



# Analyzing absolute paleointensity determinations: Acceptance criteria and the software ThellierTool4.0

**R. Leonhardt, C. Heunemann, and D. Krása,**

*Geophysics Section, Department for Earth and Environmental Sciences, Ludwig-Maximilians-Universität,  
Theresienstr. 41, 80333 Munich, Germany (leon@geophysik.uni-muenchen.de)*

[1] The ThellierTool4.0 is an intuitive and easy-to-use software which provides the possibility to analyze a wide range of different modifications of the Thellier absolute paleointensity experiment (available at <http://earthref.org/tools/>). Besides the Arai plot for paleointensity determination, orthogonal projections of the direction, decay of NRM during thermal demagnetization, and additional plots regarding alteration and multidomain checks enable the user to visualize the quality of individual determinations. Experimental checks for magnetomineralogical changes, either in-field or zero-field pTRM\* checks, are evaluated regarding their differences to the corresponding pTRM\* acquisition in two most commonly used ways. Furthermore, a measure for the cumulative alteration differences beginning at room temperature is calculated, and the possibility to correct for magnetomineralogical changes is provided. Two different experimental methods to check for multidomain bias are supported and analyzed by the software. Intensity differences recorded by pTRM\*-tail checks are calculated. Accounting for the directional difference between applied laboratory field and magnetization of the sample, the effective pTRM\*-tail is determined, and thus failures of Thellier's law of independence are monitored. Failures of the law of additivity, experimentally observed by additivity checks, are also evaluated by the software. The vectorial character of individual measurements is fully considered for all calculations. Uniform selection criteria for acceptance and rejection of determinations can be applied, and a set of such criteria with emphasis on minimal bias due to alteration, multidomain remanence, and analysis/experimental inaccuracies is suggested.

**Components:** 3497 words, 4 figures, 1 table.

**Keywords:** Paleomagnetism; absolute paleointensity; Thellier method.

**Index Terms:** 1521 Geomagnetism and Paleomagnetism: Paleointensity; 1594 Geomagnetism and Paleomagnetism: Instruments and techniques.

**Received** 22 July 2004; **Revised** 26 October 2004; **Accepted** 16 November 2004; **Published** 31 December 2004.

Leonhardt, R., C. Heunemann, and D. Krása (2004), Analyzing absolute paleointensity determinations: Acceptance criteria and the software ThellierTool4.0, *Geochem. Geophys. Geosyst.*, 5, Q12016, doi:10.1029/2004GC000807.

## 1. Introduction

[2] The Thellier method [Thellier and Thellier, 1959] and, in particular, derived modifications [e.g., Coe, 1967a; Aitken et al., 1988; McClelland and Briden, 1996; Riisager and Riisager, 2001] are the most commonly used paleomagnetic techniques for the determination of the intensity of the past Earth's magnetic field. In principle, all these techniques rely on a comparison of an artificial thermoremanence acquired in a known laboratory

field with the natural remanent magnetization (NRM) of the sample, assuming that the NRM is also a pure thermoremanent magnetization which remained essentially unchanged since emplacement of the rock. Almost all modifications of the original Thellier method follow either the approach of Coe [1967a, 1967b], where stepwise demagnetization of the NRM in zero-field is followed by stepwise acquisition of partial thermoremanent magnetizations (pTRM) at the same temperature steps as used for demagnetization, or the reverse

order by firstly imparting the pTRM followed by demagnetization to the same temperature [Aitken *et al.*, 1988]. In a strict sense, a pTRM is acquired by heating a sample to the Curie temperature  $T_C$  and applying a laboratory field during cooling between temperatures  $T_i < T_C$  and room temperature  $T_0$ . During Thellier type experiments, however, pTRM's are acquired by heating the sample to the actual heating step  $T_i$  and applying a field during cooling to room temperature  $T_0$ , hereinafter called pTRM\*. It has been shown that these two pTRM acquisition processes produce differing results for samples containing multidomain (MD) grains [e.g., Shcherbakov *et al.*, 1993; Dunlop and Özdemir, 2000; Shcherbakova *et al.*, 2000]. In the presence of MD particles this discrepancy between pTRM and pTRM\* can lead to a spurious paleointensity estimate [Fabian, 2001; Coe *et al.*, 2004; Leonhardt *et al.*, 2004]. Another commonly observed reason for failures of the Thellier experiment is chemical alteration of the sample during laboratory heating/cooling cycles [e.g., Perrin, 1998; Goguitchaichvili *et al.*, 1999]. In order to detect magnetomineralogical changes and the presence of biasing MD effects several different experimental checks have been proposed. Alteration processes are monitored by pTRM checks [Coe, 1967a] conducted to  $T_k < T_i$  either in a laboratory field directly after demagnetization to  $T_i$  (in-field checks) or zero-field checks, conducted after previous pTRM\* acquisition to  $T_i$ .

[3] The influence of MD remanences can be assessed using two different methodological approaches which monitor failures to Thellier's laws [Thellier, 1941] which have to be fulfilled to extract paleointensity information: (1) Repeated demagnetization to  $T_i$  after previous pTRM\* acquisition to  $T_i$ , so called pTRM\*-tail checks, test the independence of different pTRM\*s [Riisager and Riisager, 2001; Leonhardt *et al.*, 2004]. (2) Violations of the law of additivity of pTRM\*s are detected by the additivity check [Krása *et al.*, 2003]. This check is essentially the same as the zero-field alteration check. Yet, when conducting in-field plus zero-field checks, a comparison of both values indicates possible failures of Thellier's law of additivity.

[4] Some basic statistical parameters for the analysis and classification of the paleointensity experiment were introduced by Coe *et al.* [1978]. In order to evaluate these checks and thus the significance and reliability of the experimental data, a number of additional parameters and criteria were suggested by several authors [e.g., Prévot *et al.*,

1985; Aitken *et al.*, 1988; Tauxe, 1998; Selkin and Tauxe, 2000; Riisager and Riisager, 2001; Laj *et al.*, 2002; Biggin and Thomas, 2003; Kissel and Laj, 2004]. However, in contrast to conventional paleodirectional analyzes there is no commonly agreed parameter set and criteria range. Moreover, most of the standard calculation routines for the analyzes of paleointensity do not take into account the vectorial character of the remanence measured and differ significantly in the methods used to normalize relative errors.

[5] Here, we present a software for analyzing Thellier experiments, the ThellierTool4.0. This 32bit Windows program uses a similar data format as the Linux Pmag program [Tauxe, 1998] in order to facilitate platform and laboratory spanning comparisons of experimental data. Additionally, it allows the use of full vector analysis for all calculations involved in Thellier analysis. The most commonly used modifications of Thellier's technique are supported and the evaluation of all the quality checks mentioned above is provided. A wide range of different analysis parameters is calculated and reliability thresholds for these parameters can be defined. Furthermore, a default set of thresholds for paleointensity determination and for the classification of different checks is suggested and discussed.

## 2. Data Format and User Interface

### 2.1. Input File Format

[6] The data file, which can be read by the ThellierTool4.0, should be of the format shown in Table 1. The file can be "space" or "tab" delimited. The first two lines are optional and contain header information: If "Thellier-tdt" is found in the first line of the file, then the second header line will be used. This line contains in the following order the laboratory field ( $\mu T$ ), bearing, plunge, direction of dip and dip. The directional information only affects the orthogonal projection and has no influence on the paleointensity results. Plunge and bearing are used to obtain "in situ" coordinates, dip and direction of dip define the bedding correction. Data files without the two header lines are also accepted. In this case a default value of 35  $\mu T$  is assumed for the laboratory field. The actually used laboratory field has to be inserted manually (Figure 1a).

[7] The data of the Thellier measurement is given in 5 columns (Table 1): Column 1 contains the sample name (maximum length of 16 characters),

**Table 1.** File and Data Format<sup>a</sup>

File Structure	Sample	T, °C, and Type	M, mA/m	Dec, deg	Inc, deg	Data Description
Header (optional)	<i>Thellier-tdt</i>					
	25.0(a)	340.0(b)	50.0(c)	120.0(d)	5.0(e)	
	MGH1	20.00	4090.8	295.6	−42.8	NRM
	MGH1	200.00	3734.2	302.4	−42.4	thermal demagnetization (T + “.00”)
	MGH1	200.11	3972.4	303.0	−46.3	pTRM* acquisition (T + “.11 or .1”)
Data	MGH1	200.13	3738.2	296.5	−42.6	pTRM*-tail check (T + “.13 or .3”)
	MGH1	250.00	3617.1	300.2	−40.7	
	MGH1	250.11	3303.9	300.2	−33.9	
	MGH1	300.00	3447.4	297.4	−42.1	
	MGH1	300.11	3918.4	293.8	−49.5	
	MGH1	340.00	3284.2	297.9	−42.3	
	MGH1	250.12	2984.2	293.1	−34.7	pTRM* check (T + “.12 or .2”)
	MGH1	340.11	2796.1	295.0	−29.1	
	MGH1	250.14	3059.2	296.5	−37.2	additivity check (T + “.14 or .4”)
	...	...	...	...	...	

<sup>a</sup> Structure of a Thellier data file (\*.tdt) with demagnetization steps first, in-field pTRM\* checks, pTRM\*-tail checks, and additivity checks. The two header lines are optional. If the file description “Thellier-tdt” is found in the first line of the file, then the second line containing the following parameters is loaded: (a) laboratory field in  $\mu\text{T}$ , geographic data for “in situ” orientation (b) bearing and (c) plunge) and bedding data ((d) direction of dip and (e) dip). The data part of the input file is described in the right column.

column 2 the temperature (in °C) and type of measurement, column 3 the intensity (in  $\text{mA/m}$ ), column 4 the declination and column 5 the inclination in core coordinates. The decimal digits of the temperature value (column 2) indicate the type of measurement: .00 (or.0) stands for thermal demagnetization (further on referred to in the text as TH), .11 (or.1) is acquisition of pTRM\* (PT), .12 (or.2) defines the pTRM\*-check (CK), .13 (or.3) repeated demagnetization steps (TR) and .14 (or.4) indicates additivity checks (AC).

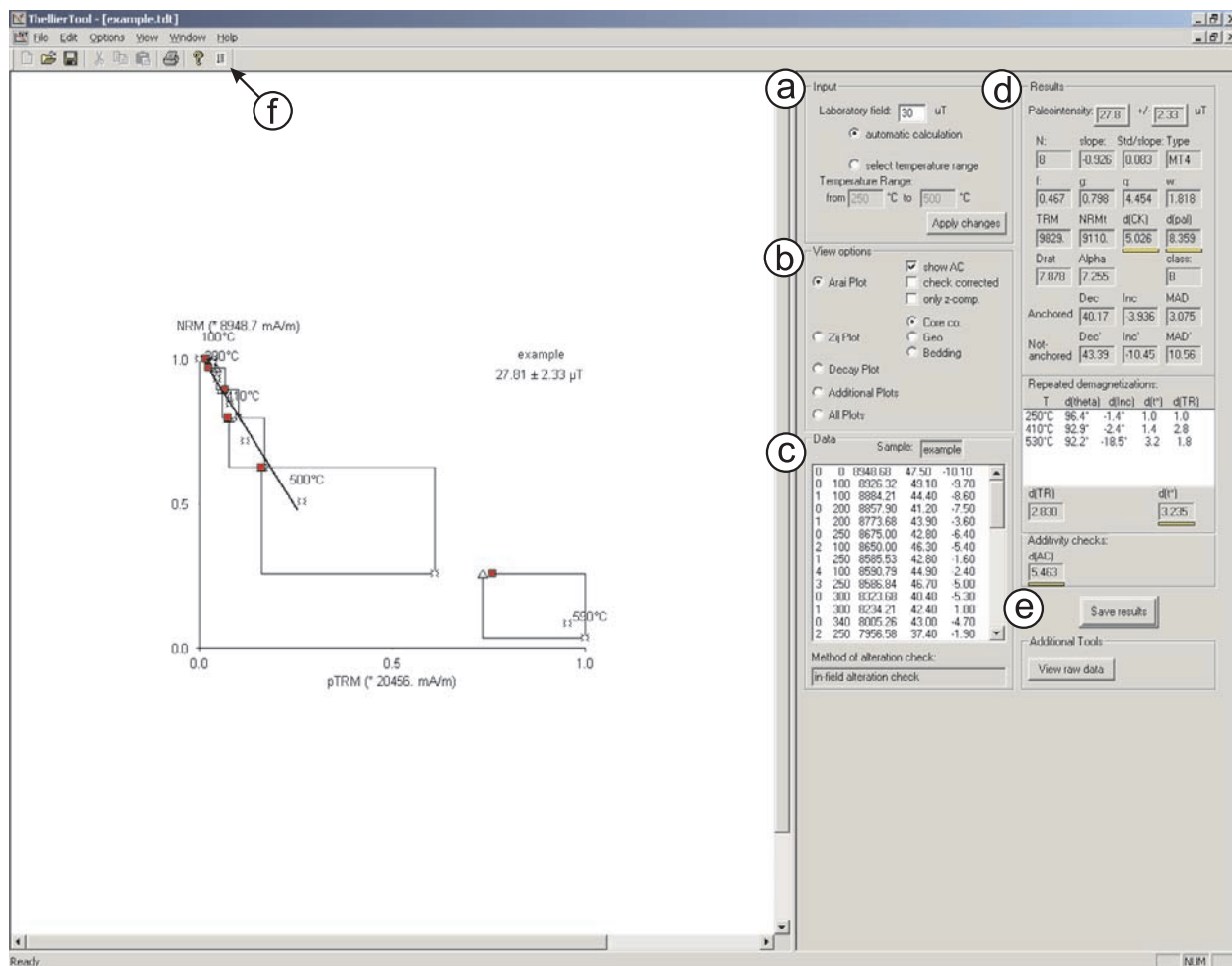
## 2.2. Main Window

[8] The “Main Window” (Figure 1) is split into two main sections: The graph with the selected plot is displayed on the left side. The form view on the right-hand side contains the results and several options regarding the data analyses.

[9] The “Input” field (Figure 1a) on the form view shows the applied laboratory field and the type of calculation method: The default option when opening a new file is “automatic calculation” (see below). If manual calculation is selected, the two edit boxes for choosing the temperature range for the calculation of the linear fit are enabled.

[10] The display options can be changed in the field labeled “View options” (Figure 1b; see also Figure 2). “Arai plot” shows the NRM/TRM diagram [Arai, 1963] (Figure 2a). Additional options for this diagram are the plotting of additivity checks, applying corrections for mag-

netomineralogical changes and z component only calculations. The “Zij plot” option shows the orthogonal projection of the demagnetization data [Zijderveld, 1967] (Figure 2b) either in core coordinates, geographic in situ coordinates or bedding corrected coordinates, if such data is provided in the file’s header. The mean direction calculated in the selected temperature interval is indicated by a dashed green line. The “Decay diagram” shows the decay of the intensity during demagnetization (Figure 2c). If repeated demagnetizations were measured then these data are also shown in the diagram as black squares. The option “Additional plots” shows up to four plots depending on the used modification of the Thellier experiment (Figure 2d). In Figure 2d (upper left panel) the difference between the applied field direction and the direction of the acquired pTRM\* is plotted. Figure 2d (upper right panel) shows the individual check errors normalized to the TRM. Positive values indicate increased capacity of pTRM\* acquisition, negative values show decreased capacity. If check correction is applied and additivity checks were measured, then the AC-errors are plotted in Figure 2d (upper right panel). Figure 2d (lower left panel) shows the tail of the pTRM\* corrected for the angular difference between the applied field and the NRM. Here, positive values indicate an acquisition of a tail in direction of the applied field. Negative values can not be related to tails and point rather to alteration or stabilization processes during repeated heating steps affecting blocking temperature ranges above the actual



**Figure 1.** The Main window, split into a form view on the right-hand side and the selected plot of the experimental data on the left: (a) input, (b) view options, (c) display of raw data, (d) results and statistical parameter, (e) save results, and (f) open criteria dialog.

heating step. In Figure 2d (lower right panel) the intensity difference between first demagnetization TH and repeated demagnetization TR is shown. The option “All plots” shows all the above described plots together on one page. Using a post-script printer driver, the print-to-page option will generate a post-script file of the selected plot.

[11] The content of the data file and the alteration check method used are shown on the lower left of the form view (Figure 1c). The field “Results” (Figure 1d) contains the calculated paleointensity, as well as all the associated statistical parameters of the linear fit and the results of the checks. If one of the obtained parameters violates the quality criteria of a class A determination (see below), a small yellow bar appears below this value. Red bars indicate that this

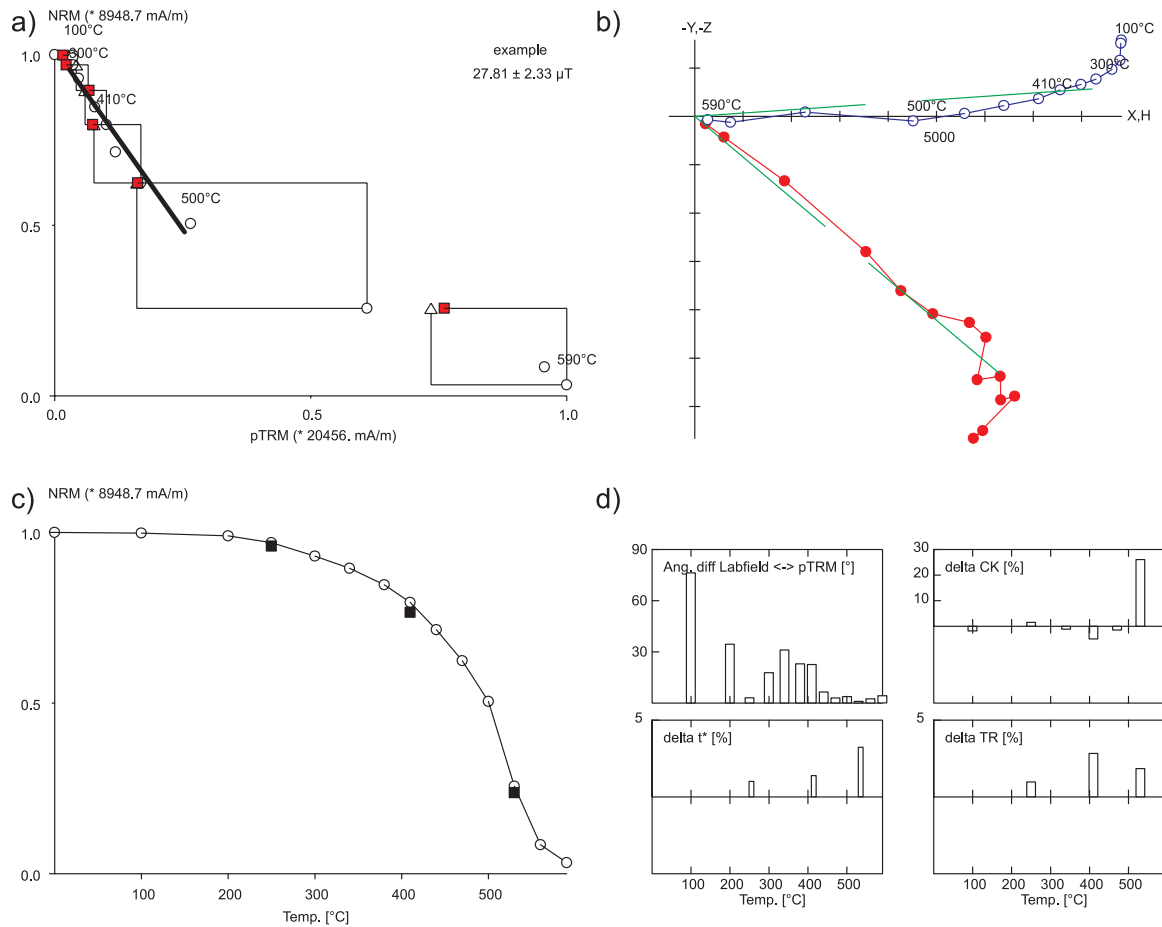
value violates the class B criteria. These threshold values of these criteria can be edited in the “Criteria Dialog”.

[12] The “Save results” button writes, or appends if the selected file already exists, all calculation results of Figure 1d in an Tab-delimited text file. A header with column labels is provided in this file. The “View raw data” button opens the Thellier data file in Notepad.

### 2.3. Criteria Dialog

[13] Whether paleointensity determinations are accepted to be reliable records of the past geomagnetic field strength is typically decided on the basis of the quality of the checks and the statistical parameters of the linear fit. Such a set of criteria, classifying the quality of the determination and the experimental checks can





**Figure 2.** The different plots according to the “View options” selection (Figure 1b): (a) Arai plot with pTRM checks (triangles) and additivity checks (red squares). (b) Zijderveld plot with the calculated mean direction (green line) associated with the temperature interval chosen. Open (blue) symbols represent projections on the vertical plane, and solid (red) symbols show projections on the horizontal plane. (c) Decay of the NRM intensity. Black squares indicate the results of the repeated demagnetization (TR). (d) Visualizes further information as, e.g., pTRM check error, tail of pTRM\*, etc. (see text).

be defined in the “Criteria Dialog” (Figure 3). These criteria are subdivided in several groups. Determination criteria, like the minimum number of successive measurement steps ( $N$ ), standard deviation of the linear fit ( $Std$ ), fraction of NRM ( $f$ ), and the quality factor ( $q$ ) [Coe *et al.*, 1978] define the first group. The selected temperature segment for intensity analyses must match the temperature range which carries the characteristic remanent magnetization of the sample. By principle component analysis (PCA) Kirschvink [1980], such directional aspects are monitored using the parameters of the second group (MAD,  $\alpha$ ). Depending on the applied experimental checks further criteria for classifying CK, TR (pTRM-tail checks) and AC can be provided. It is possible to define a maximum of three different quality classes using specific criteria for

classes A and B, as well as an users choice C if at least one parameters violates both class A and B criteria.

### 3. Analyses of Paleointensity Determination

#### 3.1. Basic Parameters

[14] After opening a data file using Thellier-Tool4.0, the pTRM\*-gained values are obtained by full vector subtraction between the TH and the respective PT acquisition. Full vector subtraction is also applied to extract CK and AC. Depending on the checks used and the measurement protocol, five different types of modified Thellier techniques are distinguished:

**Criteria** criteria for class A and B determinations

**Class A**

Linear fit criteria

Number of points (N)  $\geq$  5

Standard deviation (Std)  $\geq$  0.1

Fraction of NRM (f)  $\geq$  0.3

Quality factor (q)  $\geq$  1

Directional criteria

MAD (anchored)  $\leq$  6

MAD' (not-anchored)  $\leq$  999

Alpha  $\leq$  15

Alteration criteria

Relative check error: d(CK)  $\leq$  5

Cumulative check diff: d(pal)  $\leq$  5

Difference ratio (Drat)  $\leq$  999

Repeated demagnetization steps

Normalized tail of pTRM: d(t\*)  $\leq$  3

Relative intensity diff  $\leq$  10

Additivity checks

Relative AC error: d(AC)  $\leq$  5

**Class B**

Linear fit criteria

Number of points (N)  $\geq$  5

Standard deviation (Std)  $\geq$  0.15

Fraction of NRM (f)  $\geq$  0.3

Quality factor (q)  $\geq$  0

Directional criteria

MAD (anchored)  $\leq$  15

MAD' (not-anchored)  $\leq$  999

Alpha  $\leq$  15

Alteration criteria

Relative check error: d(CK)  $\leq$  7

Cumulative check diff: d(pal)  $\leq$  10

Difference ratio (Drat)  $\leq$  999

Repeated demagnetization steps

Normalized tail of pTRM: d(t\*)  $\leq$  5

Relative intensity diff  $\leq$  15

Additivity checks

Relative AC error: d(AC)  $\leq$  10

**Class C**

Manual determination which does not satisfy class A or B criteria.

modification of criteria

Criteria file

DefaultCriteria

Load Save Default

Automatic calculation parameter

Linear fit determination by maximizing

☒ weighting parameter (w)

☐ quality factor (q)

Allow automatic calculation with check correction in case of MT4:

☐ Enable as option for automatic calculation

General View Options

Arai diagram:

☒ normalize both axes separately

☐ normalize both axes equally

changes the style of the Arai diagram

Cancel Apply

**Figure 3.** The criteria dialog shows the chosen criteria for class A and class B determinations. Criteria can be changed and saved to a file (\*.cri). Other options are related to the automatic calculation, which searches for a slope with either maximal  $w$  or maximal  $q$ . In the case of a MT4 experiment (section 5.6), check corrected analysis can be included in the automatic algorithm. The style of the Arai diagram (equal or nonequal intensity axes) can be changed as well.

[15] *MT0*: Thellier-type method without any checks

[16] *MT1*: “Field-off first” method with pTRM\*-checks

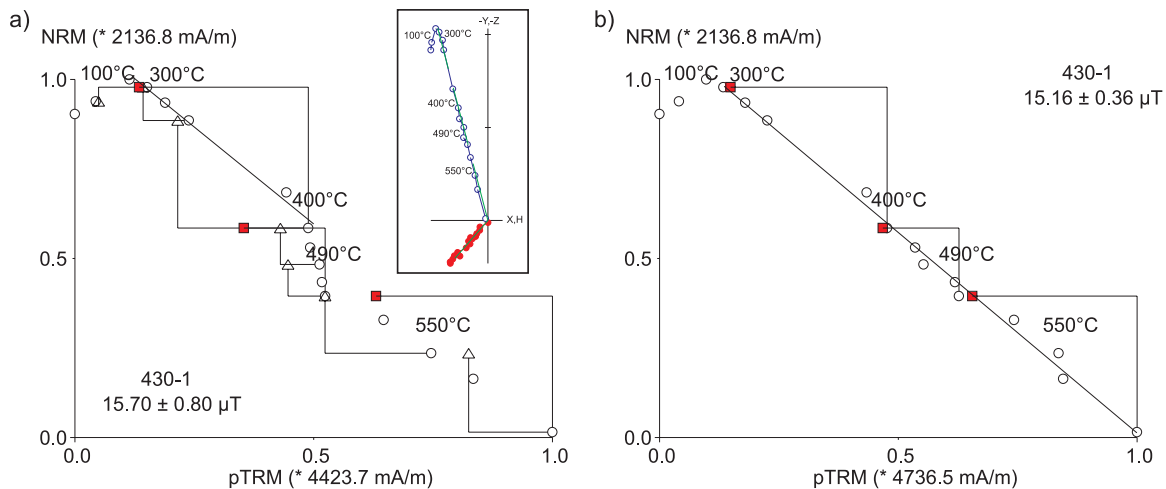
[17] *MT2*: “Field-on first” method with pTRM\*-checks

[18] *MT3*: Method *MT1* including pTRM\*-tail checks

[19] *MT4*: Method *MT1* including pTRM\*-tail and additivity checks

[20] The slope of the best fit line, the standard deviation, the fraction of NRM ( $f$ ), gap factor ( $g$ ), quality factor ( $q$ ) [Coe et al., 1978] as well as the weighting factor ( $w$ ) [Prévot et al., 1985] are

determined for a chosen segment of the Arai diagram. The true NRM ( $NRM_t$ ) is the intersection between linear fit and y-axis, whereas the  $TRM$  is defined as the intersection between linear fit and x-axis. The remanence direction obtained from the TH step is determined using PCA. Inclination ( $Inc$ ), Declination ( $Dec$ ), and maximum angular deviation ( $MAD$ ) are calculated for both anchored-to-the-origin and not-anchored fits. Furthermore, the angular difference between anchored and not-anchored solution ( $\alpha$ ) is determined. A quality class is assigned to the determination by comparing the results with the given criteria. If manual determination is selected and the results do not comply with criteria A and B values, then the determination is termed to be of class C.



**Figure 4.** (a) Noncorrected Arai plot of a sample showing magnetomineralogical changes above 400°C and (b) corresponding corrected data. Additivity checks fall on the corresponding pTRM\* values after correction, indicating a successful correction.

[21] When opening the data file an algorithm is used to find automatically the best linear segment for the available data. At first, the data file is searched for a paleointensity determination which satisfies the criteria of class A. From all the possible solutions, the one with the maximum weighting/quality factor is displayed. The used weighting factor can be either  $w$  or  $q$  and is selected in the “Criteria Dialog”. If no solution is found for class A, then the algorithm tries to find a best fit satisfying class B criteria. If again no solution is found, then all results are zero.

[22] By default, all calculations are done using full vector subtraction. If view option “z-comp only” (Figure 1b) is selected, the vector subtraction is done by using only the values for the measured z component (in core coordinates). Selecting this option for the calculation of a paleointensity value requires that the applied field is parallel to the core coordinate z component of the sample. All parameters are then recalculated. Such single component vector subtraction is also used by the Pmag Thellier analysis program [Tauxe, 1998]. Therefore selecting this option is necessary for comparison of the results obtained by the two programs.

### 3.2. Magnetomineralogical Changes During the Experiment

[23] Three parameters which are used to monitor the effect of magnetomineralogical changes from pTRM\*-checks are determined by the program.  $\delta(CK)$  [Leonhardt et al., 2000] and DRAT [Selkin

and Tauxe, 2000] describe deviations of pTRM\*-checks at a given temperature step. Both parameters give a relative measure of the individual deviation of the pTRM\* check from the corresponding pTRM\* value at a specific temperature. The difference between pTRM\*-check and related pTRM\* acquisition is normalized to the TRM for calculation of  $\delta(CK)$  and to the length of the selected segment for DRAT [Selkin and Tauxe, 2000].

[24] The cumulative check error ( $\delta_{pat}$ ) [Leonhardt et al., 2003] is related to the cumulative difference of the individual checks from room temperature up to the maximum temperature used for the best fit line. The usage of a cumulative alteration check analysis was previously suggested by Laj et al. [2002]. This parameter estimates the overall alteration, as even small individual differences between checks and pTRM\* values can sum to significant alteration errors. To quantify the effect of the cumulative alteration difference, a correction method for magnetomineralogical changes which uses the cumulative sum of alteration differences [Valet et al., 1996] is applied to the selected segment and the check corrected paleointensity value is compared to the noncorrected value. The ratio of uncorrected to corrected paleointensity normalized to the uncorrected value is  $\delta_{pat}$ .

[25] If alteration checks are continuously and subsequently performed over the entire temperature range of the experiment, and assuming that alteration occurs predominantly below the temperature of the respective check, the method of Valet et al. [1996] can be used to correct for magnetominera-

logical changes during laboratory treatment. It allows thus to obtain valid paleointensity estimates from otherwise noninterpretable experimental data [Leonhardt *et al.*, 2003]. For this technique, the cumulative sum of the individual differences between checks and associated pTRM\* values up to heating step  $i-1$  is subtracted from the measured pTRM\* value at step  $i$ . Such correction is conducted by selecting the view option “check corrected” (Figure 1b), resulting in a recalculation of pTRM\*-acquisition values and all dependent vector subtractions.  $\delta_{CK}$ ,  $\delta_{pal}$  and  $DRAT$  are for obvious reasons zero after correction. The *class* is extended by a star (e.g., A\*) if check correction is selected. A further fundamental prerequisite for this correction method is the absence of MD remanence, since such remanence biases the pTRM\*-checks used for cumulative difference calculations [Leonhardt *et al.*, 2004]. In case of measurements with additivity checks, which should fall on the corrected pTRM\* values in the absence of MD grains, it is also possible to include check corrected analysis to the automatic determination (a check box appears). If selected, first noncorrected results satisfying class A will be searched. Then check correction is applied and a result with higher weighting factor is searched satisfying class A criteria. If both attempts are unsuccessful the calculation is repeated with class B criteria values. An example of a check corrected determination is shown in Figure 4. Figure 4a exhibits magnetomineralogical changes above 400°C as indicated by deviating pTRM\*-checks. The TR steps show no significant influence of MD remanence for this example (see next paragraph). After check correction, the additivity checks coincide with the pTRM\* values indicating successful correction and a linear segment covering most of the blocking temperature spectrum is obtained.

### 3.3. Detecting Multidomain Bias

#### 3.3.1. Independency Check

[26] Repeated demagnetization to  $T_i$  after a previous field-on step to  $T_i$  (TR step) is commonly used in absolute paleointensity experiments. Various different aspects were suggested to be monitored by the TR check. This check is applied for identifying thermal stabilization processes, continuous alteration, and magnetomineralogical changes affecting blocking temperatures above the actual heating step [Aitken *et al.*, 1988; McClelland and Briden, 1996; Valet *et al.*, 1996], as well as for monitoring tails of pTRM\* [Riisager and Riisager,

2001]. In general, the TR step monitors whether a pTRM\* ( $T_0$ ,  $T_i$ ) is completely removed during a zero-field heating/cooling cycle to  $T_i$  and thus failures to Thellier’s law of independence [Thellier, 1941]. The ThellierTool4.0 analyzes the differences between the first demagnetization step (TH) and the TR step regarding intensity and directional changes (Figure 1d). Decrease or increase of intensity due to pTRM\*-tails is dependent on the angular difference between magnetization of the sample and applied laboratory field [Yu and Dunlop, 2003; Leonhardt *et al.*, 2004]. If pTRM\*-tails are exclusively responsible for differences between TH and TR and do not affect unblocking temperatures above the next heating step to  $T = T_{i+1}$ , the extent of the pTRM\* tail can be estimated by

$$t^* = \frac{H_n}{H_{lab}} \left( \pm \left( dZ - \frac{dH}{\tan(\Delta\theta)} \right) \right) \text{ for } 180^\circ > \Delta\theta > 0^\circ, \quad (1)$$

where  $dH$  and  $dZ$  are the observed differences between TH and TR step and  $\Delta\theta$  is the angle between the applied field and the remaining NRM after the TH step [Leonhardt *et al.*, 2004]. Plus or minus ( $\pm$ ) is chosen dependent on the quadrant of the tangent, resulting in a positive value for  $t^*$  in case of a tail acquisition in direction of the applied field. For  $\Delta\theta = 0^\circ$ , the tail  $t^*$  cannot be identified. For  $\Delta\theta = 180^\circ$  the tail  $t^*$  corresponds to  $|H_{lab}/(H_n + H_{lab})dZ|$ . The tail parameter  $t^*$  normalized to the NRM ( $\delta t^*$ ) is shown in Figures 1d and 2d (lower left panel). Only positive values of  $\delta t^*$  can be attributed to tails.

#### 3.3.2. Additivity Check

[27] The additivity check was introduced by Krása *et al.* [2003] to detect multidomain behavior by checking the validity of Thellier’s law of additivity [Thellier, 1941]. For the additivity check a pTRM\* ( $T_0$ ,  $T_i$ ) is demagnetized partially by a heating/cooling cycle to  $T_k$  ( $T_k < T_i$ ). The remaining remanence  $M_{rem}$  is measured and vectorially subtracted from the pTRM\* ( $T_0$ ,  $T_i$ ) without prior isolation of this pTRM\*. Using this technique, any previous tail bias is subtracted as well. The resulting additivity check value can then be compared directly to the previously isolated pTRM\* ( $T_0$ ,  $T_k$ ). In the case of pure SD remanence,

$$M_{pTRM^*}(T_0, T_i) - M_{rem} = M_{pTRM^*}(T_0, T_k). \quad (2)$$

If the remanence is carried by MD particles the left-hand side of the equation will be larger than  $M_{pTRM^*}(T_0, T_k)$ . This test is sensitive to MD remanences with  $T_{ub} < T_b$ , which are causing the



concave up curvature of the Arai plot [Dunlop and Özdemir, 2000; Fabian, 2001].

[28] The additivity check also monitors alteration in the same way as the zero-field pTRM\*-check. Essentially, the measurement as well as the calculation of both zero-field pTRM\*-check as well as additivity check are the same. The true value of the additivity check, however, lies in its comparison with in-field pTRM\*-checks. This comparison allows us to distinguish between magnetomineralogical alteration and multidomain bias. This is not possible by applying any of the three checks alone. It thus allows us to validate results obtained by the check correction method of [Valet *et al.*, 1996]. In case of SD particles and added alteration the in-field pTRM\* check and the additivity check will both show the same value after check correction. This does not hold if MD particles are present.

#### 4. Determination Criteria and Discussion

[29] Standardization of the determination criteria is still an pressing issue in order to allow a more “objective” assessment of the published paleointensity data. This approach is supported by the program with the possibility to define sets of criteria. A set of criteria to analyze individual determinations is proposed in Figure 3. The values represent a set that has been shown to yield consistent results in paleointensity investigations on more than 500 samples of various locations, ages and volcanic rock types [e.g., Leonhardt and Soffel, 2002; Leonhardt *et al.*, 2003; Heunemann *et al.*, 2004]. Yet, these criteria, in particular  $f$ ,  $q$ ,  $N$ , directional and alteration limits are admittedly subjective. In comparison to other proposed criteria for paleointensity determination [Coe *et al.*, 1978; Selkin and Tauxe, 2000; Biggin and Thomas, 2003; Kissel and Laj, 2004] the suggested thresholds are rather rigorous. For  $f$ , however, Biggin and Thomas [2003] proposed a threshold of  $>50\%$ , in order to avoid the analysis of curved diagrams due to the presence of MD remanence. Other techniques to avoid such biases are suggested here and analyzed by the ThellierTool4.0. Therefore  $f \geq 30\%$  is assumed to be a reasonable limit as long as independency and/or additivity checks point to negligible MD bias.

[30] For estimating alteration the program calculates three parameters from which we use  $\delta(CK)$  and  $\delta(pal)$  as criteria.  $\delta(CK)$  is preferred over  $DRAT$  for two reasons: it does not overemphasize low temper-

ature steps, where the pTRM acquired is rather small and the amount of data points often is very high and it does not tolerate large check errors if the selected segment is long, which could occur when only few data points at high temperature steps are used.  $\delta(CK)$  generally shows smaller values than  $DRAT$ . From the analyzes of Brazilian and Siberian volcanics it is found that  $DRAT < 10\%$  if  $\delta(CK) < 7\%$  (class B criteria). Regarding the interpretation of  $\delta(pal)$ , one has to keep in mind that small paleointensities lead to relatively higher experimental errors, in particular regarding small variations of the applied field. Thus, having very low paleointensities, experimental variations and errors are likely to lead to an exceeding of the 5% (class A) or 10% (B) limit. In this case a lower limit for the absolute difference between corrected and noncorrected analysis of 1  $\mu T$  should be used to evaluate the determination. Prerequisite for an optimal calculation of  $\delta(pal)$  are consecutively performed checks over the whole temperature range.

[31] The thresholds for  $\delta(AC)$  and  $\delta(t^*)$  are based on experiments with synthetic magnetite samples with varying grain size [Krása *et al.*, 2003] and numerical modeling [Leonhardt *et al.*, 2004], which underlined the suitability of these criteria. The value of  $\delta(t^*)$ , however, is not significant for very small  $\Delta\theta$ , which has to be checked manually. Furthermore, the direction of the applied field has to be known for  $\delta(t^*)$  calculation, as well as for alteration correction. Only laboratory fields parallel to the z-axis of the sample are recognized by the software. For other field orientations independency checks, alteration correction and  $\delta(pal)$  are not calculated correctly. Negative values for  $\delta(t^*)$  are ignored as selection criteria by the program. Such negative values can be related to continuous changes of amount and configuration of domains [Heider *et al.*, 1988] or continuous destruction of remanence during repeated heating steps. Not supported by the program are criteria regarding within-site variations of paleointensity. Allowing only a 25% variation of the paleointensity values [Selkin and Tauxe, 2000] within a cooling unit creates problems when dealing with low intensities. For example, a variation of 3  $\mu T$  around a site mean paleointensity of 60  $\mu T$  is generally regarded as a highly reliable result. The same scatter around a mean value of 10  $\mu T$  would lead to a rejection of all results obtained from this cooling unit. Consequently, applying this criteria leads to a systematical bias of the accepted results toward higher values. Systematical bias in analyzing individual paleointensity experiments and/or large sets of data

can obscure important features of the variation of the Earth's magnetic field strength throughout its history.

[32] The ThellierTool4.0 supports the data format of the widely used Pmag Thellier program [Tauxe, 1998]. Therefore the laboratory exchange of raw data is simplified which is of importance in view of a public database for raw paleointensity data.

## 5. Conclusion

[33] The ThellierTool4.0 is an interactive software that is easy to use (available at <http://earthref.org/tools/>). It provides full vector analyses for all calculations. The data format is similar to that used by other programs, which allows direct comparison and might be a step toward a database of raw paleointensity data.

[34] Most of the modifications and improvements of the Thellier method are supported. The ThellierTool4.0 calculates all standard analysis parameters and allows assessment of the quality of determinations by evaluating different checks and thresholds as proposed in the literature.

[35] On the basis of published rock magnetic considerations we suggest a set of acceptance criteria which is, admittedly, also subjective. However, the ThellierTool4.0 allows the user to define its own criteria set and therefore to test the influence of certain thresholds on the results.

[36] Selection criteria can lead to a systematical bias of published paleointensity values and thus of the database. Avoiding such bias represents an very important issue when studying the variation of geomagnetic field throughout its past.

## Acknowledgments

[37] We would like to thank Yongxin Pan, Peter Riisager, and Fabio Donadini for helpful suggestions during development of the software. The journals referees and the associate editor are acknowledged for their helpful and constructive comments. Funding was provided by the German Science Foundation (DFG) in the framework of the priority program "Geomagnetic Variations" (R.L.: So72/67-3, C.H.: So72/66-2, D.K.: Pe173/12-2) and a fellowship of the German Academic Exchange Service (D.K.).

## References

Aitken, M. J., A. L. Allsop, G. D. Bussell, and M. B. Winter (1988), Determination of the intensity of the Earth's magnetic field during archaeological times: Reliability of the Thellier technique, *Rev. Geophys.*, **26**, 3–12.

- Arai, Y. (1963), *Secular variation in intensity of the past geomagnetic field*, M.Sc. thesis, 84 pp., Univ. Tokyo, Tokyo.
- Biggin, A. J., and D. N. Thomas (2003), The application of acceptance criteria to results of Thellier paleointensity experiments performed on samples with pseudo-single-domain-like characteristics, *Phys. Earth Planet. Inter.*, **138**, 279–287.
- Coe, R. S. (1967a), Paleointensity of the Earth's magnetic field determined from tertiary and quaternary rocks, *J. Geophys. Res.*, **72**, 3247–3262.
- Coe, R. S. (1967b), The determinations of paleointensities of the Earth's magnetic field with emphasis on mechanisms which could cause non-ideal behavior in Thelliers method, *J. Geomagn. Geoelectr.*, **19**, 157–179.
- Coe, R. S., S. Grommé, and E. A. Mankinen (1978), Geomagnetic paleointensities from radiocarbon-dated lava flows on Hawaii and the question of the Pacific nondipole low, *J. Geophys. Res.*, **83**, 1740–1756.
- Coe, R. S., J. Riisager, G. Plenier, R. Leonhardt, and D. Krása (2004), Multidomain behavior during Thellier paleointensity experiments: Results from the 1915 Mt. Lassen flow, *Phys. Earth Planet. Inter.*, **147**, 141–153.
- Dunlop, D. J., and O. Özdemir (2000), Effect of grain size and domain state on thermal demagnetization tails, *Geophys. Res. Lett.*, **27**, 1311–1314.
- Fabian, K. (2001), A theoretical treatment of paleointensity determination experiments on rocks containing pseudo-single or multi domain magnetic particles, *Earth Planet. Sci. Lett.*, **188**, 45–58.
- Goguitchaichvili, A., M. Prévot, J. Thompson, and N. Roberts (1999), An attempt to determine the absolute geomagnetic field intensity in southwestern Iceland during the Gauss-Matuyama reversal, *Phys. Earth Planet. Inter.*, **115**, 53–66.
- Heider, F., S. L. Halgedahl, and D. J. Dunlop (1988), Temperature dependence of magnetic domains in magnetite crystals, *Geophys. Res. Lett.*, **15**, 499–502.
- Heunemann, C., D. Krása, H. C. Soffel, E. Gurevitch, and V. Bachtadse (2004), Directions and intensities of the Earth's magnetic field during a reversal: Results from the Permo-Triassic Sibirian trap basalts, Russia, *Earth Planet. Sci. Lett.*, **218**, 197–213.
- Kirschvink, J. L. (1980), The least-squares line and plane and the analysis of paleomagnetic data, *Geophys. J. R. Astron. Soc.*, **62**, 699–718.
- Kissel, C., and C. Laj (2004), Improvements in procedure and paleointensity selection criteria (PICRIT-03) for Thellier and Thellier determinations: Application to Hawaiian basaltic long cores, *Phys. Earth Planet. Inter.*, **147**, 155–169.
- Krásá, D., C. Heunemann, R. Leonhardt, and N. Petersen (2003), Experimental procedure to detect multidomain remanence during Thellier-Thellier experiments, *Phys. Chem. Earth*, **28**, 681–687.
- Laj, C., C. Kissel, V. Scao, J. Beer, D. M. Thomas, H. Guillou, R. Muscheler, and G. Wagner (2002), Geomagnetic intensity and inclination variations at Hawaii for the past 98 kyr from core SOH-4: A new study and a comparison with existing contemporary data, *Phys. Earth Planet. Inter.*, **129**, 205–243.
- Leonhardt, R., and H. C. Soffel (2002), A reversal of the Earth's magnetic field recorded in mid-Miocene lava flows of Gran Canaria: Paleointensities, *J. Geophys. Res.*, **107**(B11), 2299, doi:10.1029/2001JB000949.
- Leonhardt, R., F. Hufenbecher, F. Heider, and H. Soffel (2000), High absolute paleointensity during a mid Miocene excursion of the Earth's magnetic field, *Earth Planet. Sci. Lett.*, **184**, 141–154.

- Leonhardt, R., J. Matzka, and E. A. Menor (2003), Absolute paleointensities and paleodirections from Fernando de Noronha, Brazil, *Phys. Earth Planet. Inter.*, **139**, 285–303.
- Leonhardt, R., D. Krása, and R. S. Coe (2004), Multidomain behavior during Thellier paleointensity experiments: A phenomenological model, *Phys. Earth Planet. Inter.*, **147**, 127–140.
- McClelland, E., and J. C. Briden (1996), An improved methodology for Thellier-type paleointensity determination in igneous rocks and its usefulness for verifying primary thermoremanence, *J. Geophys. Res.*, **101**, 21,995–22,013.
- Perrin, M. (1998), Paleointensity determination, domain structure, and selection criteria, *J. Geophys. Res.*, **103**, 30,591–30,600.
- Prévot, M., E. A. Mankinen, R. S. Coe, and S. Grommé (1985), The Steens Mountain (Oregon) geomagnetic polarity transition: 2. Field intensity variations and discussion of reversal models, *J. Geophys. Res.*, **90**, 10,417–10,448.
- Riisager, P., and J. Riisager (2001), Detecting multidomain magnetic grains in Thellier paleointensity experiments, *Phys. Earth Planet. Inter.*, **125**, 111–117.
- Selkin, P. A., and L. Tauxe (2000), Long-term variations in paleointensity, *Phil. Trans. R. Soc. London, Ser. A*, **358**, 1065–1088.
- Shcherbakov, V. P., E. McClelland, and V. V. Shcherbakova (1993), A model of multidomain thermoremanent magnetization incorporating temperature-variable domain structure, *J. Geophys. Res.*, **98**, 6201–6216.
- Shcherbakova, V. V., V. P. Shcherbakov, and F. Heider (2000), Properties of partial thermoremanent magnetization in pseudosingle domain and multidomain magnetite grains, *J. Geophys. Res.*, **105**, 767–781.
- Tauxe, L. (1998), *Paleomagnetic Principles and Practice*, 299 pp., Springer, New York.
- Thellier, E. (1941), Sur la vérification d'une méthode permettant de déterminer l'intensité du champ magnétique terrestre dans le Passé, *C. R. Hebd. Seances Acad. Sci.*, **212**, 281–283.
- Thellier, E., and O. Thellier (1959), Sur l'intensité du champ magnétique terrestre dans le passé historique et géologique, *Ann. Géophys.*, **15**, 285–376.
- Valet, J.-P., J. Brassart, I. Le Meur, V. Soler, X. Quidelleur, E. Tric, and P.-Y. Gillot (1996), Absolute paleointensity and magnetomineralogical changes, *J. Geophys. Res.*, **101**, 25,029–25,044.
- Yu, Y., and D. J. Dunlop (2003), On partial thermoremanent magnetization tail checks in Thellier paleointensity determination, *J. Geophys. Res.*, **108**(B11), 2523, doi:10.1029/2003JB002420.
- Zijderveld, J. D. A. (1967), AC demagnetization of rocks: Analysis of results, in *Methods in Palaeomagnetism*, edited by D. W. Collinson, K. M. Creer, and S. K. Runcorn, pp. 254–287, Elsevier, New York.