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# OSLThermo and ESRThermo: Libraries of codes for trapped-charge thermochronometry

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20 **Abstract.** Over the past fifteen years, trapped-charge (T-C) thermochronometry has been established as an ultra-low temperature (<80 °C) thermochronometric system. Its novelty is its ability to resolve rock cooling within the final few km of Earth's surface, as well as rock-surface temperature changes since the Last Glacial Maximum to the present day. Deriving temperature histories from the luminescence signals of feldspar minerals, or the electron spin resonance signals of quartz minerals, requires the modelling of both signal accumulation and signal loss in response to mineral exposure to ionizing radiation and temperature, as well as athermal signal losses for feldspar minerals. Two open-source libraries have been developed in MATLAB that allow different numerical models to be used for this purpose; the first is applicable to the infrared stimulated luminescence (IRSL) of feldspar minerals (OSLThermo) and the second to the electron spin resonance (ESR) signal of quartz minerals (ESRThermo). These libraries have been made available in GITHUB and this contribution describes their broad structure, the T-C models that have been implemented and their practical use.

Codes are available for download on GitHub: <a href="https://github.com/GeorginaKing/OSLThermo">https://github.com/GeorginaKing/OSLThermo</a> for luminescence thermochronometry & <a href="https://github.com/GeorginaKing/ESRThermo">https://github.com/GeorginaKing/ESRThermo</a> for ESR thermochronometry.

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## 1 Introduction

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The development of trapped-charge thermochronometry over the past fifteen years (e.g., Herman et al., 2010; Guralnik et al., 2015a; Wu et al., 2015; King et al., 2016a; Brown et al., 2017; Biswas et al., 2018; King et al., 2020; Zhang et al., 2025) and recent investigations of trapped-charge thermometry (e.g., Guralnik and Sohbati, 2019; Biswas et al., 2020) have built upon both previous applications of the method (e.g., Houtermans et al., 1957; Ronca and Zeller, 1965; Grün et al., 1999) and earlier fundamental research describing the accumulation and loss of trapped-charge signals (e.g., Prokein and Wagner, 1994; Toyoda and Ikeya, 1991). The premise of the technique is that, as the luminescence and electron spin resonance (ESR) signals of feldspar and quartz minerals are thermally sensitive, they can be used to determine temperature histories. Temperature changes occur, for example, as rocks are exhumed towards the Earth's surface (e.g., King et al., 2016c; Bouscary et al., 2024), or as atmospheric temperature changes due to climatic variations and affects rock surface temperatures (e.g., Guralnik and Sohbati, 2019; Biswas et al., 2020).

Luminescence and ESR thermochronometry have been applied in a variety of settings to determine rock-thermal histories, including the Southern Alps of New Zealand (Herman et al., 2010), the Himalayas (De Sarkar et al., 2013; King et al., 2016c; Bouscary et al., 2024), the European Alps (Lambert, 2018; Wen et al., 2024), Taiwan (Wu et al., 2015), the Chilean Andes (Stalder et al., 2022), and in the Japanese Alps (King et al., 2023; Bartz et al., 2024) and alpine foreland (Ogata et al., 2022). Recent reviews are given by King et al. (2016b) and Herman and King (2018).

Luminescence and ESR thermochronometry rely on the combination of laboratory measurements with numerical models, that allows the conversion of trapped-charge concentrations into thermal histories. Two or three laboratory experiments are typically used to build an ESR or luminescence thermochronometry measurement, respectively (e.g., Herman et al., 2010; Guralnik et al., 2015b; King et al., 2016a; Biswas et al., 2018; Fang and Grün, 2020; King et al., 2020) (Fig. 1). The first experiment (Fig. 1B and Fig. 1E) measures the concentration of trapped charge within the sample, and is usually done using a single aliquot regenerative dose method (e.g., Murray and Wintle, 2000; Tsukamoto et al., 2015). The measurement comprises construction of a sample-specific calibration curve, for sample signal response to laboratory irradiation, known as a dose response curve (DRC). As trapped-charge thermochronometry data are often described as saturation ratios, i.e. the proportion of electrons trapped (n) relative to the maximum possible number of trapped electrons (N), laboratory DRC are generally measured until signal saturation (i.e. no further increase in sample signal for increasing dose). For some samples, the exceptionally high saturation level of the quartz ESR Al-centre makes this impractical, and for this signal, the system may be treated as non-saturating (e.g., King et al., 2020). The second experiment (Fig. 1C and Fig. 1F) measures the thermal decay of the luminescence or ESR signals in response to temperature. Generally, it comprises an isothermal decay experiment whereby signal loss relative to a fixed temperature is measured following different isothermal heating durations (e.g., Bouscary and King, 2022). The final experiment is only applicable to the luminescence of feldspar minerals and consists of measuring the rate of anomalous fading (Wintle, 1973; Visocekas et al., 1994) by measuring signal loss at ambient temperature following different delay durations (Fig. 1A).



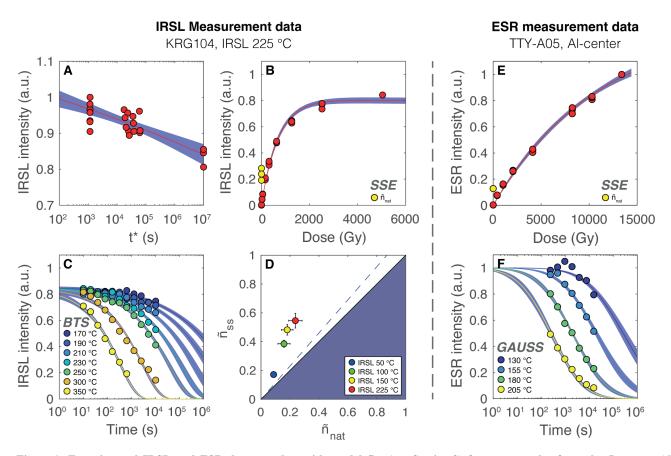


Figure 1: Experimental IRSL and ESR data together with model fits (see Section 2) for two samples from the Japanese Alps. (A) Athermal signal loss, (B) dose response, (C) and isothermal decay for the IRSL<sub>225</sub> signal of the K-feldspar extract of sample KRG104 (King et al., 2020). (D) Comparison of luminescence natural saturation ratios,  $\tilde{n}_{nat}$ , with those calculated for athermal steady state,  $\tilde{n}_{ss}$ , (dashed line indicates 15% deviation from unity) for the four IRSL signals of sample KRG104. (E) Dose response and (F) isothermal decay for the Al-centre of sample TTY-A05 (Bartz et al., 2024).

Fitting these experimental data using models that describe signal accumulation, thermal or athermal decay, allows the experimental data to be reduced to several kinetic parameters, as illustrated in Eq. (1):

$$\frac{\mathrm{d}\tilde{n}}{\mathrm{d}t} = \frac{\dot{p}}{D_0} \left( 1 - \tilde{n} \right)^{\alpha} - s \, \tilde{n}^{\beta} \, e^{\left( \frac{-E_a}{k_B T} \right)} - \tilde{s} \, \tilde{n} \, e^{\left( -\rho'^{-\frac{1}{3}} r' \right)} \tag{1}$$

The trapped-charge population  $\tilde{n}$  at a given time t (Ma) is given by three terms. The first term on the right-hand side of the equation describes trapped-charge accumulation where  $\dot{D}$  (Gy·Ma<sup>-1</sup>) is the environmental dose rate,  $D_0$  (Gy) is the characteristic dose of saturation and  $\alpha$  is an exponent  $\geq 1$ , depending on whether electron trapping is described as first ( $\alpha = 1$ ) or general ( $\alpha > 1$ ) order. The second term describes thermal loss at a given temperature, T (K), where s (s<sup>-1</sup>) is the frequency factor,  $E_a$  (eV) is the activation energy of the electron trap,  $k_B$  (eV·K<sup>-1</sup>) is the Boltzmann constant, and  $\beta$  the order of kinetics

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 $\geq$ 1. The final term describes athermal loss where  $\tilde{s}$  (3 x 10<sup>-15</sup> s<sup>-1</sup>) is a frequency factor,  $\rho'$  is a dimensionless description of the density of recombination centres and r' is a dimensionless distance between traps and recombination centres (Huntley, 2006). A variety of different models describing signal accumulation and athermal or thermal signal loss have been investigated for use in trapped-charge thermochronometry/thermometry applications (e.g., Guralnik et al., 2015b; Biswas et al., 2018; Lambert, 2018; Biswas et al., 2020; King et al., 2020), and have been validated against data collected in the laboratory as well as independent temperature measurements (e.g., Lambert, 2018; Bouscary and King, 2022). These kinetic parameters can then be used together with Eq. (1), to predict a trapped-charge concentration for a particular time-temperature history, allowing the natural trapped charge concentration of a sample to be inverted for its thermal history.

In this contribution, we present two MATLAB libraries, OSLThermo and ESRThermo, that are available for the processing of trapped-charge thermochronometry data. We first outline the T-C models implemented in the codes and then describe the structure of the OSLThermo and ESRThermo libraries as well as the required input format of experimental data. Note that we do not comment on the suitability of different models for specific datasets, but rather list those models that have been implemented in the libraries at present. We anticipate that these libraries will be further updated in the future.

## 95 2 Model overview

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In this section, the specific T-C models implemented in the OSLThermo and ESRThermo libraries are described. Although athermal signal losses are often not measured first, here we begin with fitting these data as athermal losses must also be accounted for when constraining the trapped-charge concentration and fitting isothermal decay data of feldspar minerals in the OSLThermo library.

## 100 2.1 Athermal signal loss (OSLThermo library only)

Athermal signal losses are known to affect the luminescence of feldspar minerals (Visocekas et al., 1994) and must be accounted for when fitting luminescence data to derive the kinetic parameters of signal dose response and thermal decay. The OSLThermo library uses the model of Huntley (2006), as implemented by Kars et al. (2008), to compute the natural dose response curve of feldspar signals by correcting the data for athermal fading, and to calculate the natural steady-state luminescence signal,  $\tilde{n}_{ss}$ . This signal is expressed as the ratio between the trapped-charge concentration, n, and the maximum possible trapped-charge concentration in the absence of anomalous fading, N. Signal saturation is the main limitation of luminescence thermochronometry (e.g., Valla et al., 2016), and accurate screening of luminescence signals for saturation is essential.

The rate of anomalous fading induced signal loss can be calculated from:

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$$n(t^*) = n(0) \cdot \varphi(t^*)$$
 (2)

where n(0) is the initial trapped-charge concentration at time 0,  $n(t^*)$  is the signal remaining after fading time  $t^*(s)$ , which is calculated following Appendix F of Aitken (1985), and





$$\varphi(t^*) = e^{-\rho' \ln{(1.8\,\tilde{s}\,t^*)^3}} \tag{3}$$

in which  $\rho' \equiv \frac{4\pi\rho}{3\alpha^3}$ , where  $\rho$  is the density of recombination centres and  $\alpha$  is a constant (Huntley, 2006; Kars et al., 2008).

To compute the athermal steady-state value of feldspar luminescence signals,  $\tilde{n}_{ss}$ , the following equation is used (Li and Li, 2008; King et al., 2016a):

$$\tilde{n}_{SS} = \int_{r'=0}^{\infty} \frac{3 r'^2 e^{-r'^3}}{1 + \frac{D_0}{2} \tilde{s} e^{-\rho'} \frac{1}{3} r'} dr'$$
(4)

where the dimensionless distance  $r' \equiv \left\{\frac{4\pi\rho}{3}\right\}^{\frac{1}{3}}r$ , with r the tunnelling distance from a trap to a recombination centre, and the probability that the nearest recombination centre is at a distance between r' and r' + dr' is given by  $p(r')dr' = 3r'^2e^{-r'^3}dr'$  (Huntley, 2006).

## 2.2 Signal growth

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Trapped-charge signals accumulate in response to the exposure of feldspar and quartz minerals to ionizing radiation. Various models have been proposed for luminescence and ESR signal growth. In the OSLThermo library, the single-saturating exponential (SSE; Apers et al., 1981) and general order kinetic (GOK; Guralnik et al., 2015b) growth functions have been implemented. In the ESRThermo library in addition to SSE and GOK, a linear (LIN) growth function has also been implemented for signals that do not appear to experience saturation (King et al., 2020).

In trapped-charge thermochronometry, the saturation ratio of the centre under investigation is usually considered, rather than the age, consequently,  $\tilde{n}$  ratios are calculated for all of the signal growth fitting options with the exception of the LIN model, where N, the maximum possible trapped-charge concentration, cannot be constrained, and  $\tilde{n}$  thus only represents the trapped-charge population. For this model, rather the total dose, D (Gy), accumulated, i.e., the equivalent dose,  $D_e$  (Gy), of the natural sample is considered.

The different dose response models are given below:

(i) Single saturating exponential (SSE) growth

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$$\tilde{n}(t) = \varphi(t^*) \cdot A\left(1 - e^{-\frac{\dot{D}_{lab}t}{D_0}}\right)$$
 (5)

where  $\tilde{n}(t)$  is the ratio of trapped electrons at time t (s), A is a pre-exponential multiplier,  $\dot{D}_{lab}$  (Gy·s<sup>-1</sup>) is the laboratory dose rate and  $\varphi$  accounts for athermal detrapping (Eq. (2) and Eq. (3)). Note that athermal detrapping is only applicable for luminescence signals from feldspar and this term is not incorporated in the ESRThermo library. Single saturating exponential fits have been used previously to fit both luminescence (e.g., Herman et al., 2010) and ESR (e.g., Grün et al., 1999) thermochronometry data.





(ii) General order kinetic (GOK) growth

$$\tilde{n}(t) = \varphi(t^*) \cdot A \left( 1 - \left( 1 + \left( \frac{\dot{D}_{lab}}{D_0} \right) c \ t \right) \right)^{-\frac{1}{c}} \tag{6}$$

Where the kinetic order of trapping,  $\alpha = c + 1$  (Guralnik et al., 2015b). General order kinetic models have been used to fit both IRSL (e.g., Guralnik et al., 2015a; Lambert, 2018) and thermoluminescence data (Biswas et al., 2018).

(iii) Linear (LIN) growth

$$\tilde{n}(t) \approx D_e(t) = t \, \dot{D}$$
 (7)

Linear growth has been used to describe the ESR response of the Al-centre within the context of ESR-thermochronometry (King et al., 2020).

## 2.3 Thermal signal loss

The thermal sensitivity of trapped-charge signals is well known (e.g., Aitken, 1985). The following models have been implemented in the OSLThermo and ESRThermo libraries: (i) the band-tail states model (BTS; Li and Li, 2013), (ii) the general order kinetics model (GOK; Guralnik et al., 2015a), and (iii) the Gaussian distribution model (GAUSS; Lambert, 2018). The mathematical basis of the models is described below:

(i) Band-tail states (BTS)

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$$\frac{n(t)}{n(0)} = \varphi(t^*) \cdot \int_0^{E_t} P(E_b) e^{\left(-s t e^{-\frac{E_t - E_b}{k_B T}}\right)} dE_b$$
 (8)

where  $E_t$  (eV) is the trap depth of the electron trap, and  $E_b$  (eV) is the depth of the band-tail state below the conduction band. The probability of thermally evicting electrons into band-tail states of energy in the range of  $E_b + dE_b$ ,  $P(E_b) dE_b$ , is given by (Poolton et al., 2009; Li and Li, 2013):

$$P(E_b) dE_b = C e^{\left(-\frac{E_b}{E_u}\right)} dE_b \tag{9}$$

where C is a pre-exponential multiplier and  $E_u$  (eV) is the width of the Urbach tail. King et al. (2016a; 2016c), Herman and King (2018), King et al. (2020), Bouscary and King (2022) and Ogata et al. (2022) used the BTS model to describe their multiluminescence-thermochronometry data from feldspar minerals.

(ii) General order kinetics (GOK)

$$\frac{n(t)}{n(0)} = \varphi(t^*) \cdot \left[ n(0)^{1-\beta} - (1-\beta) s t e^{-\frac{E_t}{k_B T}} \right]^{\frac{1}{1-\beta}}$$
 (10)





Note that if the kinetic order,  $\beta$ , is fixed at 1 or 2, the model reverts to first-order or second-order kinetics respectively. Guralnik et al. (2015b) used GOK thermal decay to fit their infra-red stimulated luminescence thermochronometry for samples from the KTB borehole, whilst Biswas et al. (2018) and Stalder et al. (2022) used a similar approach to fit their thermoluminescence thermochronometry data. Wu et al. (2015) employed first-order kinetics to fit quartz luminescence data for samples from Taiwan, while Toyoda and Ikeya (1991) used second-order kinetics to describe the thermal decay of the ESR Al- and Ticentres of quartz minerals, noting their potential for thermochronometry.

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(iii) Gaussian distribution model (GAUSS)

The GAUSS distribution model assumes a Gaussian distribution of trap depths, with mean trap depth  $\mu(E_t)$  (eV) and width  $\sigma(E_t)$  (eV) (Lambert, 2018), with:

$$\frac{n(t)}{n(0)} = \varphi(t^*) \cdot \int_0^{E_a(max)} P_t(E_t) e^{\left(-s t e^{-\frac{E_t}{k_B T}}\right)} dE_t$$
 (11)

where  $E_a(max)$  is arbitrarily set to 9 eV, corresponding to the maximum optical bandgap for amorphous quartz (DiStefano and Eastman, 1971), and the probability of eviction  $P_t(E_t)$  given by:

$$P_t(E_t) = \frac{1}{\sigma(E_t)\sqrt{2\pi}} e^{\left(-\frac{1}{2}\left(\frac{E_t - \mu(E_t)}{\sigma(E_t)}\right)^2\right)}$$
(12)

Lambert (2018) used the GAUSS model to describe thermal losses from the IRSL signals of feldspar minerals from the Mont Blanc massif, whilst King et al. (2020) and Bartz et al. (2024) used the GAUSS model to describe thermal signal losses from the ESR Al- and Ti-centres of quartz samples from Japan.

## 2.4 Data inversion

Using the kinetic parameters derived from fitting experimental data with the T-C models described above, it is possible to use the rate equation Eq. (1) to invert for a thermal history. For the luminescence of feldspar, the model must be integrated over the range of recombination centre distances r' and, for the BTS and GAUSS models, over the range of activation energies  $E_a$  described by Eq. (8) and Eq. (11) (where  $E_a = E_t - E_b$  for the BTS model, and  $E_a = E_t - \mu(E_t)$  for the GAUSS model). For quartz ESR data, as quartz minerals do not experience athermal fading, the third term on the right-hand side of the equation can be discarded. In this case, it is only necessary to integrate over the range of activation energies:

$$\frac{\mathrm{d}\tilde{n}}{\mathrm{d}t} = \frac{\dot{D}}{D_0} (1 - \tilde{n})^{\alpha} - s \, \tilde{n}^{\beta} \, e^{\left(-\frac{E_t}{k_B T}\right)} \tag{13}$$

Finally for a non-saturating system exhibiting linear dose response, Eq. (14) is used:

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$$\frac{\mathrm{d}\tilde{n}}{\mathrm{d}t} \approx \frac{\mathrm{d}D}{\mathrm{d}t} = \dot{D} - s D e^{\left(-\frac{E_t - \mu(E_t)}{k_B T}\right)} \tag{14}$$



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### 3 Structure of OSLThermo and ESRThermo

The two libraries described here are structured in a similar manner (Table 1), that allows the input of partially processed trapped-charge data into MATLAB. Each library can be divided into two main parts: data fitting and inversion. Data fitting relates to the derivation of the kinetic parameters that describe signal growth and decay, and inversion to using these parameters to predict thermal histories from the natural trapped-charge concentrations of the sample under investigation (Table 1).

Table 1: Overview of the structure of the OSLThermo and ESRThermo libraries.

|              | Script name           | Description   | Output                                   |  |
|--------------|-----------------------|---|--|--|
|              | OSLThermo/            | The main script that calls the other scripts, where the | Depends on the scripts that are run (see |  |
| Data fitting | ESRThermo             | user selects the T-C models to use and which scripts    | Stage1 to Stage4b below).                |  |
|              |                       | to run (see Stage1 to Stage4b below).                   |  |  |
|              | Stage1_ExceltoStruct  | Uploads the data from a pre-defined Excel               | filename.mat containing structure,       |  |
|              |                       | spreadsheet format (see Fig. 2).                        | 'records', of the raw data               |  |
|              | Stage2a_Fitparameters | Fits the raw data with the selected T-C models to       | fitpar.mat containing structure,         |  |
|              |                       | obtain kinetic parameters.                              | 'records.params', of the kinetic         |  |
|              |                       |   | parameters                               |  |
|              | Stage2b_PlotFit       | Plots raw data with model fits.                         | Figures of the data fitting (see Fig. 1) |  |
|              | Stage3a_Invesion      | Inverts for a cooling history using the selected T-C    | 'Tt.mat', structure containing the       |  |
|              |                       | models and output from Stage2a.                         | inversion results                        |  |
| ü            | Stage3b_PlotTt        | Plots cooling inversion results.                        | Figures of the cooling inversion results |  |
| Inversion    |                       |   | (see Fig. 3)                             |  |
|              | Stage4a_InversionExh  | Inverts for exhumation rate using the selected T-C      | 'Zt.mat', structure containing the       |  |
|              |                       | models and output from Stage2a.                         | inversion results                        |  |
|              | Stage4b_PlotExh       | Plots exhumation inversion results.                     | Figures of the exhumation inversion      |  |
|              |                       |   | results (see Fig. 4)                     |  |

## 4 Experimental data

The OSLThermo and ESRThermo libraries are designed for the following three experimental data types but could be modified for different types of experimental data if required. (i) Luminescence or ESR dose response data measured in a regenerative dose protocol until saturation (except in the case of some ESR Al-centre signals that do not saturate at laboratory doses), i.e. the luminescence or ESR response to a range of laboratory irradiation doses including zero dose. The laboratory irradiation source dose rate (Gy·s·¹) must be listed in the data input file, as well as the irradiation times (ks) (Fig. 2). (ii) Isothermal decay data for a minimum of one isothermal holding temperature, however, we strongly recommend including at least two isothermal holding temperatures. Using only one isothermal holding temperature often results on large and poorly constrained errors in the derived thermal kinetic parameters, whereas two or more temperatures significantly improve the accuracy and reliability of the fit. The isothermal holding temperatures (°C) must be listed in the data input file together with the isothermal holding times (ks) (Fig. 2). (iii) Anomalous fading data for feldspar luminescence data only. The fading time (ks), derived from the irradiation times and the time delay between irradiation and the start of the trapped-charge measurement, should be calculated



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following Appendix F of Aitken (1985). These times can be directly extracted from the t\* (hrs) values given in Analyst (see Duller, 2018).

The data format for the Excel data input file is shown in Fig. 2 for an example luminescence sample. The background subtracted integrated signals for each of the measurements (e.g., Lx/Tx values for luminescence) should be input into the Excel spreadsheet for each measurement point. Templates populated with the example data shown here are available for download from GitHub [https://github.com/GeorginaKing/OSLThermo & https://github.com/GeorginaKing/ESRThermo, "Data" folder]. Where fewer dose response, isothermal holding temperatures, or athermal fading data have been measured, the rows should be deleted and the values of 'nSAR' (number of measurements or aliquots measured for dose response curve measurements), 'nITH' (number of isothermal temperatures used in the isothermal holding experiment), and 'nFAD' (number of aliquots measured for athermal fading for IRSL) updated in the OSLThermo/ESRThermo script (see Section 5.1). This spreadsheet (Fig. 2) must be saved in the "Data" folder of the MATLAB library so that it can be called by the script Stage1\_ExcelToStruct script (see Table 1 and further details below). It should then only be necessary for the user to modify the OSLThermo/ESRThermo script to read in, fit and invert their data.

|  | A B                     |                     | С  | D                              | E      | F      | G         | Н            | 1             | J         | K      | L      | M      | N     | 0    |
|--|-------------------------|---------------------|--|--------------------------------|--------|--------|-----------|--------------|---------------|-----------|--------|--------|--------|-------|------|
| Samp   | ole                     | (KRG104)            |  | Signal (type, temperature) IRS |        | (IRSL  | 225)—     | — Туре с     | of signal mea | asured    |        |        |        |       |      |
| Natu   | tural T (°C)            |                     | (10.0 2.0)—— Average surface temperature and uncertainty |                                |        |        |           |              |               |           |        |        |        |       |      |
| Natu   | ral Ď (Gy/ka)           | Sample              | e name   | (6.16                          | 0.83)  | Env    | ironmenta | al dose rate | and und       | certainty |        |        |        |       |      |
| Labc   | alibration:             |                     |  |                                |        |        |           |              |               |           |        |        |        |       |      |
|  | <b>T(°C)</b> 15         |                     | t (ks)   | Nat                            | 0.000  | 0.250  | 0.500     | 1.500        | 3.000         | 6.000     | 12.000 | 24.000 | 48.000 | 0.000 | 0.2  |
| Ĺ  | <b>Ö (Gy/s)</b> 0.105   | Se                  | $L_x/T_x$  | 1.154                          | 0.004  | 0.283  | 0.518     | 1.196        | 1.951         | 2.878     | 3.905  | 4.653  | 5.087  | 0.016 | 0.2  |
|  | <b>T(°C)</b> 15         | Dose response       | t (ks)   | Nat                            | 0.000  | 0.250  | 0.500     | 1.500        | 3.000         | 6.000     | 12.000 | 24.000 | 48.000 | 0.000 | 0.2  |
| Ĺ  | <b>Ó (Gy/s)</b> 0.105   | _00 ds_             | $L_x/T_x$  | 1.778                          | 0.006  | 0.281  | 0.519     | 1.219        | 1.928         | 3.009     | 3.949  | 4.623  | 5.294  | 0.020 | 0.2  |
|  | <b>T(°C)</b> 15         | 9                   | t (ks)   | Nat                            | 0.000  | 0.250  | 0.500     | 1.500        | 3.000         | 6.000     | 12.000 | 24.000 | 48.000 | 0.000 | 0.2  |
| Ĺ  | <b>Ö (Gy/s)</b> 0.105   |                     | $L_x/T_x$  | 1.410                          | 0.008  | 0.264  | 0.493     | 1.238        | 1.987         | 2.889     | 3.778  | 4.590  | 4.976  | 0.022 | 0.2  |
|  | <b>T(°C)</b> 170        |                     | t (ks)   | 0.000                          | 0.010  | 0.020  | 0.040     | 0.080        | 0.160         | 0.320     | 0.640  | 1.280  | 2.560  | 5.120 | 10.2 |
| Ĺ  | <b>Ö (Gy/s)</b> 0.105   |                     | L <sub>x</sub> /T <sub>x</sub>                           | 0.928                          | 0.931  | 0.916  | 0.915     | 0.917        | 0.901         | 0.906     | 0.924  | 0.895  | 0.879  | 0.825 | 0.8  |
|  | <b>T(°C)</b> 190        |                     | t (ks)   | 0.000                          | 0.010  | 0.020  | 0.040     | 0.080        | 0.160         | 0.320     | 0.640  | 1.280  | 2.560  | 5.120 | 10.2 |
| Ĺ  | <b>Ö (Gy/s)</b> 0.105   |                     | L <sub>x</sub> /T <sub>x</sub>                           | 0.956                          | 0.929  | 0.911  | 0.910     | 0.917        | 0.924         | 0.917     | 0.860  | 0.868  | 0.827  | 0.828 | 0.8  |
|  | <b>T(°C)</b> 210        | _                   | t (ks)   | 0.000                          | 0.010  | 0.020  | 0.040     | 0.080        | 0.160         | 0.320     | 0.640  | 1.280  | 2.560  | 5.120 | 10.  |
| Ĺ  | <b>Ö (Gy/s)</b> 0.105   | sothermal<br>decay  | L <sub>x</sub> /T <sub>x</sub>                           | 0.952                          | 0.901  | 0.912  | 0.923     | 0.911        | 0.886         | 0.903     | 0.874  | 0.830  | 0.793  | 0.771 | 0.1  |
|  | <b>T(°C)</b> 230        | therm<br>decay      | t (ks)   | 0.000                          | 0.010  | 0.020  | 0.040     | 0.080        | 0.160         | 0.320     | 0.640  | 1.280  | 2.560  | 5.120 | 10.  |
| Ĺ  | <b>Ö (Gy/s)</b> 0.105   | _de_de_             | L <sub>x</sub> /T <sub>x</sub>                           | 0.910                          | 0.926  | 0.918  | 0.887     | 0.861        | 0.895         | 0.836     | 0.782  | 0.759  | 0.714  | 0.643 | 0.5  |
|  | <b>T(°C)</b> 250        | lso                 | t (ks)   | 0.000                          | 0.010  | 0.020  | 0.040     | 0.080        | 0.160         | 0.320     | 0.640  | 1.280  | 2.560  | 5.120 | 10.  |
| Ĺ  | <b>Ö (Gy/s)</b> 0.105   |                     | L <sub>x</sub> /T <sub>x</sub>                           | 0.908                          | 0.896  | 0.888  | 0.860     | 0.824        | 0.799         | 0.792     | 0.754  | 0.687  | 0.613  | 0.533 | 0.   |
|  | <b>T(°C)</b> 300        |                     | t (ks)   | 0.000                          | 0.010  | 0.020  | 0.040     | 0.080        | 0.160         | 0.320     | 0.640  | 1.280  | 2.560  | 5.120 | 10.  |
| Ĺ  | <b>Ö (Gy/s)</b> 0.105   |                     | L <sub>x</sub> /T <sub>x</sub>                           | 0.815                          | 0.803  | 0.772  | 0.725     | 0.668        | 0.596         | 0.509     | 0.437  | 0.363  | 0.286  | 0.221 | 0.:  |
|  | <b>T(°C)</b> 350        |                     | t (ks)   | 0.000                          | 0.010  | 0.020  | 0.040     | 0.080        | 0.160         | 0.320     | 0.640  |        |        |       |      |
| Ĺ  | <b>Ö (Gy/s)</b> 0.105   |                     | L <sub>x</sub> /T <sub>x</sub>                           | 0.677                          | 0.571  | 0.537  | 0.454     | 0.371        | 0.292         | 0.226     | 0.155  |        |        |       |      |
|  | <b>T(°C)</b> 15         | (A)                 | t (ks)   | 1.156                          | 17.546 | 23.576 | 35.626    | 59.706       | 1.159         | 10007.395 | 1.152  | 1.152  |        |       |      |
| Ĺ  | <b>Ö (Gy/s)</b> 0.105   | - on 6              | L <sub>x</sub> /T <sub>x</sub>                           | 0.921                          | 0.920  | 0.911  | 0.903     | 0.916        | 0.953         | 0.806     | 0.935  | 0.891  |        |       |      |
|  | <b>T(°C)</b> 15         | Anomalous<br>fading | t (ks)   | 1.156                          | 19.051 | 25.085 | 37.134    | 61.218       | 1.159         | 10008.891 | 1.152  |        |        |       |      |
|  | <b>Ó (Gy/s)</b> 0.105   |                     | L <sub>x</sub> /T <sub>x</sub>                           | 0.916                          | 0.901  | 0.865  | 0.886     | 0.861        | 0.955         | 0.817     | 0.915  |        |        |       |      |
|  | T(°C) (15)              |                     | t (ks)   | 1.156                          | 20.556 | 26.593 | 38.646    | 62.734       | 1.159         | 10010.387 | 1.152  |        |        |       |      |
|  | <b>Ö (Gy/s)</b> (0.105) | //                  | L <sub>x</sub> /T <sub>x</sub>                           | 0.898                          | 0.910  | 0.887  | 0.898     | 0.901        | 0.992         | 0.800     | 0.925  |        |        |       |      |
| Measurement temperature Instrument dose rate Individual sheet for each signal measured |                         |                     |  |                                |        |        |           |              |               |           |        |        |        |       |      |
|  |                         |                     |  |                                |        |        |           | KBC104 IBS   | 1 005         |           |        |        |        |       |      |

Figure 2: Example Excel data input sheet for the OSLThermo library. Note that all of these data, except for the average surface temperature (that can be manually inputted in *Stage3a\_Inversion* and *Stage4a\_InversionExh* of the OSLThermo and ESRThermo scripts) and laboratory dose rates for the isothermal decay and fading measurements, are mandatory for the codes to run.





# 5 Running the code

The code comprises multiple stages, which are available on GitHub, and can be download at:

<a href="https://github.com/GeorginaKing/OSLThermo">https://github.com/GeorginaKing/ESRThermo</a>. Users will need both a MATLAB license and the Statistics and Machine Learning Toolbox to run the code. Example datasets are provided from King et al. (2016a) for OSLThermo and Bartz et al. (2024) for ESRThermo. The libraries contain the different MATLAB codes, with OSLThermo/ESRThermo being the main code/launcher that calls the other code stages that have been selected. Four folders are contained in the libraries: "Data" where the Excel files with the luminescence or ESR input data need to be placed, "Functions" which regroups the different functions used in the MATLAB codes, "ComputeData" where the computed data is output, and "Figures" where the computed figures are saved.

## 5.1 OSLThermo/ESRThermo

In OSLThermo/ESRThermo the user must provide the filename and select which models will be used to fit and invert the data ('SAR\_fittype' and 'ITH\_fittype'). The number of aliquots or measurements for the dose response curve, the number of isothermal temperatures investigated ('nITH'), and the number of aliquots or measurements for athermal fading ('nFAD', only for OSLThermo) must also be stated.

```
OSI Thermo
                                                        ESRThormo
 %%% List of file names %%%%
                                                          %%% List of file names %%%%
 filenamevec = {'KRG104'};
                                                          filenamevec = {'TTY-A05'};
 %%% Number of measurements %%%%
                                                          %%% Number of measurements %%%
 nSARvec = 3; % number of aliquots measured for SAR
                                                          nSARvec = 3; % number of SAR measurements
 nITHvec = 7;
               % number of isothermal decay temperatures
                                                          nITHvec = 4;
                                                                        % number of isothermal decay temperatures
 nFADvec = 3; % number of aliquots measured for fading
                                                          %%% Select models %%%
 %%% Select models %%%
                                                          SAR_fittype = 1; % 1=SSE; 2=GOK; 3=LIN
 SAR fittype = 1; \% 1=SSE; 2=GOK
                                                          ITH fittype = 3; % 2=GOK; 3=GAUSS
 ITH fittype = 1; % 1=BTS; 2=GOK; 3=GAUSS
```

250 The user then selects which codes should be run for that particular sample, e.g., *Stage1\_ExcelToStruct*, *Stage 2a\_Fitparameters*, etc. Once a code has been run for a sample, the output is saved (see Table 1), so it is not necessary to run the code again unless the raw data have changed, or the data should be fitted with a different model.

## 5.2 Stage1 ExcelToStruct

This function imports the Excel data, stored in the subfolder "Data", into MATLAB and creates a MATLAB structure called 'records' that is called in *Stage2a\_Fitparameters*:

```
    OSLThermo
    ESRThermo

    run Stage1_ExcelToStruct
    run Stage1_ExcelToStruct
```





```
>> records =
                                                                 >> records =
1×4 struct array with fields
                                                                 1x2 struct array with fields:
       id: 'KRG104 IRSL225'
                                                                         id: 'TTY-A05-Al'
       typeMeasurement: 'IRSL'
                                                                         typeMeasurement: 'ESR'
       typeSignal: 225
                                                                         typeSignal: 'Al-centre'
       params: [1×1 struct]
                                                                         params: [1×1 struct]
       rawdata: [1×13 struct]
                                                                         rawdata: [1×7 struct]
>> records.params =
                                                                 >> records.params =
struct with fields:
                                                                 struct with fields:
                                                                         natT: [10 5]
       natT: [10 2]
       natDdot: [1.9533e-10, 2.62693e-11]
                                                                         natDdot: [1.2406e-10 1.1725e-11]
>> records.rawdata =
                                                                 >> records.rawdata =
1×13 struct array with fields:
                                                                 1×7 struct array with fields:
       Τ
                                                                         T
       labDdot
                                                                         labDdot
       t
       L
                                                                         ESR
```

This structure is saved as a .mat file in the subfolder "ComputeData", with the name *filename.mat*, and can be accessed without running *Stage1\_ExcelToStruct* again. If multiple sheets are present in the Excel file, 'records' will comprise multiple datasets, which can be accessed separately by inputting records(*i*) where *i* is the record number, into the MATLAB Command Window. The different rows of rawdata, *j* can also be accessed directly, for example to access the duration of dose/isothermal annealing time (Table 2), one can input *records(i).rawdata(j).t* into the command line.

Table 2: Variable names and description of data stored in the MATLAB structure 'records' after running Stage1 ExcelToStruct.

| Excel ID                        | MATLAB ID                          | Description  |
|---------------------------------|------------------------------------|--|
| Sheet name                      | records(i).id                      | Excel sheet name   |
| Type of measurement             | $records (i). type \\ Measurement$ | Type of measurement (IRSL, ESR)                          |
| Type of signal                  | records(i).typeSignal              | Type of signal (temperature of IRSL (°C), or ESR defect) |
| Natural T (°C)                  | records(i).params.natT             | Natural temperature (°C)                                 |
| Natural D (Gy·s <sup>-1</sup> ) | records (i).params.nat Ddot        | Natural environmental dose rate (Gy·s <sup>-1</sup> )    |
| T (°C)                          | records(i).rawdata(j).T            | Measurement temperature (°C)                             |
| $\dot{D}$ (Gy·s <sup>-1</sup> ) | records (i). rawdata (j). lab Ddot | Instrument dose rate (Gy·s <sup>-1</sup> )               |
| t (ks)                          | records(i).rawdata(j).t            | Duration of dose/isothermal annealing (ks)               |
| Lx/Tx                           | records(i).rawdata(j).L            | Luminescence data (OSLThermo only)                       |
| ESR                             | records(i).rawdata(j).ESR          | ESR data (ESRThermo only)                                |





# 5.3 Stage2a\_Fitparameters

This script calls *filename.mat*, created by *Stage1a\_ExcelToStruct*, and fits the raw data using the T-C models specified in the OSLThermo/ESRThermo script. The dose response and athermal fading data are fitted independently for each aliquot/measurement to account for individual laboratory dose rates and varying maximum trapped-charge signal values. The kinetic parameters output by the script are averaged per signal type across the different aliquots/measurements, and depend on the T-C models used. They are summarised in Table 3 per T-C model. In the MATLAB codes, these parameters are stored in the structure 'records' as 'records.params', and are exported in an Excel table. In addition to the kinetic parameters, the modelled data fits are stored in the structure 'records' as 'records.plot' for plotting in *Stage2b PlotFit*.

```
OSLThermo
                                                                ESRThermo
 >> records =
                                                                 >> records =
 1 x 4 struct array with fields:
                                                                 1 x 2 struct array with fields:
         id: 'KRG104 IR225'
                                                                         id: 'TTY-A05-A1'
         typeMeasurement: 'IRSL'
                                                                         typeMeasurement: 'ESR'
         typeSignal: 225
                                                                         typeSignal: 'Al-centre'
         params: [1×1 struct]
                                                                         params: [1×1 struct]
         rawdata: [1×13 struct]
                                                                         rawdata: [1×7 struct]
         SAR model: 'SSE'
                                                                         SAR model: 'SSE'
         ITH model: 'BTS'
                                                                         ITH model: 'GAUSS'
         plot: [1×1 struct]
                                                                         plot: [1×1 struct]
 >> records.params =
                                                                 >> records.params =
 struct with fields:
                                                                 struct with fields:
         natT: [10, 2]
                                                                         natT: [10, 5]
         natDdot: [1.9533e-10, 2.6269e-11]
                                                                         natDdot: [1.2406e-10, 1.1725e-11]
         rhop10: [-5.6606, 0.0573]
                                                                         De: [1.5093e+03, 48.2475]
         g2d: [2.6846, 0.3351]
                                                                         D0: [1.1030e+04, 965.1034]
         D0: [708.8781, 30.9929]
                                                                         GOK a: [NaN, NaN]
         GOK a: [NaN, NaN]
                                                                         s10: [13.5306, 0.6237]
         Et: [1.3831, 0.0443]
                                                                         Et: [1.5338, 0.0561]
         Eu: [0.1244, 0.0071]
                                                                         GOK b: [NaN, NaN]
                                                                         sigmaEt: [0.0897, 0.0049]
         GOK b: [NaN, NaN]
         sigmaEt: [NaN, NaN]
                                                                         AgeESR: [385.5232, 38.4629]
         s10: [8.0616, 0.3714]
                                                                         nNnat: [0.1279, 0.0041]
         NatFadedDe: [386.9116, 82.5055]
         NatFadedD0: [687.1585]
         AgeOSL: [62.7696, 15.8248]
         maxAgeOSL: [222.9586]
         nNnat: [0.2391, 0.0497]
         nNss: [0.5555, 0.0441]
```





Table 3: Description of the parameters output by Stage2a\_Fitparameters and stored in 'records.params', depending on the T-C models selected. Additional useful values are calculated in the codes but are not extensively discussed in this manuscript, which focuses on the key parameters used in the different scripts.

| Parameter   | OSLThermo MATLAB ID | ESRThermo MATLAB ID |
|---|---------------------|---------------------|
| Environmental parameters  |                     |                     |
| $T_{nat}(^{\circ}C)$ – average surface temperature                      | natT                | natT                |
| D (Gy·s <sup>-1</sup> ) – natural environmental dose rate               | natDdot             | natDdot             |
| Athermal detrapping model (OSLThermo script only)                       |                     |                     |
| $\rho$ ' (-) – recombination centre density                             | rhop10              | -                   |
| $g_{2d}$ (%/dec.) – fading rate normalised to 2 days                    | g2d                 | -                   |
| $\tilde{n}_{ss}$ (-) – athermal steady-state signal (fading corrected)  | nNss                | -                   |
| Trapping models SSE   |                     |                     |
| $\tilde{n}_{nat}$ (-) – natural signal                                  | nNnat *             | nNnat               |
| D <sub>e</sub> (Gy) – equivalent dose                                   | NatFadedDe*         | De                  |
| $D_0$ (Gy) – characteristic dose of saturation                          | D0 *                | D0                  |
| $D_{0\_nat}\left(Gy\right)-D_{0}$ for the natural faded signal          | NatFadedD0 *        | -                   |
| GOK   |                     |                     |
| $\tilde{n}_{nat}$ (-) – natural signal                                  | nNnat *             | nNnat               |
| D <sub>e</sub> (Gy) – equivalent dose                                   | NatFadedDe*         | De                  |
| $D_0$ (Gy) – characteristic dose of saturation                          | D0 *                | D0                  |
| $D_{0 \text{ nat}}(Gy) - D_{0}$ for the natural faded signal            | NatFadedD0 *        | -                   |
| $\bar{a}$ (-) – kinetic order of trapping                               | GOK_a               | GOK_a               |
| LIN   |                     |                     |
| D <sub>e</sub> (Gy) – equivalent dose                                   | -                   | De                  |
| Detrapping models   |                     |                     |
| BTS   |                     |                     |
| $E_t$ (eV) – trap depth   | Et                  | -                   |
| $E_u$ (eV) – Urbach width   | Eu                  | -                   |
| $s(s^{-1})$ – frequency factor  | s10                 | -                   |
| GOK   |                     |                     |
| $E_t$ (eV) – trap depth   | Et                  | Et                  |
| b (-) – kinetic order of detrapping                                     | GOK_b               | GOK_b               |
| s (s <sup>-1</sup> ) – frequency factor                                 | s10                 | s10                 |
| GAUSS   |                     |                     |
| $\mu(E_t)$ (eV) – mean trap depth                                       | Et                  | Et                  |
| $\sigma(E_t)$ (eV) – standard deviation of trap depth (width)           | sigmaEt             | sigmaEt             |
| s (s <sup>-1</sup> ) – frequency factor                                 | s10                 | s10                 |
| Ages  |                     |                     |
| Age (ka) – Apparent age   | AgeOSL *            | AgeESR              |
| Age <sub>max</sub> (ka) – Max. age, calculated for 2.D <sub>0 nat</sub> | maxAgeOSL *         | -                   |

Note: for the OSLThermo script, all data with an asterisk (\*) are fading corrected values.



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# 5.4 Stage2b\_PlotFit

Stage 2b\_PlotFit calls filename.mat, created in Stage 1\_ExcelToStruct and updated in Stage 2a\_Fitparameters, and produces plots of the raw data and model fits. In the OSLThermo library, the output of the Huntley (2006) model to test for luminescence signal saturation due to anomalous fading (Kars et al., 2008; Valla et al., 2016) is also plotted ( $\tilde{n}_{ss}$  vs.  $\tilde{n}_{nat}$ ; Fig. 1D). The figures produced for the two example datasets are shown in Fig. 1 and are automatically saved as either .png, .svg, or .eps files to the subfolder "Figures". Whilst it is not necessary to run Stage 2b\_PlotFit prior to running Stage 3a\_Inversion as no additional data fitting occurs in the script, it is good practice to make a visual inspection of the quality of data fitting before proceeding to the data inversion.

## 290 5.5 Stage3a Inversion

Stage3a\_Inversion inverts trapped-charge data for rock cooling history, using the parameters calculated in  $Stage2a\_Fitparameters$ , assuming monotonic cooling. All the data from a single Excel file are inverted together, for example different temperature IRSL data saved on different sheets of the same Excel file (Fig. 2). Note that the same T-C models used for fitting the data, must be used for the inversion. For OSLThermo, default parameters are setup for the model to run for 1 Myr assuming cooling from Tmax = 150 °C to Tmin =  $10 \pm 5$  °C using niter = 5000 iterations; and for ESRThermo, the model is setup to run for 5 Myr assuming cooling from Tmax = 200 °C to Tmin =  $10 \pm 5$  °C using niter = 5000 iterations. These conditions can be changed by editing the following lines of code:

```
%%% Model parameters
300
                                                               % maximum temperature in (°C)
                Tmax = 150;
                Tsurf = 10; TsurfErr = 5;
                                                               % average modern surface or sample temperature in (°C), and uncertainty
                                                               % maximum time in (Ma)
                tmax = 1;
                tmin = 0;
                                                               % minimum time in (Ma)
                                                               % discretisation of the model in time
                nstep = 501;
305
                time = linspace(tmin,tmax,nstep);
                %%% Number of iterations
                niter = 5000;
                                                               % number of random realisations / Monte Carlo iterations
```

More iterations will require a longer computational time. The principles of the inversion are fully described in King et al. (2016a) and King et al. (2020) and are outlined briefly here. Random monotonic cooling histories are generated, and for each history, the accumulation of trapped-charge is calculated using Eq. (1) (Fig. 3B-E, H) and the sample specific kinetic parameters determined in  $Stage2a\_Fitparameters$ . The quality of each model fit to the natural measured data is assessed by comparing the final modelled  $\tilde{n}_{mod}$  value,  $\tilde{n}_{mod,f}$  (i.e. the value calculated after 1 Ma for OSLThermo, and 5 Ma for ESRThermo) to the natural measured value  $\tilde{n}_{nat}$  using a misfit function, M (Eq. (15); Fig. 3F, I). This function has been updated since King et al. (2016a) following Wheelock et al. (2015), and as described by King et al. (2020) and Biswas et al. (2020):



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$$M = \left(\frac{1}{2} \frac{\tilde{n}_{nat}}{\sigma \tilde{n}_{nat}} \log \left(\frac{\tilde{n}_{nat}}{\tilde{n}_{mod,f}}\right)\right)^2 \tag{15}$$

where,  $\sigma \tilde{n}_{nat}$  is the uncertainty on  $\tilde{n}_{nat}$ . The value of  $\sigma \tilde{n}_{nat}$  can be determined either from the measured uncertainty or set arbitrarily, for example as 5 or 10% of  $\tilde{n}_{nat}$ , or as a fixed value, e.g., 0.05.

```
%%% Redefine uncertainties (OPTIONAL) % snNnat(snNnat<0.05) = 0.05; % set the uncertainty to 0.05 when it is <0.05 % snNnat(snNnat./nNnat<0.05) = 0.05*nNnat; % set the uncertainty to 5% of \tilde{n}_{nat} when it is <5% set the uncertainty on \tilde{n}_{nat} to 5% of \tilde{n}_{nat}
```

The results of the inversion (time-temperature paths,  $\tilde{n}_{mod}$  vectors, and misfit values) are saved in a MATLAB structure called 'Tt', which is saved in the "ComputeData" subfolder.

```
OSLThermo
                                                              ESRThermo
 >> Tt =
                                                                >> Tt =
 struct with fields:
                                                                struct with fields:
         misfit: [5000×1 double]
                                                                       misfit: [5000×1 double]
         time: [5000×501 double]
                                                                       time: [5000×501 double]
         temp: [5000×501 double]
                                                                       temp: [5000×501 double]
         nNmod: [5000×501×4 double]
                                                                       nNmod: [5000×501×2 double]
         nNnat: [0.0866; 0.1577; 0.1802; 0.2391]
                                                                       nNnat: [0.1279; 0.4754]
         snNnat: [0.0043; 0.0079; 0.0090; 0.0120]
                                                                       snNnat: [0.0064; 0.0238]
                                                                       AgeESR: c1 [385.52; 508.76]
         AgeOSL: c1 [81.37; 57.61; 56.93; 62.77]
                  c2 [15.39; 16.01; 14.02; 15.82]
                                                                                 c2 [38.46; 50.24]
         maxAgeOSL: [236.95; 219.70; 243.70; 222.96]
                                                                       TypeMeasurement: {'ESR' 'ESR'}
         TypeMeasurement: {'IRSL' 'IRSL' 'IRSL' 'IRSL'}
                                                                       TypeSignal: {'Al-centre' 'Ti-centre'}
         TypeSignal: [50 100 150 225]
```

In addition to investigating rock cooling, it is also possible to investigate isothermal histories or specific thermal histories by replacing the random cooling history generated using the randpathAD function with a specific time-temperature history.

# 5.6 Stage3b PlotTt

Stage3b\_PlotTt uses the output from Stage3a\_Inversion and computes a probability density function from the inversion results.

335 The likelihood, L, of a particular cooling history is computed from the misfit scores:

$$L = e^{-M} \tag{16}$$

and normalised by the maximum likelihood ( $L_{max}$ ), before these values are passed through a rejection algorithm whereby values of L are contrasted with a random number between 0 and 1, and only values that are greater than the random number are retained (Tarantola, 2005). The cooling histories retained are then used to compute a probability density function. This is done by dividing the time-temperature space into equal-size cells and calculating the number of time-temperature paths passing through each cell. The results of inverting the example datasets are shown in Fig. 3.





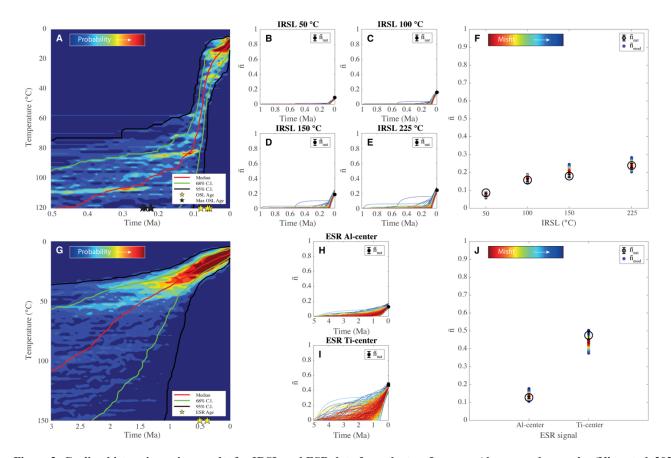


Figure 3: Cooling history inversion results for IRSL and ESR data from the two Japanese Alps example samples (King et al, 2020; Bartz et al., 2024). Probability density function of the accepted time-temperature history (cooling path) (A) for all four IRSL signals of sample KRG104 and (G) for the Al-centre and Ti-centre of sample TTY-A05; modelled signal accumulation (B-E, H-I) and misfit between measured and modelled values (F, J) for the time-temperature paths that passed the rejection algorithm. In (A, G), the red line is the median cooling path, and the green and black lines are the 68% and 95% confidence intervals, respectively.

## 5.7 Stage4a InversionExh

350 Stage4a\_InversionExh allows the inversion of trapped-charge data for an exhumation history; the approach is fully described in Biswas et al. (2018) and is only briefly explained here. In this script, random time-temperature histories are first generated over a specified time-period and depth. Rock cooling histories for each time-depth path are then computed using the 1D heat-transfer equation, and the accumulation of trapped-charge is calculated using Eq. (1) and the sample-specific kinetic parameters determined in Stage2a\_Fitparameters. As for Stage3a\_Inversion, the quality of each model fit to the natural measured data is assessed by comparing the final modelled ñ value, ñ<sub>mod.f</sub>, using Eq. (15).



390



The model is set-up to run over the last 5 Ma ('tmax') over a depth of 15 km ('Lz') with an initial geothermal gradient of 30 °C·km<sup>-1</sup> ('G'). The thermal diffusivity ('kappa0'), number of iterations ('niter') and discretization of the model ('nstep') can also be modified. This code is more computationally expensive than *Stage3a\_Inversion* and it requires more iterations to yield a similar number of accepted paths.

```
%%% Physics
                                              % thermal diffusivity (km<sup>2</sup>·Myr<sup>-1</sup>)
           kappa0 = 30;
           Lz = 15;
                                              % depth (km), use 25 km for high temperature thermochronometers
365
                = 30;
                                              % initial temperature gradient (°C·km<sup>-1</sup>)
           Tsurf=10; TsurfErr=5;
                                              % surface temperature (°C) and its uncertainty
           %%% Numerics: discretization, time steps and plotting frequency
           nz = 31:
                                              % number of nodes
370
           dz = Lz/(nz-1);
                                              % node size (km)
           %%% Choose the depth time history (i.e. exhumation rate history)
                                              % maximum depth in (km)
           Zmax = Lz;
                                              % surface, i.e. Z=0 km
            Zmin = 0;
375
                                              % time in Ma (today)
           tmax = 5;
           tmin = 0:
           nstep = 6000;
                                              % timestep, to ensure high resolution over the timescale
                 = (tmax-tmin)./(nstep-1);
                                              % calculate timestep, dt (Myr)
                                              % create time vector
           tvec = (tmin:dt:tmax);
380
           %%% Number of iterations
           niter = 100000;
                                              % number of iterations
```

# 5.8 Stage4b PlotZt

Stage4b\_PlotZt plots the inversion results from  $Stage4a\_InversionExh$ . The depth and time-period of interest are defined in the plotting script (and are usually smaller than the modelled domain), as is the matrix resolution for computing the exhumation history. As the geothermal gradient (G) evolves throughout the inversion, a final geothermal gradient that is unfeasibly high may be obtained. For this reason, a threshold value can be defined ( $G\_cut$ ) to exclude results with a final  $G > G\_cut$  (see Stalder et al., 2022 for a discussion).  $G\_cut$  is set to 100 °C·km<sup>-1</sup> in the code, but this value can be modified.

```
%%% Define parameters for plotting
           DoI = 2;
                                              % depth of interest, last xx (km)
           ToI = 0.3:
                                              % time of interest, last xx (Ma)
           G cut = 100;
                                             % cut-off for geothermal gradient (°C·km<sup>-1</sup>)
395
                                             % restrict to a time-window of interest for plotting
           time window = ToI;
           %%% Resolution of matrix
           nAvM = 1200:
                                              % temporal dt = ToI/nAvM and spatial dZ = DoI/nAvM resolutions
           resampling = 100;
                                              % how many times median is resampled (min. 100)
400
           nb path = 0.10;
                                              % number of resampled paths in % of total accepted paths (min. 10\% = 0.10)
            vel interval = 10;
                                              % define velocity smoothing interval in (kyr)
```





This script produces a range of figures, including a probability density function of time-depth for the accepted paths (Fig. 4A, D), as well as a comparison between modelled ( $\tilde{n}_{mod}$ ) and measured ( $\tilde{n}_{nat}$ ) values, and in the case of luminescence data, the predicted field saturation values,  $\tilde{n}_{ss}$ , for the sample under investigation (Fig. 4B, E). It also produces a figure showing the time series of the modelled exhumation history in linear and log space (Fig. 4C, D).

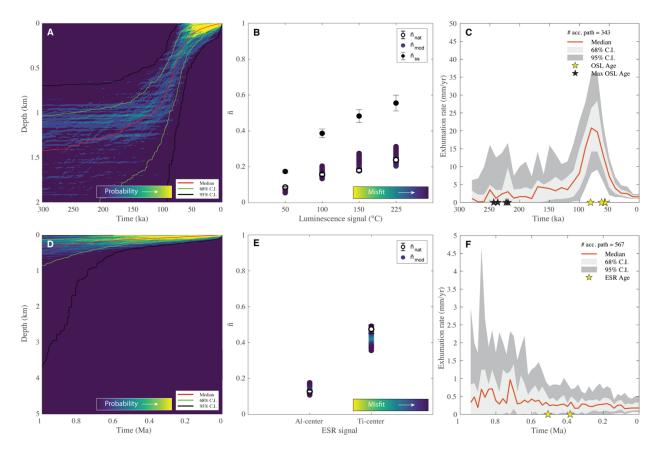


Figure 4: Exhumation rate inversion results for IRSL (A-C) and ESR (D-F) data following 10,000 iterations. Probability density function of the accepted time-depth history (exhumation path) (A) for all four IRSL signals of sample KRG104 and (D) for the ESR Al- and Ti-centre of sample TTY-A05; misfit between measured and modelled values (B, E) and time-series of exhumation rate changes (C, F) plotted in linear space. In (A, D), the red line is the median cooling path, and the green and black lines are the 68% and 95% confidence intervals respectively.

## 6 Outlook

We hope that by sharing the codes that we have developed for the modelling of trapped-charge thermochronometry data for feldspar OSL and quartz ESR, we will encourage broader application and further development of trapped-charge

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thermochronological and geochronological community.

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thermochronometry and thermometry techniques. The codes can easily be adapted for other trapped-charge signals, such as quartz OSL or thermoluminescence. We will continue to update the OSLThermo and ESRThermo libraries as new T-C models emerge and as the trapped-charge community advances efforts to improve thermochronometric analysis, for example, by incorporating averaging thermal kinetic parameters (Bouscary and King, 2024), enabling more complex thermal histories (e.g., reheating), or integrating trapped-charge data with other thermochronometric systems. By fostering open-source development and collaboration, we aim to support the growth and integration of trapped-charge thermochronometry within the broader

425 Codes are available for download on GitHub: <a href="https://github.com/GeorginaKing/OSLThermo">https://github.com/GeorginaKing/OSLThermo</a> for luminescence thermochronometry & <a href="https://github.com/GeorginaKing/ESRThermo">https://github.com/GeorginaKing/ESRThermo</a> for ESR thermochronometry.

#### **Author contributions**

CB, GEK, MB, AD, BG, and FH contributed to the conceptualization and methodological design of the study. Data curation was performed by CB and GEK, while formal analyses were carried out by CB, GEK, MB, LB, AD, BG, FH, NS, and VV.

The investigation and methodological implementation involved almost all authors (CB, GEK, MKB, MB, RHB, AD, BG, FH, UN, PGV, VV, and XW), with validation contributions from CB, GEK, MKB, MB, BG, FH, and XW. Software development and implementation were undertaken by CB, GEK, MKB, MB, RHB, AD, BG, FH, UN, and VV. Supervision was led by GEK, FH, and BG. Project administration and resource provision were coordinated by GEK and FH, and funding was acquired by CB, GEK, and FH. The original manuscript draft was written by CB and GEK, and all authors contributed to the review, editing, or validation of the final version.

## Code and Data availability

The codes used in this study are publicly available on GitHub: for OSL thermochronometry on feldspar at <a href="https://github.com/GeorginaKing/OSLThermo">https://github.com/GeorginaKing/OSLThermo</a> and for ESR thermochronometry on quartz at <a href="https://github.com/GeorginaKing/ESRThermo">https://github.com/GeorginaKing/ESRThermo</a>. For each code, the Excel input file corresponding to the sample analysed in this manuscript is provided, allowing direct reproduction of the results.

## **Competing interests**

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One of the co-authors serves on the Editorial Board of the journal GChron.





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