dm)
    list(res)  })}
hrVar<-function(hr){
parms  <- c(p=p,s1=s1,s2=s2,An=An,Am=Am,
            B=B,N=N,E1=E1,E2=E2,kb=kb)
y <- xstart <- c(n = 1e11, m=1e11)
out <-  ode(xstart, times, PagonisHR, parms) }
```

```
p<-1e9
s1<-1e9
s2<-1e12
An<-1e-8
Am<-1e-6
B<-1e7
N<-1e13
E1<-0.8
E2<-0.5
kb<-8.617e-5
times  <- seq(0, 350,by=1)
Lc<-Lb<-temps<-matrix(NA,nrow=length(times),ncol=4)
areaLb<-areaLc<-vector(length=4)
for (i in 1:4){
  hr<-i
  a<-hrVar(hr)
  Lc[,i]<- Am*a[,"m"]*(a[,"m"]-a[,"n"])/hr
  Lb[,i]<-B*  ((An*(N-a[,"n"])*(a[,"m"]-a[,"n"])+s1*a[,"n"]*
 exp(-E1/(kb*(273+hr*times)))))/( s2*exp(-E2/(kb*
(273+hr*times)))+p+B))/hr
   temps[,i]<-273+hr*times
  areaLc[i]<-sum(Lc[,i],rm.NA=TRUE)*hr
  areaLb[i]<-sum(Lb[,i],rm.NA=TRUE)*hr
}
par(mfrow=c(1,3))
var<-c(NA,NA,NA,1:4)
matplot(cbind(temps),cbind(Lb),lty="solid",typ="o",pch=1:4,
xlim=c(370,550),ylim=c(0,22e8),lwd=2, col=1:4 ,
xlab=expression("Temperature [K]"), ylab="LB [a.u.])")
legend("topleft",bty="n",pch=var,lty="solid",col=var,
legend=c("(a)",
"Pagonis","SLT model: LB","1 K/s","2 K/s","3 K/s","4 K/s"))
matplot(cbind(temps),cbind(Lc),lty="solid",typ="o",pch=1:4,
xlim=c(370,550),ylim=c(0,5e8),lwd=2,col=1:4,
xlab=expression("Temperature [K]"), ylab="LC [a.u.])")
legend("topleft",bty="n",pch=var,lty="solid",col=var,
legend=c("(b)"," ","LC emissions","1 K/s","2 K/s","3 K/s",
"4 K/s"))
matplot(1:4,cbind(areaLc,areaLb,areaLb+areaLc),lty="solid",
typ="o",lwd=3, pch=1:3,col=1:3,ylim=c(0,1.7e11),
xlab="Heating rate [K/s]",ylab="TL Areas: LB,  LC,  LB+LC")
legend("topleft",bty="n",pch=c(NA,NA,1:3),lty="solid",
col=c(NA,NA,
1:3),legend= c("(c)"," ","LC area","LB area","LC+LB area"))
```

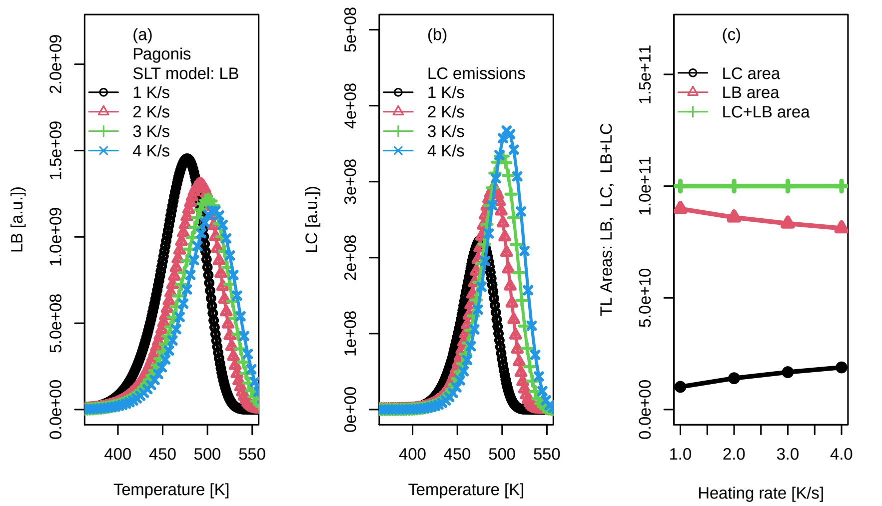

Fig. 7.12: Simulations of the anomalous heating rate effect using the simplified SLT model by Pagonis et al. [31], with the parameters given in the text, and for four different values of the heating rate $\beta = 1 - 4$ K/s. (a) The L_B peaks due to localized transitions in the model; (b) The L_C peaks from delocalized transitions; (c) The areas under the TL glow curves in (a),(b) and their sum $L_C + L_B$, as a function of the heating rate.