

TLD-MC : ThermoLuminescence Deconvolution in MathCad

Last revised: 2013-06-01

Folder containing the data files: DataFolder := "data"

▢ General _____

▢ Models _____

▢ Temp _____

===== **Experimental data** =====

Click [here](#) for info about accepted file formats.

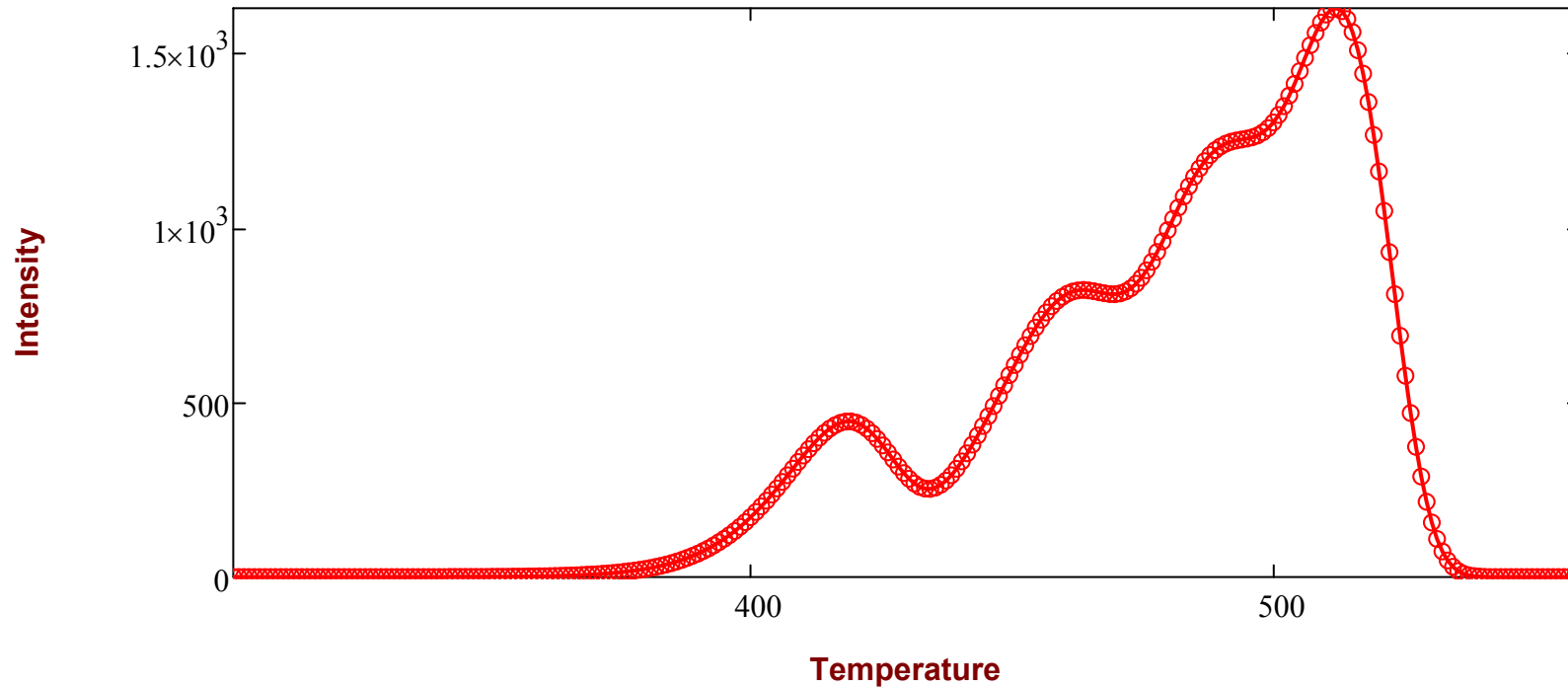
Relative file path is allowed.

Current working directory: CWD = "E:\MyDocs\Worksheets\McadApps\TLD-MC\" .

Options: BETA, T1, T2, TEMPSCALE, XSHIFT, YSHIFT, YSCALE, NORM, SKIP, F
(click [here](#) for more info)

Load := $\begin{pmatrix} \text{FILE} & \text{"sample.dat"} \\ \text{BETA} & 8.4 \end{pmatrix}$

▢ Processing



===== Model selection =====

$$\begin{pmatrix} \text{Model} \\ \text{Background} \end{pmatrix} := \begin{pmatrix} \text{FOK_A1} \\ \text{ZERO} \end{pmatrix}$$

FOK	Randall-Wilkins first-order kinetics (exact)
FOK_A1	First-order kinetics approximation by Kitis et al.
FOK_A2	First-order kinetics approximation by a quotient of polynomials
FOK_A3	First-order kinetics approximation by Podgorsak et al.
FOK_W	First-order kinetics approximation by Weibull distribution
SOK	Garlick-Gibson second-order kinetics (exact)
SOK_A1	Second-order kinetics approximation by Kitis et al.
GOK	May-Partridge general-order kinetics (exact)
GOK_A1	General-order kinetics approximation by Kitis et al.
MOK	Mixed-order kinetics (exact)
GA	General approximation (independent traps)
CGA	General approximation (coupled traps)

Background functions:

ZERO	Zero
CONSTANT	A constant value (e.g. detector dark signal).
EXP	Exponential $y(x) = B_1 + B_2 \cdot \exp(B_3 \cdot x)$
POLY	Polynomial $y(x) = B_1 + B_2 \cdot x + B_3 \cdot x^2 + \dots$

===== Parameter initialization =====

Each column of guess values contains ordered data for single trap

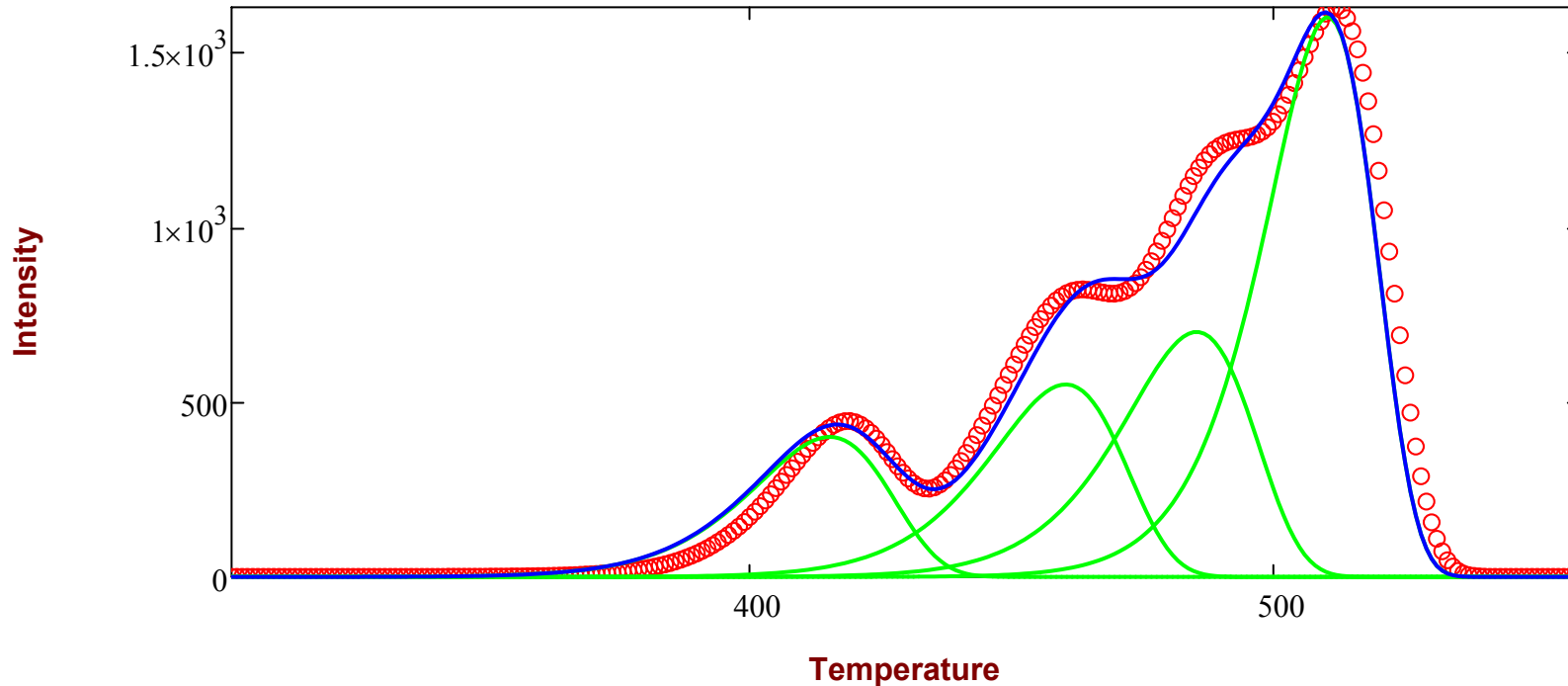
GuessValues := $\begin{pmatrix} 1.1 & 1.4 & 1.6 & 2.1 \\ 415 & 460 & 485 & 510 \\ 400 & 550 & 700 & 1600 \end{pmatrix}$

Info = $\begin{pmatrix} "E" & "Activation\ energy\ (eV)" \\ "Tm" & "Peak\ temperature\ (K)" \\ "Im" & "Peak\ intensity\ (a.u.)" \end{pmatrix}$

BkgGuessValues := 0

▢ Processing

FOM = 10.0515·%



▢ Archive

▢ Processing

===== **Constraints** =====

Predefined functions: Energy(P), PeakTemp(P), PeakInt(P), Dose(P), Traps(P), Freq(P), Order(P), Alpha(P), Deep(P) and Retrap(P). s, b, α , M and R are represented by their natural log. Click [here](#) for more info.

▾ Processing

===== **Optimized result** =====

If necessary, copy-paste the parameter matrix as new input to repeat optimization

OptimizedValues = $\begin{pmatrix} 1.382328 & 1.48185 & 1.581807 & 2.001031 \\ 417.185399 & 456.522684 & 484.011703 & 511.668348 \\ 398.154476 & 543.139247 & 835.592463 & 1623.056803 \end{pmatrix}$

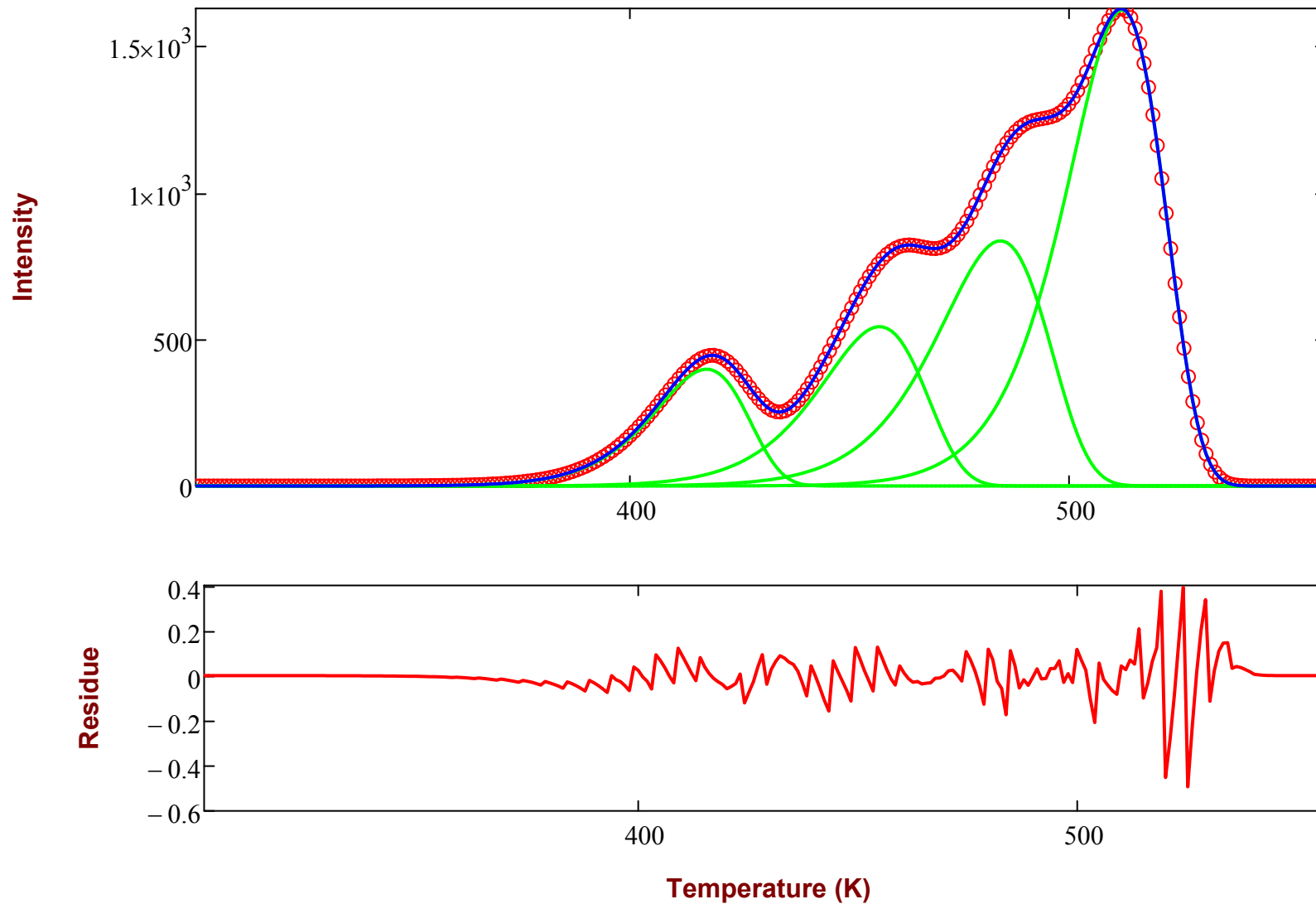
OptimizedBkg = 0

▾ Archive

▾ Processing

FOM = 0.01105·%

Full report was written to the file ReportFile = "data\sample.FOK_A1.report"
Glow curves were written to the file PeaksFile = "data\sample.FOK_A1.fit"



===== End of Program =====