Chapter 4
DOSE RESPONSE OF DOSIMETRIC MATERIALS

Abstract In this chapter we discuss theoretical and experimental aspects of the dose response of dosimetric materials, and use analytical equations to fit experimental data. We define the superlinearity index $g(D)$, and the supralinearity index $f(D)$, and discuss various functions commonly used to describe shape of dose response curves in TL, OSL, OA and ESR signals: the saturating exponential, double saturating exponential, single exponential plus linear and the recently derived equation using the Lambert W function. We show how to numerically integrate the equations for the irradiation stage in the OTOR model, and compare with the analytical solution based on the Lambert W function. Several detailed R codes are given of fitting experimental data ESR, TL, OSL data, including situations with superlinear dose response. We simulate experiments in which the sample temperature is variable during the irradiation process, and which may affect the dose response of the material. We discuss superlinear dose response as the result of competition between two electron traps during the irradiation, and present experimental data analysis using the new analytical Pagonis-Kitis-Chen (PKC) equation which describes superlinearity effects. This chapter will conclude with an overview of the analytical dose response equations based on the Lambert function, and with a discussion of the importance of the Lambert function in the description of luminescence phenomena.

Code 4.1: Fit dose response data with saturating exponential

```
#Fit dose response data with Saturating Exponential
rm(list = ls(all=T))
options(warn=-1)
library("minpack.lm")
library("lamW")
```

```
## fit to saturation exponential ----
t = c( 0,50.7117,100.534,152.135,204.626,272.242)
y = c(0,33.144,42.205,43.1055,44.4157,43.7098)
fit_data <-data.frame(  t ,y)
plot(fit_data,ylim=c(0,max(y)),xlab="Dose [Gy]",
ylab="OSL (L/T)")
fit <- minpack.lm::nlsLM(
  formula = y ~ N * (1-exp(-b* t)),
  data = fit_data,
  start = list(N= max(y),b = .01))
N_fit <- coef(fit)[1]
b_fit <- coef(fit)[2]
## plot analytical solution
t1<-0:300
lines(x = t1,  y = N_fit  * (1-exp(-b_fit* t1)),col = "blue")
legend("right",bty="n",legend=c("Quartz OSL"," ",
"Libyan quartz"))
## print results
cat("\nfitted N: ", N_fit)
cat("\nfitted Do: ", round(1/b_fit,2), "Gy")
```

```
  ##
  ## fitted N:  44.16116
  ## fitted Do:  35.83 Gy
```

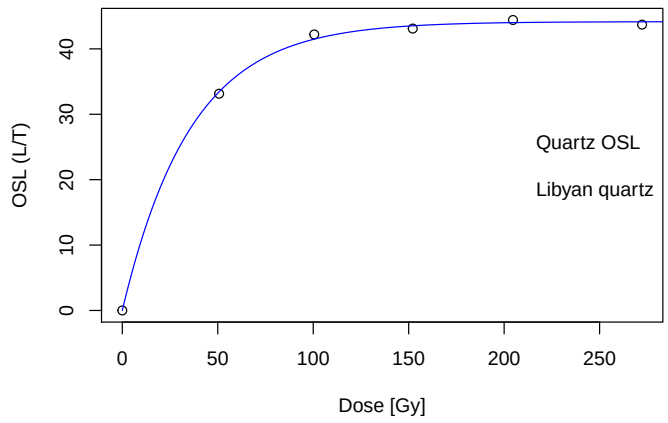

Fig. 4.1: Fitting dose response data with a saturating exponential. For more details see Pagonis et al. [38], original data from Li et al. [22].

Code 4.2: Irradiation: OTOR, Lambert analytical solution

```
# OTOR MODEL- IRRADIATION Lambert solution code
rm(list = ls(all=T))
options(warn=-1)
library(lamW)
library("deSolve")
## Plot  analytical solution of OTOR irradiation stage, using W
t<-0:100
N<-1E10
R<-.1
X<-1e10
k<-function(u){1+(1/(1-R))*lambertW0((R-1)*exp(-(R*X*u/N)+R-1))}
y1<-lapply(t,k)
x<-unlist(t)
y<-unlist(y1)
plot(x,y,xlab="Irradiation time t, s",ylab="Filled Traps n/N",
pch=1)
# Numerically Solve GOT equation for IRRADIATION  using  deSolve
n.0 <- 0  # initial concentration of filled traps
# Calculate numerical ODE solution
ODE <- function(t, state, parmameters){
  with(as.list(c(state, parameters)),{
    dn <-   (N-n) * X*R / ((N - n) * R + n )
    list(c(dn)) })}
parameters <- c(N=N, X = X, R =R)
state <- c(n = n.0)
num_ODE <- ode(y = state, times =t,func=ODE,parms=parameters)
lines(x = num_ODE[,1],y = num_ODE[,2]/N,xlab ="Time[s]",
type="l",col = "red")
legend("right",bty="n",pch=c(NA,1),legend =c("W(t)", "ODE"),
       col = c("red","black"), lwd = 1)
```

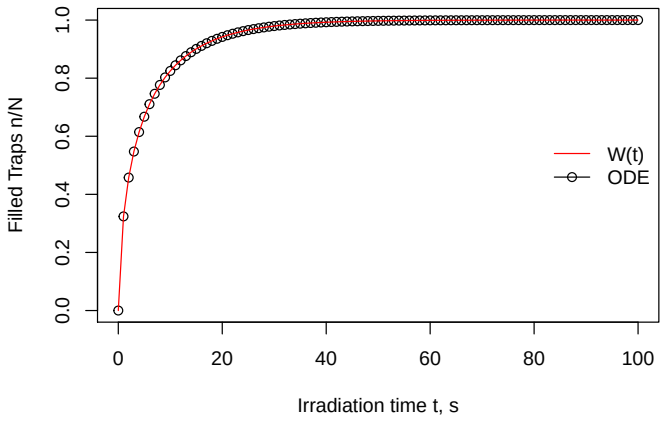

Fig. 4.2: Dose response in the OTOR model, using the Lambert analytical solution Eq.(**??**). The analytical solution (solid line) is compared with the numerical solution of the differential Eq.(**??**) shown as circles.

Code 4.3: Fit of experimental TL dose response data using W(x)

```
rm(list = ls(all=T))
options(warn=-1)
library("minpack.lm")
library("lamW")
## fit to Lambert equation  ----
t = c(0.00394056,0.00451523,0.39225,0.412035,0.703062,0.741318,
 0.742221,1.49553,1.49758,1.5158,2.98473,3.00304,3.02282,
 5.99852, 6.05755)
y = c(2.45103,2.80847,3.97964,4.28586,5.30465,5.10007,5.66177,
6.21706,7.49364,6.82965,8.50226,7.88934,8.19555,11.0809,11.7953)
fit_data <-data.frame(  t ,y)
plot(fit_data,ylim=c(0,max(y)),xlab="Dose [Gy]",
     ylab="OSL (L/T)",xlim=c(-.5,6.5))
fit <- minpack.lm::nlsLM(
  formula =y~N*(1+lambertW0((abs(R)-1)*exp(abs(R)-1-abs(b)*
   (t+abs(f))))/(1-abs(R))),
  data = fit_data,
```

```
  start = list(N= max(y),R=.9, b = .1,f=0.3))
N_fit <- coef(fit)[1]
R_fit <- abs(coef(fit)[2])
b_fit <- abs(coef(fit)[3])
f_fit <- abs(coef(fit)[4])
## plot analytical solution
t<- seq(from=-0.5,to=7,by=.02)
lines(
  x = t,
  y=N_fit*(1+lambertW0((R_fit-1)*exp(R_fit-1-b_fit*
                                       (t+f_fit)))/(1-R_fit)),
  col = "blue")
legend("right",bty="n",legend=c("Berger (1990)",
                                "Volcanic glass"," "))
## print results
cat("\nfitted N: ", N_fit)
cat("\nfitted R: ", R_fit)
cat("\nfitted Dc: ", round(1/b_fit,2), "Gy")
cat("\nfitted f: ", f_fit)
```

```
  ##
  ## fitted N:  19.14201
  ## fitted R:  5.276899e-06
  ## fitted Dc:  21.6 Gy
  ## fitted f:  0.2279443
```

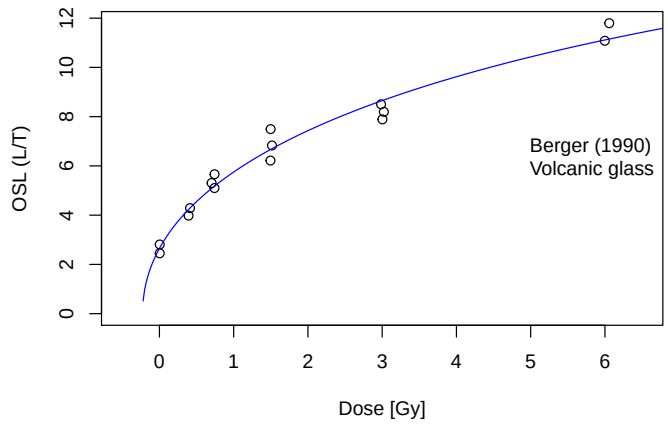

Fig. 4.3: Fit of experimental TL dose response data using the Lambert Eq.(**??**), with a non-zero intercept on the dose axis. For more details see Pagonis et al. [38], original data from Berger [2].

Code 4.4: Fit of experimental ESR dose response data using Lambert equation

```
rm(list=ls())
options(warn=-1)
library("minpack.lm")
library("lamW")
# Load the data
TLqzx<-c(174.13, 345.027, 931.847, 1603.74, 2524.39, 4031.12,
6372.18,9044.09,12217.5,15058.3,19981.5,25072.3,30082.3,40011.4)
TLqzy<-c(1.07478, 1.68389, 2.18591, 2.93875, 3.51271, 4.48122,
5.59377,6.3484,7.3184,8.39557,9.33133,10.4105,11.8478,13.6478)
plot(TLqzx,TLqzy,type="p",pch=1,col="red",
xlab=expression("Dose [Gy]"),ylab ="ESR signal [a.u.]",
ylim=c(0,20))
legend("topleft",bty = "n",
legend = c("Quartz"," ","ESR dose response"))
## fit to Lambert equation  ----
t <-TLqzx
y<-TLqzy
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= max(y),R=.9, b = .01)
)
N_fit <- coef(fit)[1]
R_fit <- abs(coef(fit)[2])
b_fit <- coef(fit)[3]
## plot analytical solution
t<- seq(from=0,to=40000,by=100)
lines(  x = t,
y=N_fit*(1+lambertW0((R_fit-1)*exp(R_fit-1-b_fit*t))/(1-R_fit)),
  col = "blue")
```

```
## print results
cat("\nfitted N: ", N_fit)
cat("\nfitted R: ", R_fit)
cat("\nfitted Dc: ", 1/b_fit, " Gy")

  ##
  ## fitted N:  51.24355
  ## fitted R:  1.432573e-08
  ## fitted Dc:  995428.2  Gy
```

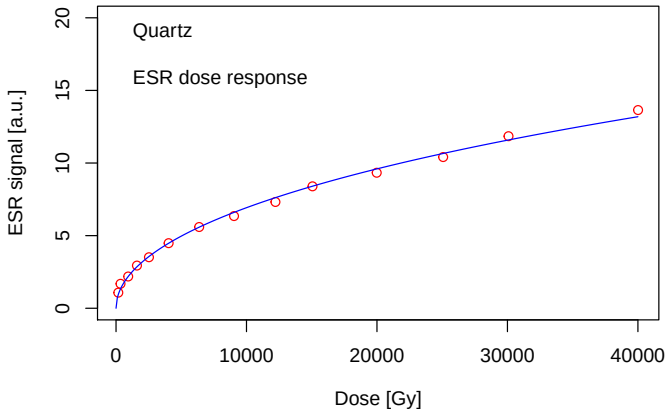

Fig. 4.4: Fit of experimental ESR dose response data using the Lambert Eq.(**??**). For more details see Pagonis et al. [38], original data from Duval [9].

Code 4.5: Fit of experimental OSL dose response data using W(x)

```
rm(list = ls(all=T))
options(warn=-1)
library("minpack.lm")
library("lamW")
par(mfrow=c(1,2))
## fit to saturation exponential ----
t = c(-34.2466, 34.2466, 68.4932, 273.973, 1027.4,1986.3,3013.7,
      5000, 7979.45, 10000)
```

```
y = c(1.04664, 0.000978474, 2.76386, 7.24592,12.6008,14.5329,
      15.8956,  17.1905, 17.847, 18.0952)
fit_data <-data.frame(  t ,y)
plot(fit_data,ylim=c(0,max(y)),xlab="Dose [Gy]",
ylab="OSL (L/T)")
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=.9, b = .01))
N_fit <- coef(fit)[1]
R_fit <- abs(coef(fit)[2])
b_fit <- coef(fit)[3]
## plot analytical solution
t<- seq(from=0,to=10000,by=100)
lines(  x = t,
y=N_fit*(1+lambertW0((R_fit-1)*exp(R_fit-1-b_fit* t))/
(1-R_fit)),  col = "blue")
legend("right",bty="n",legend=c("(a)"," ","Fine grain",
"Quartz"," "))
## print results
cat("\nFine grain"," ")
cat("\nfitted N: ", N_fit)
cat("\nfitted R: ", R_fit)
cat("\nfitted Dc: ",round( 1/b_fit,2), "Gy")
## fit to Lambert equation ----
t = c(0, 3.5583, 44.1822, 258.718, 1051.62, 2044.98, 3003.94,
      5024.61, 7046.32, 9992.29)
y = c(0, 0.93512, 2.61108, 4.99104, 6.36704, 6.42148,
      6.43643, 6.46792, 6.77215, 6.97391)
fit_data <-data.frame(  t ,y)
plot(fit_data,ylim=c(0,max(y)),xlab="Dose[Gy]",ylab="OSL (L/T)")
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=10, b = 1e-4))
N_fit <- coef(fit)[1]
R_fit <- abs(coef(fit)[2])
b_fit <- coef(fit)[3]
## plot analytical solution
t<- seq(from=0,to=10000,by=100)
lines(  x = t,
y=N_fit*(1+lambertW0((R_fit-1)*exp(R_fit-1-b_fit*t))/(1-R_fit)),
```

```
  col = "blue")
legend("right",bty="n",legend=c("(b)"," ","Coarse grain",
"Quartz"," "))
## print results
cat("\nCoarse grain"," ")
cat("\nfitted N: ", N_fit)
cat("\nfitted R: ", R_fit)
cat("\nfitted Dc: ",round( 1/b_fit,2)," Gy")

  ##
  ## Fine grain
  ## fitted N:  17.57116
  ## fitted R:  0.3971654
  ## fitted Dc:  1325.83 Gy
  ## Coarse grain
  ## fitted N:  6.610193
  ## fitted R:  1.938374e-06
  ## fitted Dc:  403.02  Gy
```

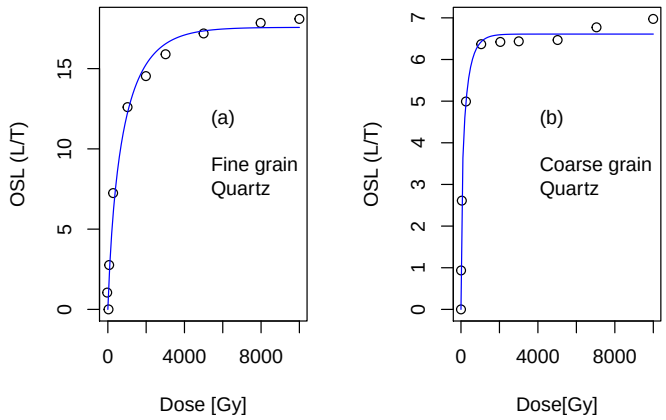

Fig. 4.5: Fit of experimental SAR-OSL experimental dose response data, for (a) fine grain and (b) coarse grain quartz samples, using the Lambert equation. For more details see Pagonis et al. [38], original data by Timar-Gabor et al. [51] (their Figure 3).

Code 4.6: Irradiation of thermally unstable trap (OTOR)

```
# OTOR MODEL- IRRADIATION of thermally unstable trap (OTOR)
rm(list = ls(all=T))
options(warn=-1)
library(lamW)
library("deSolve")
## Plot the numerical solution of OTOR irradiation stage,
## at different irradiation temperatures
t<-0:100
N<-1E10
R<-.1
X<-1e10
E<-1
s<-1e12
kb<-8.617e-5
TISO<-20
p<-s*exp(-E/(kb*(273+TISO)))
# Numerically Solve GOT equation for IRRADIATION  using  deSolve
n.0 <- 0  # initial concentration of filled traps
# Calculate numerical ODE solution
ODE <- function(t, state, parmameters){
  with(as.list(c(state, parameters)),{
    dn <-  ( (N-n) * X*R-(p*(n**2))) / ((N - n) * R + n )
      list(c(dn))  })}
parameters <- c(N=N, X = X, R =R, p=p)
state <- c(n = n.0)
num_ODE <- ode(y = state,times = t,func = ODE,parms=parameters)
plot(x = num_ODE[,1], y = num_ODE[,2]/N,pch=2,ylim=c(0,1.1),
xlab = "Time[s]", ylab = "Trap filling ratio, n/N",type="b",
      col = "red")
# Change the irradiation temperature TISO
TISO<-100
p<-s*exp(-E/(kb*(273+TISO)))
parameters <- c(N=N, X = X, R =R, p=p)
num_ODE2 <- ode(y = state, times = t, func=ODE,parms=parameters)
lines(x = num_ODE2[,1],    y = num_ODE2[,2]/N, pch=3,
col = "Black",type="b")
legend("right",bty="n",pch=c(2,3),expression("T=" ~ 20^o ~C ~"",
"T=" ~ 100^o ~C ~""),col=c("red","black"),lwd=2)
```

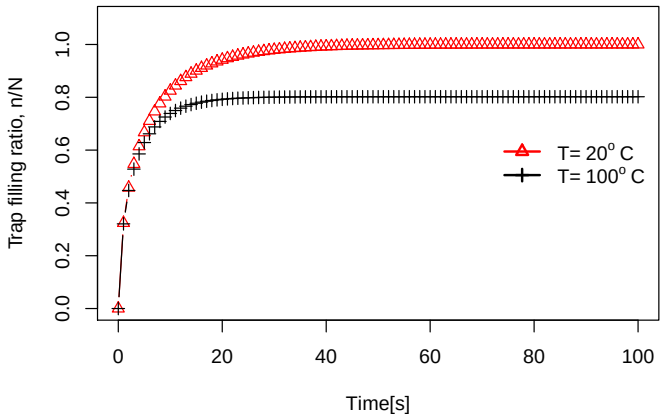

Fig. 4.6: Simulation of the effect of sample temperature during the irradiation process, within the OTOR model. For a more detailed study of this effect, see Chen et al. [7].

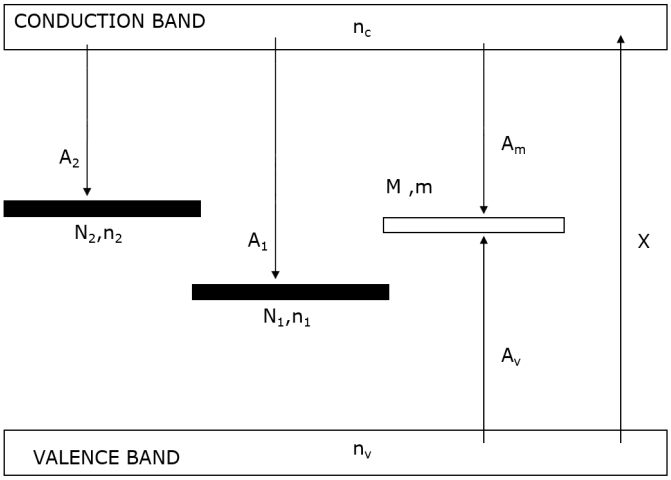

Fig. 4.7: The 2T1C model of Bowman and Chen [4], describing competition effects during the irradiation stage. Various electronic transitions are shown during the irradiation process. Transition X: Creation of electron-hole pairs by radiation. Transitions A_v and A_m: Trapping of holes and recombination of electrons at the recombination centers (RC). Transitions A_1,A_2: Trapping of electrons in the dosimetric and competitor trap. For more details, see Pagonis et al. [39] .

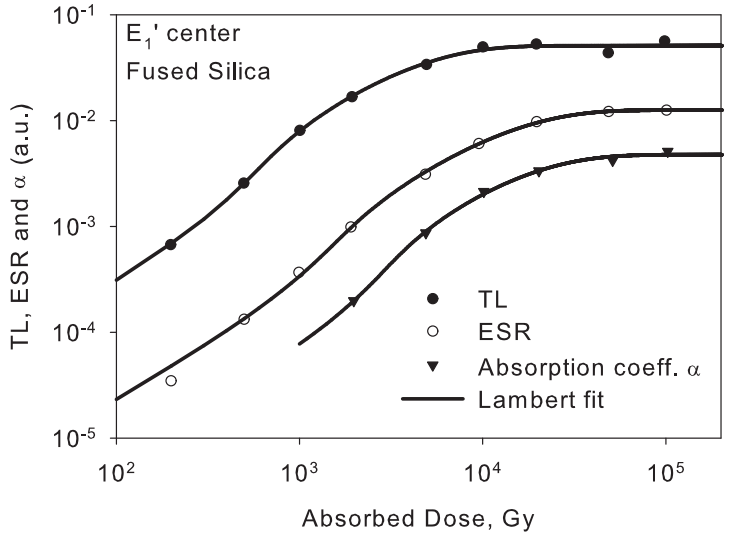

Fig. 4.8: Superlinear dose dependence of the E_1' center concentration (ESR), TL and OA signals, from a single sample of fused silica. Note the log scale in both axes. The solid lines are fitted using the PKC Eq.(**??**). For more details see Pagonis et al. [39], original data from Wieser [53].

Code 4.7: TL dose response of anion deficient aluminum oxide

```
rm(list = ls(all=T))
options(warn=-1)
library("minpack.lm")
library("lamW")
## fit to Pagonis-Kitis-Chen PKC superlinearity equation ----
t=c(0.0537568,0.103385,0.156481,0.211929,0.260776,
0.321015,0.36483,0.414625,0.478926,0.535569,0.589476,
0.638899,0.824344,0.951985,1.18991,1.63688,3.19332)
y=c(6694.89,15592.6,24767.6,39360.5,52176.2,78075.6,
101463,131855,189548,227223,272406,376197,469268,
634929,792121,1.16105e6,1.6992e6)
fit_data <-data.frame(  t ,y)
fit <- minpack.lm::nlsLM(
formula=y~N*(1-(lambertW0(abs(B)*exp(abs(B)-lamda*t))/
abs(B))**beta),
  data = fit_data,
```

```
  start = list(N= max(y),B=5, lamda = 10,beta=0.1))
N_fit <- coef(fit)[1]
B_fit <- coef(fit)[2]
lamda_fit <- coef(fit)[3]
beta_fit <- coef(fit)[4]
## print results
cat("\nfitted N: ", N_fit)
cat("\nfitted B: ", B_fit)
cat("\nfitted Dc: ", round(1/lamda_fit,2)," Gy")
cat("\nfitted beta: ", beta_fit)
## plot analytical solution
t<- seq(from=0,to=4,by=.01)
plot(fit_data,log="xy",xlab="Dose [Gy]",ylab="TL")
legend("topleft",bty="n",legend=c("Nikiforov et al. (2014)",
"Anion-deficient","Aluminum Oxide"))
lines( x = t,
y=N_fit*(1-(lambertW0(abs(B_fit)*exp(abs(B_fit)-lamda_fit*
t))/abs(B_fit))**beta_fit),
       col = "blue",log="xy")

  ##
  ## fitted N:  2095289
  ## fitted B:  6.870824
  ## fitted Dc:  0.05  Gy
  ## fitted beta:  0.02999771
```

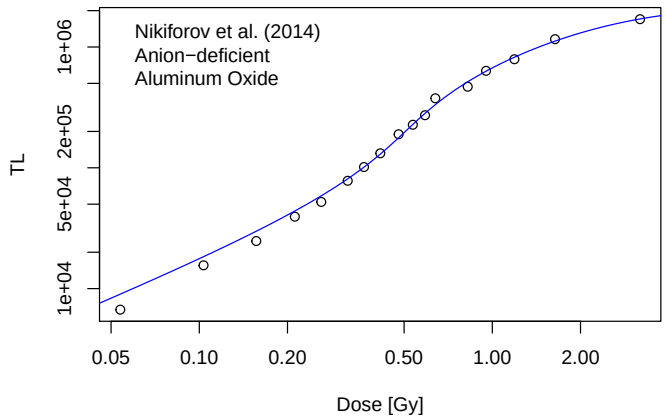

Fig. 4.9: TL dose response of an anion deficient aluminum oxide single crystal, which had low initial sensitivity to irradiation. The superlinear dose response is fitted with the PKC equation. For more details see Nikiforov et al. [26], see also the discussion in Pagonis et al. [39].

Code 4.8: Fit to Supralinearity index f(D) using Lambert W

```
rm(list = ls(all=T))
options(warn=-1)
library("minpack.lm")
library("lamW")
## fit g(D) to Lambert equation ----
t = c(0.0811131, 0.171804,0.450923,0.857988,1.88341,
4.44069,8.44947,17.2683,40.7152,83.2104,176.246,
415.552,819.456,1674.74,3948.68,8983.32)
y = c(1.03326,0.983911,1.08074,1.10465,1.12844,1.28023,
1.37731,1.50481,1.76636,1.79021,1.45428, 0.813382,
0.428722,0.208669,0.0799713,0.0305689)
fit_data <-data.frame(  t ,y)
fit <- minpack.lm::nlsLM(
  formula = y ~ N * (1-(lambertW0(abs(B)*exp(abs(B)- t/Dc))/
  abs(B))**beta)/t,
  data = fit_data,
  start = list(N= max(y),B=1.2, Dc = 5,beta=0.1)
)
N_fit <- coef(fit)[1]
B_fit <- abs(coef(fit)[2])
Dc_fit <- coef(fit)[3]
beta_fit <- coef(fit)[4]
## print results
cat("\nfitted N: ", N_fit)
cat("\nfitted B: ", B_fit)
cat("\nfitted Dc: ", round(Dc_fit,2)," Gy")
cat("\nfitted beta: ", beta_fit)
## plot analytical solution
t<- seq(from=0.01,to=10000,by=.2)
plot(fit_data,log="x",ylab="Supralinearity Index f(D)",
xlab="Irradiation Dose, Gy")
lines( x = t,
y=N_fit*(1-(lambertW0(abs(B_fit)*exp(abs(B_fit)-t/Dc_fit))/
abs(B_fit))**beta_fit)/t,       col = "blue",log="x")
legend("topright",bty="n",legend=c("Edmund (2007)",
```

```
"figure 5.11","Probe A"))

  ##
  ## fitted N:  375.0032
  ## fitted B:  1.237203
  ## fitted Dc:  5.07  Gy
  ## fitted beta:  0.03240109
```

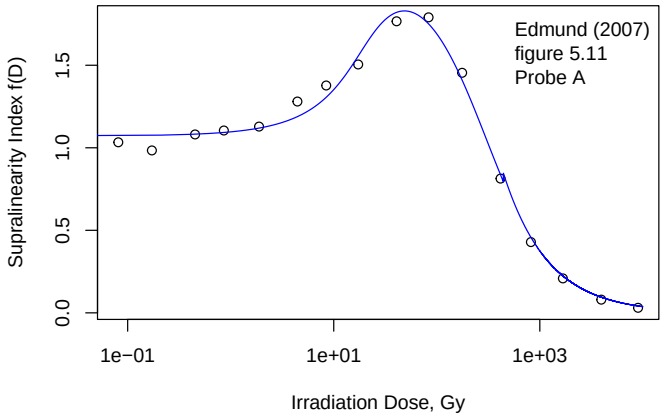

Fig. 4.10: Fit to the superlinear behavior of an Al_2O_3:C probe using the PKC superlinearity equations. For more details of the analysis see Pagonis et al. [39], original experimental data from Edmund [10].