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Temperature dependence of the relationship of thermal diffusivity versus thermal conductivity for crystalline rocks

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Abstract Thermal diffusivity governs the transient heat transport equation. Thus, a realistic characterisation of this parameter and its temperature dependence is crucial for geothermal modelling. Due to sparse information from boreholes, lack of samples, and elaborate measurement procedures, there is often insufficient data on thermal diffusivity at elevated temperatures. We make use of existing data on crystalline (metamorphic and magmatic) rock samples from the Kola Peninsula and the Eastern Alps and develop a general relationship for the temperature dependence of thermal diffusivity up to 300°C. The temperature dependence of thermal conductivity is parameterised itself, using an empirical relationship which is set up for both data sets as well. Hence, only thermal conductivity at ambient temperatures is required for determining the temperature dependence of thermal diffusivity. We obtain different coefficients for both data sets which can be explained by different geological settings, and therefore different mineral compositions and internal structures. Comparisons with other expressions for these rock physical parameters show a good agreement at ambient conditions. General relations for thermal diffusivity at elevated temperatures are rare. A comparison of our results with data from two crystalline samples from the KTB and data from the Southern Indian Granulite Province highlights the need for further data, which will help to quantify uncertainties.

Keywords Geothermics · Rock physics · Temperature dependence · Thermal conductivity · Thermal diffusivity

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Introduction

The transient heat transport equation is governed by thermal diffusivity κ:

$$\frac{\partial T}{\partial t} = \kappa \nabla^2 T. \tag{1}$$

Therefore, an exact knowledge of the thermal diffusivity of rocks is of particular importance when studying the thermal regime of the Earth's crust. Thermal diffusivity is a function of thermal conductivity λ, density ρ, and specific heat capacity c_P:

$$\kappa = \frac{\lambda}{\rho\, c_P}. \tag{2}$$

Its temperature dependence is rather significant. The reason is the opposite behaviour of thermal conductivity and heat capacity with respect to temperature. While between 0 and 300°C thermal conductivity of rocks decreases in general, thermal capacity (the product of density and specific heat capacity) increases. The decrease of thermal conductivity with temperature is related to phonon scattering (Schatz and Simmons 1972; Beck 1988), described by a reciprocal behaviour and constants a (W^{-1} m) and b (W^{-1} K m):

$$\lambda = \frac{1}{aT + b}. \quad (3)$$

The temperature dependence of the specific heat capacity c_P of rocks can be described by a second-order polynomial (Kelley 1960), with coefficients A_i:

$$c_P = \sum_{i=0}^{2} A_i T^i. \quad (4)$$

From equation (4) it is obvious that specific heat capacity increases with temperature. The product of c_P and rock density ρ is called thermal capacity. Due to the small expansion coefficient of the rocks, density is considered constant within the temperature range studied here.

In this work, the main focus lies on the variation of thermal diffusivity with temperature. Based on data sets from different areas, the aim of this study is to set up an empirical relationship between thermal diffusivity at temperature T and thermal conductivity at ambient temperatures.

Measurement methods

The temperature dependence of thermal conductivity was determined by the divided bar method. The temperature ranges from ambient temperature up to 300°C. The general uncertainty of divided bar measurements is ±3%. The elaborate preparation of the samples and the duration of the measurement allow only determination of values at larger intervals and restricts the number of samples to be studied. As an example, Fig. 1 shows the measurements results for the seven samples from the Kola data set (see Sect. 2), including error bars. Measurement results for one sample (3200-612) were spoiled for temperatures above 140°C and therefore omitted. The lines in this figure represent the interpolation using Eq. (3). However, for deriving an empirical relationship for temperature dependence of thermal diffusivity, the original data is used. As far as the original orientations of the samples were known, the vertical component of thermal conductivity was determined. However, both data sets used here comprise measurements regarding anisotropy at ambient temperatures. This allowed to estimate the error of the values obtained here. The maximum anisotropy factor K, which represents the quotient of thermal conductivity parallel and perpendicular to bedding or foliation ($K = \lambda_{par}/\lambda_{per}$), is in both cases lower than 1.2 (Mottaghy et al. 2005; Vosteen and Schellschmidt 2003). The largest deviation between the vertical component and the effective thermal conductivity would occur with a dip angle of 45° of the bedding, yielding an error of about 5%. This is an acceptable uncertainty and thus is it justified to neglect anisotropy in our study.

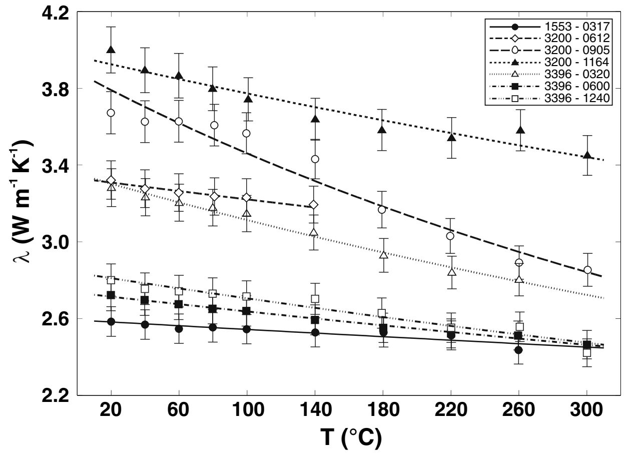

Fig. 1 Variation of thermal conductivity with temperature T for the samples from the Kola data set. *Error bars* indicate the uncertainty of the measurement of ±3%

The temperature dependence of the specific heat capacity was measured by a heat flux differential scanning calorimeter. Data was recorded every 100 m K at a heating rate of 200 m K min^{-1}. The uncertainty of this method is ±1%. Figure 2 shows the procedure of data acquisition, again for a sample from the Kola data set. The dark grey line indicates the temperature range which is used to interpolate the data [Eq. (4)].

Sample mass was measured with laboratory scales. The rock volume was determined with a gas displacement pycnometer. The uncertainty of this method is ±0.06%. From this, the rock density ρ can be computed which is needed for the determination of thermal diffusivity κ [Eq. (2)].

We neglect the influence of pressure on thermal diffusivity, since the temperature range observed here corresponds to depth of about 17 km in the Kola area and about 12–15 km in the Alps. Estimating the pressure in these depths by a lithostatic pressure gradient at a mean density of 2,900 kg m^{-3} yields about 0.5 and 0.4 GPa, respectively. As outlined in Ray et al. (2006), a first order correction of about 10% GPa^{-1} would result in an increase of about 5 and 4%, respectively. This is in the order of the uncertainty, and can therefore be neglected. Furthermore, we selected those samples which showed no thermal cracking after the measurements at elevated temperatures, assuring that no sample alteration occurred which might influence the results.

Data

Two independent data sets of crystalline rocks are used to determine the temperature dependence of thermal diffusivity, one from the Eastern Alps and one from the Kola Peninsula. Although rocks of quite similar genesis were

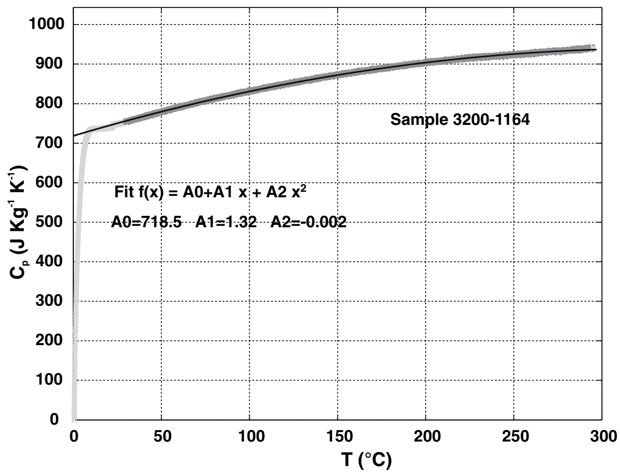

Fig. 2 Variation of specific heat capacity with temperature T for a sample of serpentinite from the Kola data set. The *light-grey line* show all acquired data, whereas the *dark-grey line* indicates the range used for interpolation. The *black line* represents the fit of which the coefficients are given. *Error bars* are omitted in favour of better viewing

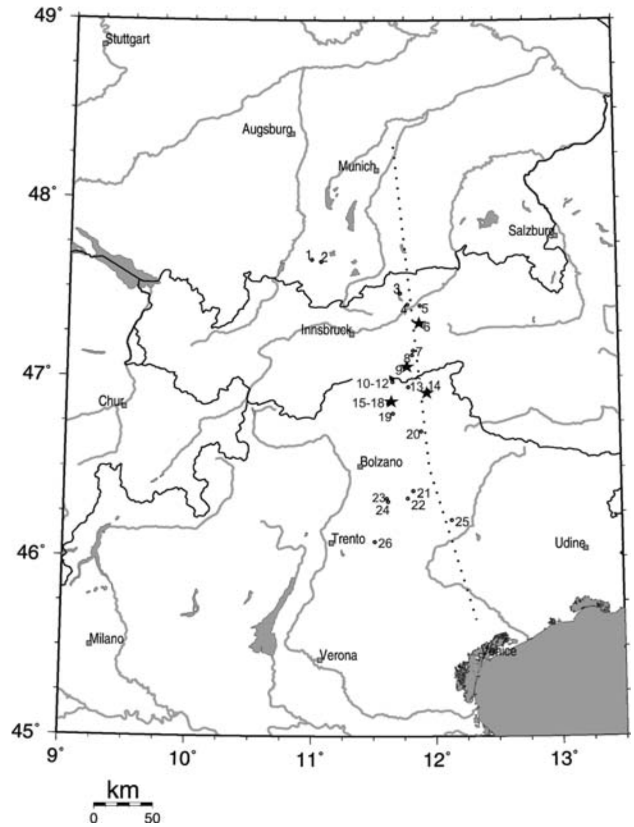

Fig. 3 TRANSALP profile (*dotted line*) and sampling locations 1–26 (from north to south). The samples for this study originate from the locations marked by *asteriks*

considered in both sets, their origin from different geological provinces and their different age might imply different thermophysical properties. Therefore, we cannot expect a universally valid relationship for the temperature dependence of thermal diffusivity.

Transalp

The objective of the TRANSALP campaign was to investigate the deep structure and the dynamic evolution of the Eastern Alps. This was mainly done by means of a reflection and refraction seismic profile between Munich and Venice (TRANSALP Working Group 2002). Besides to that, the complex geology of the Eastern Alps leads to the exposure of various strata at the Earth's surface, originating from different depth levels of the European and Adriatic plate. Keeping this in mind, a rock sampling campaign at 26 different locations along the TRANSALP profile was carried out (see Fig. 3). This yielded a set of 118 sedimentary and crystalline (magmatic and metamorphic) rocks (Vosteen et al. 2003; Vosteen and Schellschmidt 2003). At all these rock samples extensive laboratory measurements of thermal conductivity, specific heat capacity and density were carried out. The temperature dependence of thermal conductivity and specific heat capacity was determined upon 16 rock samples. A subset of seven crystalline rocks where chosen for this study, shown in Table 1. A detailed description of sampling strategy and measurement techniques can be found in Vosteen et al. (2003) and Vosteen and Schellschmidt (2003).

Kola

We also used a data set of boreholes from the immediate surroundings of the Russian ultra-deep borehole on the Kola Peninsula (SG-3), shown in Fig. 4. The details of this survey are described by Mottaghy et al. (2005). This superdeep borehole is located on the northern rim of the Fennoscandian (Baltic) Shield at 69°23′N, 30°36′E. It is the deepest borehole in the world to date. Situated in the Pechenga ore district, its distance to the Barents Sea is about 50 km (Fig. 4). During the Weichselian period the Kola Peninsula was covered by glaciers, producing a topography at elevation ranging between 300 and 400 m above sea level in the measurement area. The bedrock of Proterozoic and Archaean age is covered by Quaternary glacial sediments, typically only a few meters thick at most. The bedrock consists mainly of metavolcanic, metasedimentary or igneous rocks, and forms a syncline structure.

For SG-3 as well as for most of the shallower boreholes, laboratory measurements of thermal conductivities and heat capacities were available (1,375 samples), and for nine samples temperature-dependent properties were measured.

Table 1 Thermal conductivity (λ), rock density ρ, and specific thermal capacity (c_P) at ambient temperatures for the Transalp rock samples (Vosteen and Schellschmidt 2003)

Sample	Rock type	λ (W m^{-1}K^{-1})	ρ (kg m^{-3})	c_P (J kg^{-1}k^{-1})
L06/3	Quartz–phyllite	2.87	2.83	799
L09/5	Gabbro	1.52	2.94	771
L10/6	Amphibolite 1	2.53	2.94	774
L17/1	Amphibolite 2	2.16	3.02	769
L11/5	Ortho-gneiss	2.18	2.66	769
L14/1	Paragneiss 1	3.37	2.74	760
L16/4	Paragneiss 2	2.03	2.73	776

Seven of these samples are used for the study of the temperature dependence of thermal diffusivity. Table 2 shows all three properties for the Kola rock samples.

A general relationship between $\lambda(T)$ and $\lambda(0)$

First, a relationship for the temperature dependence of thermal conductivity is derived. The detailed procedure is described in Vosteen and Schellschmidt (2003). The resulting equations allow the determination of thermal conductivity at temperatures T if only its value at ambient conditions ($\approx$25°C) is known. With thermal conductivity at 0°C varying from 1.4 to 3.5 W m^{-1} K^{-1} and for temperatures up to 300°C, it follows from Vosteen and Schellschmidt (2003) for crystalline, alpine rocks:

$$\lambda(0)_{\text{alp}} = 0.53\lambda(25°\text{C}) + \frac{1}{2}\sqrt{1.13(\lambda(25°\text{C}))^2 - 0.42\lambda(25°\text{C})} \tag{5}$$

$$\lambda(T)_{\text{alp}} = \frac{\lambda(0)}{0.99 + T(a - b/\lambda(0))}. \tag{6}$$

Here, a = 0.0030 ± 0.0015 K^{-1} and b = 0.0042 ± 0.0006 W m^{-1} K^{-2}.

For the Kola rock samples in Table 2, the similar approach yields the relations, also for temperatures up to 300°C:

$$\lambda(0)_{\text{kola}} = 0.52\lambda(25°\text{C}) + \frac{1}{2}\sqrt{1.09(\lambda(25°\text{C}))^2 - 0.36\lambda(25°\text{C})} \tag{7}$$

$$\lambda(T)_{\text{kola}} = \frac{\lambda(0)}{1.00 + T(a - b/\lambda(0))}. \tag{8}$$

Here, a = 0.0017 ± 0.0007 K^{-1} and b = 0.0036 ± 0.0014 W m^{-1} K^{-2}. Figure 5 visualises the different relationships for both data sets, using λ = 2.5 W m^{-1} K^{-1} as an example.

Determining $\kappa(T)$ from $\lambda(0)$

In order to develop a relationship for thermal diffusivity κ at varying temperature T, we firstly plot thermal diffusivity versus thermal conductivity for every temperature where measurements are available. The result is shown for the Transalp rock samples in Fig. 6 and for the Kola rock samples in Fig. 7. The symbols in the figures indicate the measured values, whereas the lines represent linear regressions at different temperatures. The reciprocal slope of each of these linear regressions yields another linear relationship (Fig. 8). This allows to determine thermal diffusivity at any temperature, only based upon the known temperature dependence of thermal conductivity:

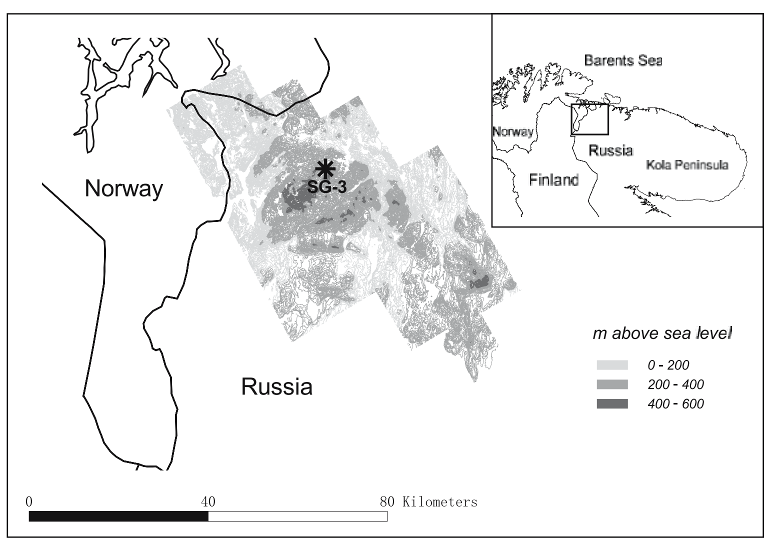

Fig. 4 Location of the Kola super-deep borehole SG-3. Samples from shallow holes in the immediate vicinity are used in this study

Table 2 Thermal conductivity (λ), rock density ρ, and specific thermal capacity (c_P) at ambient temperatures for the Kola rock samples (Mottaghy et al. 2005)

Borehole	Rock type	λ (W m^{-1}K^{-1})	ρ (kg m^{-3})	c_P (J kg^{-1}k^{-1})
1553-317	Ultramafic	2.6	3.04	784.5
3200-612	Metavolcanic	3.3	2.88	776.5
3200-905	Basic magmatic	3.7	2.97	771.8
3200-1164	Metavolcanic	4.0	2.85	816.5
3396-320	Gneiss	3.3	2.63	747.9
3396-600	Gneiss	2.7	2.62	740.7
3396-1240	Amphibolite	2.8	3.06	745.3

$$\kappa(T) = f(\lambda(T)) = \lambda(T)\frac{1}{mT+n}.(10^{-6}\,\mathrm{m}^2\,\mathrm{s}^{-1}). \qquad (9)$$

For the Transalp rock samples, the coefficients are $m = 0.0022 \pm 0.0004$ MJ m^{-3} K^{-2} and $n = 2.066 \pm 0.070$ MJ m^{-3} K^{-1}. Regarding the Kola samples we obtain $m = 0.0036 \pm 0.0005$ MJ m^{-3} K^{-2} and $n = 2.404 \pm 0.091$ MJ m^{-3} K^{-1}. With Eqs. (5)–(8) it is now possible to determine thermal diffusivity at temperatures T from 0 to 300°C. The only required input is thermal conductivity at ambient temperature. Table 3 summarises the derived equations and coefficients. Following the example for thermal conductivity from above, Fig. 9 shows variation of thermal diffusivity with temperature for $\lambda = 2.5$ W m^{-1} K^{-1} at ambient conditions.

Discussion

Our results confirm our assumption about a different thermal behaviour of crystalline rocks from different geological settings. The terms magmatic and metamorphic are based on a rock's genesis, but have little significance in terms of physical properties which can be influenced by different mineral composition and texture. From Fig. 8 it becomes obvious that a joint relationship for both data sets cannot be established. At ambient temperatures, heat capacity is about 15% higher in the case of the Kola data set. This deviation increases with temperature to slightly above 20% at 300°C. The expressions for thermal conductivity are obviously different as well [Eqs. (5)–(8)]. For the example shown in Fig. 5, the deviation increases with temperature, going up to 20% at 300°C. This in turn results in a different behaviour for the temperature dependence of thermal diffusivity, as seen in Fig. 9. In this case, both expressions differ by about 20% at ambient conditions, but they nearly match at 300°C. This figure also shows the large variation of thermal diffusivity with temperature. Regarding the Transalp samples and the Kola samples in a temperature range from 10 to 300°C, thermal diffusivity decreases by 50 and 35%, respectively.

Thus, we argue that care must be taken when using general expressions for thermal diffusivity and its temperature dependence. A realistic characterisation of thermal parameters is crucial for a wide field of research, including downward continuation of lithospheric data, geothermal energy, thermal modelling in general, as well as palaeoclimatic studies using subsurface temperatures. On the other hand only the acquisition of extensive data sets can yield reliable mean values with corresponding uncertainties.

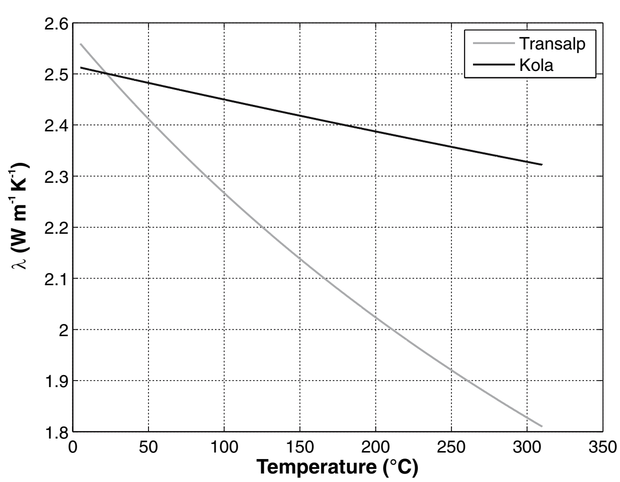

Fig. 5 Calculated variation of thermal conductivity for both data sets using Eqs. (5)–(8) and λ (25°C) = 2.5 W m^{-1} K^{-1}

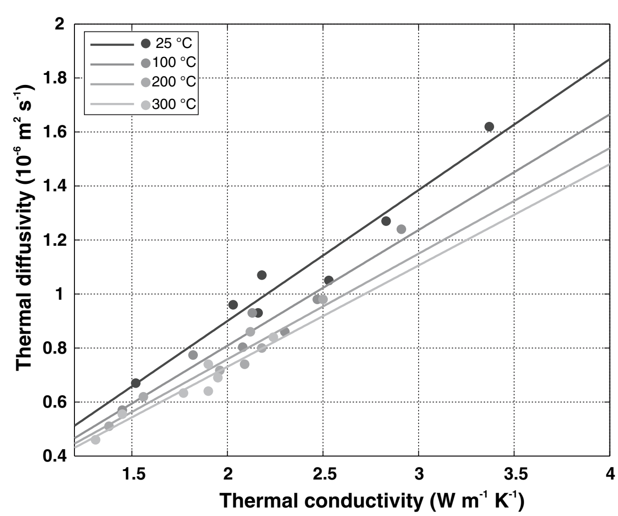

Fig. 6 Temperature dependence of the κ–λ relation for the Transalp rock samples. The *symbols* show the evaluated measurements and the *lines* indicate the associated linear regressions

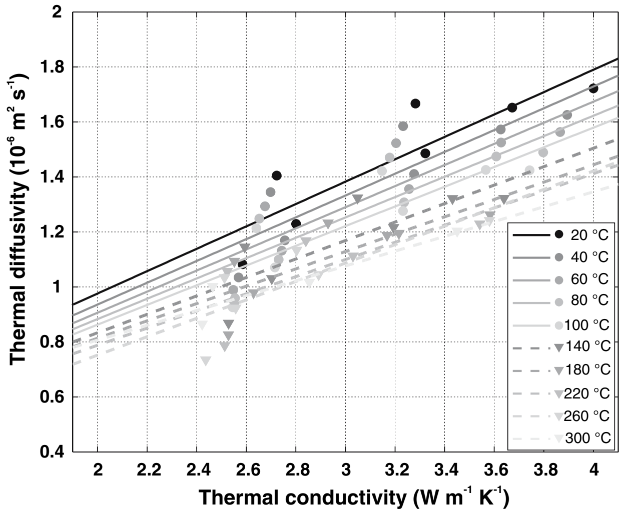

Fig. 7 Temperature dependence of the κ–λ relation for the Kola rock samples. The *symbols* show the evaluated measurements and the *lines* indicate the associated linear regressions

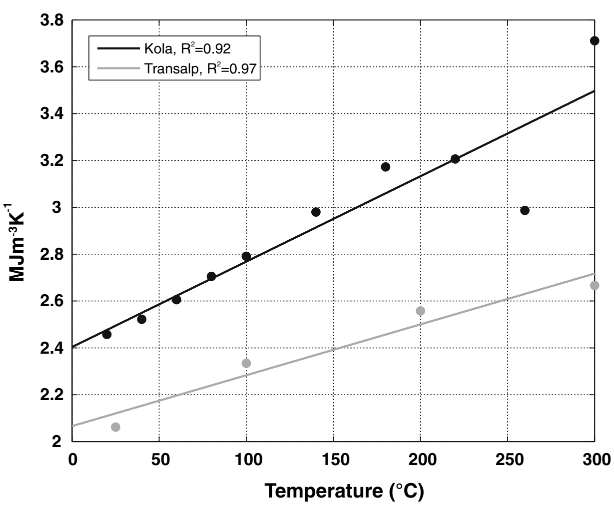

Fig. 8 Temperature dependence of the reciprocal slope (heat capacity ρ c_P) of the linear relations shown in Figs. 6 and 7

Comparison with other expressions

Beck (1988) states that thermal capacity ρc_P at ambient conditions and for a great majority is 2.3 MJ m^{-3} K^{-1} ± 20%. This allows to determine thermal diffusivity κ (10^{-6} m^2 s^{-1}) at ambient conditions from thermal conductivity λ (W m^{-1} K^{-1}):

$$\kappa = c \cdot \lambda, \tag{10}$$

with an empirical constant $c =$ 0.44 ± 0.09 MJ^{-1} m^3 K. Equation (10) agrees with both data sets [see Eq. (9); Fig. 8]. Another empirical relationship for the thermal diffusivity as a function of thermal conductivity was set up by Kukkonen and Suppala (1999), based on measurements

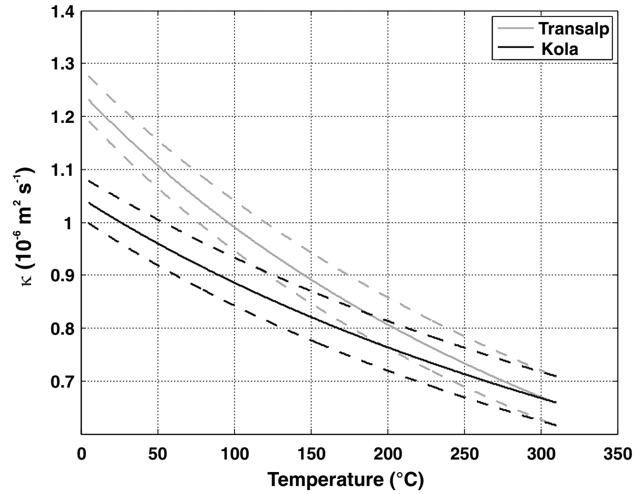

Fig. 9 Calculated variation of thermal diffusivity for both data sets using Eq. (9) and λ (25°C) = 2.5 W m^{-1} K^{-1}. The *dashed lines* give an estimation due to the uncertainties which arise from the linear regressions shown in Figs. 7 and 8, corresponding to the parameters *m* and *n* given in Table 3

on rocks from different Finnish sites (Kukkonen and Lindberg 1998). Their corresponding equation takes the form:

$$\kappa = -0.2 + c \cdot \lambda, \tag{11}$$

with c = 0.53, λ in W m^{-1} K^{-1} and κ in 10^{-6} m^2 s^{-1}. This is shown in Fig. 10, where thermal diffusivity is plotted versus thermal conductivity at ambient temperature. Both, our measurements and the empirical relations by Kukkonen and Suppala (1999) are consistent with the findings of Beck (1988): all values lie within the range which results from a variation of thermal capacity by ±20% (grey lines).

Due to a lack of the required suite of rock physical properties, there are far more studies regarding the temperature dependence of thermal conductivity than those regarding thermal diffusivity. For a comparison with the results of the Transalp project and references therein, see Vosteen and Schellschmidt (2003). Seipold and Huenges (1998) presents a study of the temperature dependence of thermal properties of samples from the KTB-borehole. The rocks (gneiss and amphibolite) are comparable to those used here. In their study, data is fitted to the following equation, valid for a temperature range from 20 to 500°C:

$$\kappa(T) = 1/(A + B \cdot T) + C \cdot T^3 (10^{-6}\,\mathrm{m}^2\,\mathrm{s}^{-1}), \tag{12}$$

with coefficients A = 1.25, B = 2.13 × 10^{-3}, and C = 1.25 × 10^{-10} for one amphibolite sample. For a paragneiss sample, they obtain A = 7.79 × 10^{-1}, B = 2.55 × 10^{-3}, and C = 1.15 × 10^{-10}. Figure 11 shows that the derived relationships for the Kola and Transalp rock samples cannot describe the temperature dependence of thermal diffusivity

Table 3 The temperature dependence of thermal conductivity λ and thermal diffusivity κ determined in this study

Location	Parameter
Transalp	$\lambda(0)_{\mathrm{alp}} = 0.53\lambda(25°\mathrm{C}) + \frac{1}{2}\sqrt{1.13(\lambda(25°\mathrm{C}))^2 - 0.42\lambda(25°\mathrm{C})}$
	$\lambda(T)_{\mathrm{alp}} = \frac{\lambda(0)}{0.99 + T(a - b/\lambda(0))}$
	$a = 0.0030 \pm 0.0015\ \mathrm{K}^{-1}$, $b = 0.0042 \pm 0.0006\ \mathrm{W\ m}^{-1}\ \mathrm{K}^{-2}$
	$\kappa(T)_{\mathrm{alp}} = \lambda(T)_{\mathrm{alp}} \frac{1}{mT+n}$
	$m = 0.0022 \pm 0.0004\ \mathrm{MJ\ m}^{-3}\ \mathrm{K}^{-2}$, $n = 2.066 \pm 0.070\ \mathrm{MJ\ m}^{-3}\ \mathrm{K}^{-1}$
Kola	$\lambda(0)_{\mathrm{kola}} = 0.52\lambda(25°\mathrm{C}) + \frac{1}{2}\sqrt{1.09(\lambda(25°\mathrm{C}))^2 - 0.36\lambda(25°\mathrm{C})}$
	$\lambda(T)_{\mathrm{kola}} = \frac{\lambda(0)}{1.00 + T(a - b/\lambda(0))}$
	$a = 0.0017 \pm 0.0007\ \mathrm{K}^{-1}$, $b = 0.0036 \pm 0.0014\ \mathrm{W\ m}^{-1}\ \mathrm{K}^{-2}$
	$\kappa(T)_{\mathrm{kola}} = \lambda(T)_{\mathrm{kola}} \frac{1}{mT+n}$
	$m = 0.0036 \pm 0.0005\ \mathrm{MJ\ m}^{-3}\ \mathrm{K}^{-2}$, $n = 2.404 \pm 0.091\ \mathrm{MJ\ m}^{-3}\ \mathrm{K}^{-1}$

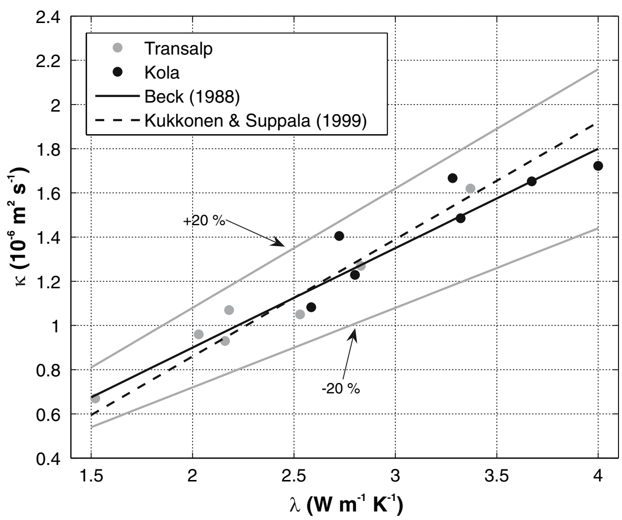

Fig. 10 Thermal diffusivity versus thermal conductivity at ambient temperatures for the samples studied, in comparison to the empirical relations found by Kukkonen and Suppala (1999) and Beck (1988). The *grey lines* define the upper and lower bound of Eq. (10)

of these two samples. It is systematically lower, with higher initial values for the gneiss sample, due to a higher thermal conductivity at ambient temperatures ($\lambda = 3.36$ W m^{-1} K^{-1}) of the quartz-rich gneiss sample. The value for the amphibolite sample is $\lambda = 2.6$ W m^{-1} K^{-1}. These two values entered Eqs. (5)–(9) for comparison. Although there are only two samples regarded by Seipold and Huenges (1998), it becomes clear that studying the temperature dependence of similar rock types does not necessarily imply a similar behaviour.

A more recent work by (Ray et al. 2006) proposes a relationship for granulitic rocks for a temperature range from 20 to 450°C. The following equation is obtained, using results from thermal diffusivity measurements on 16 samples from the Southern Indian Granulite Province:

$$\kappa(T) = 0.7 + 144\frac{\kappa_{\mathrm{amb}} - 0.7}{T - 150}\ (10^{-6}\ \mathrm{m}^2\ \mathrm{s}^{-1}), \quad (13)$$

where κ_{amb} is thermal diffusivity at ambient conditions and T is temperature in Kelvin. Figure 12 shows a comparison with our findings, using $\lambda = 2.5$ W m^{-1} K^{-1} at ambient conditions which corresponds to $\kappa_{\mathrm{alp}} = 1.19 \times 10^{-6}$ m^2 s^{-1} and $\kappa_{\mathrm{kola}} = 1.01 \times 10^{-6}$ m^2 s^{-1} at ambient conditions for the Transalp and Kola relation, respectively. These values are then used for κ_{amb} in Eq. (13). Up to 100°C, a satisfactory agreement is observed, but the deviation between the different expressions for thermal diffusivity increases and reaches about 20% at 300°C.

Conclusions

We studied the temperature dependence of thermal diffusivity of a set of crystalline rocks from different origins. Due to the inhomogeneous composition of crystalline rocks, it is nearly impossible to establish general expressions for rock properties which are universally valid. However, our study aims at a first estimation of the thermal dependence of thermal diffusivity up to 300°C. We set up an empirical relationship for both sets of rock samples, if only thermal conductivity at ambient temperatures is known. These equations can be used for numerical simulation of transient heat transport processes in the crystalline basement.

However, two important issued must be considered here. First, we are aware that the presented empirical relations only rely on few samples. However, the extensive measurement procedure, especially of the temperature dependence of thermal conductivity, limits the number of measurements. Second, the difference in the relationships developed here implies that they cannot easily be applied to crystalline rocks from other origins. Thus, we point out the importance of the choice of a particular relationship for the temperature dependence of thermal diffusivity. For geothermal studies on rocks from other areas than discussed here, we suggest either choosing appropriate

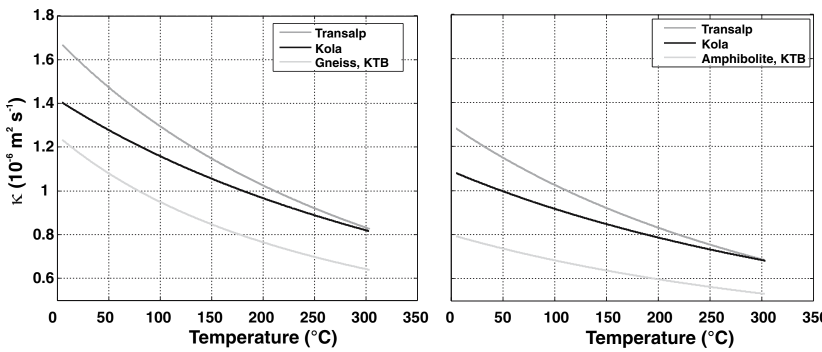

Fig. 11 The temperature dependence of thermal diffusivity determined in this study in comparison with results from two KTB samples (Seipold and Huenges 1998)

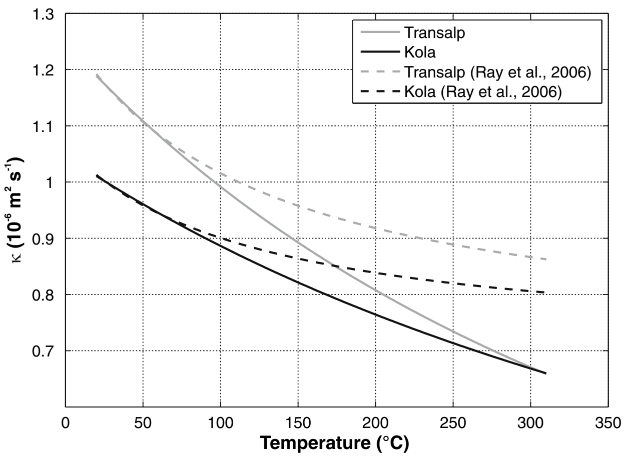

Fig. 12 The temperature dependence of thermal diffusivity determined in this study in comparison with a relationship obtained by Ray et al. (2006)

parameters from the literature, if available, sensitivity studies, or even new measurements. This is certainly welcome, since more data on the temperature dependence of thermal diffusivity is needed in general. At this point it must be emphasised that data on thermal diffusivity is also lacking for the shallow subsurface where ground heat exchangers are installed. An realistic prediction of their transient, long term behaviour depends on a precise knowledge of thermal diffusivity. However, in the shallow subsurface other effects like saturation and groundwater flow play a role, and the temperature range is between about 10 and 20°C, being much lower than the temperatures studied here. Therefore, a similar study about thermal diffusivity addressing this topic is highly desirable.

To summarise, our study will help to improve existing empirical models and constrain the the inevitable uncertainties, and therefore contribute to our understanding of the thermal regime of the crust.

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