Python in stimulated luminescence: a further step in dose response fitting

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Introduction

Recently, Pagonis et al. (2020a, 2020b) formulated two analytical expressions with the use of Lambert W function, derived from the phenomenological models; the one trap one re-combination (OTOR) and two trap one recombination (TTOR) center models. By utilizing the supralinearity index (f(D)) in both cases, they managed to accurately fit a plethora of TL/OSL dose response curves (Pagonis et al., 2020b). Moreover, a new flexible approach for mathematical formulation of stimulated luminescence phenomena was presented by Prevezanou et al. (2022). The present study presents Python scripts carry out the simultaneous fittings of both dose response and the supralinearity index f(D), that result in better understanding of the competition and the non-linear effects. Another aim of this work is the implementation of Lambert W function in routine equivalent dose estimations, using the corrected OSL dose response curves of the highly applied Single Aliquot Regenerative (SAR) dose protocol (Murray & Wintle, 2000).

Methodology

In the simpler OTOR model, the trap filling during irradiation is described by the expression n=N{1- $\frac{W[Z1]}{R-1}$}, where $Z_1=Z_R\exp(-D/D_C)$ with $Z_R=(R-1)\exp(R-1)$. Finally, using the equation f(D)= $\frac{S(D)/D}{S(D1)/D1}$ eq.(1), where D1 is a normalization dose in the initial linear range, we get the expressions for the supralinearity index f(D), presented in Table 1.

The Python codes that include the analytical expressions described in table 1 for the OTOR and TTOR models are available in GitHub (https://github.com/GeorgiaKiose/Dose-response-stimulated luminescence). The SciPy library has been imported for the fitting, using the function *optimization.curve_fit*, while the supralinearity index f(D) is calculated through the embedded in Python scripts eq.(1).

Table 1 Analytical expressions used for the two models.

OTOR	TTOR
$\frac{n(D)}{N} = 1+\frac{W[(R-1)\exp(R-1-\frac{R}{D_c})]}{1-R}$	$\frac{n_2}{N_2} = 1-\left(\frac{1}{B}W\left[B\exp(B)\exp\left(-\frac{D}{Dc}\right)\right]\right)^{\frac{A2}{A1}}$
$f(D)=\frac{1}{kD}\left(1-\frac{W[Z_1]}{R-1}\right)$, with $k=\frac{1}{(R-1)Dc}\frac{W[Z_R]}{1+W[Z_R]}$	$f(D)=\frac{1}{kD}\left[1-\left(\frac{W[Z_2]}{B}\right)^a\right]$, with $k=\left(\frac{1}{B}\right)^a\frac{a}{Dc}\frac{W[z_B]^a}{1+W[z_B]}$
$ED=-Dc\left[\frac{HB}{Io-1}(1-R)+\log\left(\frac{\frac{HB}{Io-1}(1-R)}{(R-1)\exp(R-1)}\right)\right]$	$ED=-Dc\left[B\left(1-\frac{HB}{Io}\right)^{1/A1}+\log\frac{B\left(1-\frac{HB}{Io}\right)^{1/A1}}{B\exp(B)}\right]$

Table 2 Parameters included in the analytical expressions of the two models.

OTOR	Units	Fitting Parms
Trap filling ratio: n(D)/N	-	X
Retrapping ratio: R=An/Am<1	-	√
Saturation dose: Dc=N/R>0	Rad/Gy	√
Retrapping coefficient of electrons: An	cm^3s^{-1}	X
Recombination coefficient of electrons: Am	cm^3s^{-1}	X
Total concentrations of trapping states: N	cm^{-3}	X
TTOR		
Parameter B= $\frac{N_1(A_1-A_m)}{A_2N_2+A_mN_1}$ >0	-	√
Parameter Dc= $\frac{A_2N_2+A_mN_1}{A_1}$ >0	Rad/Gy	√
Ratio of trapping coefficients of the two competing traps: a=A2/A1<1	-	√
Total concentrations of the two trapping states: N1, N2	cm^{-3}	X
Equivelent dose: ED	Rad/Gy	X

Results

The results showed that analytical equations fit simultaneously and excellently the whole simulated TL/OSL dose response and the resulted f(D) curves behavior.

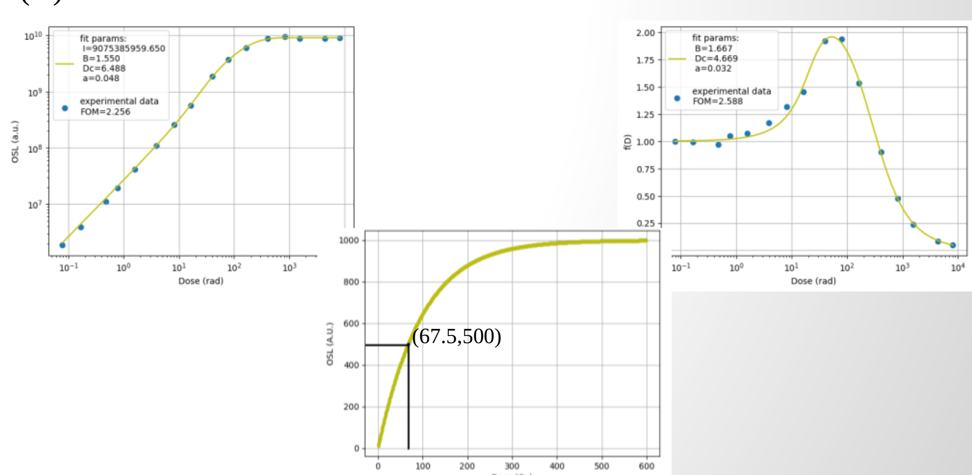

Fig.1 *(a) Fitting of the dose response and (b) the resulted f(D) curve using the TTOR model and (c) the equivalent dose estimation.*

Conclusion

The theoretical expressions of the two models were implemented with great precision in Python and has been successfully used to fit the experimental data, allowing thus to estimate much larger, than usual, equivalent doses. The estimated equivalent dose using the Lambert-W function not only is not empirical, but also incorporates lower dose, especially for the cases when the equivalent dose is located in the saturation dose region.

References

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