Some features of the temperature-pressure dependence of the effective thermal conductivity of rocks

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Abstract. We have studied the behavior of the effective thermal conductivity of rocks (as natural heterogeneous materials) for the pressure range 0.1-400 MPa (initial region) and the temperature range 273-523 K. We propose a low-parametric empirical equation with great accuracy describing the effective thermal conductivity dependence, and discuss the physical meaning of its parameters.

1. Introduction

As is well known, the temperature dependence of the thermal conductivity \( \lambda(T) \) of dielectrics is very sensitive to the crystal structure, compressibility, and elastic constants. Indeed, if heat transfer in solids with an ordered crystalline structure has a wave character and its temperature dependence is described as \( \lambda(T) \sim T^{-1} \) [1,2], then in solids with an amorphous structure then, in solids with an amorphous structure, heat transfer is of an activation nature and their temperature dependence obeys to \( \lambda(T) \sim T^{0.5} \). The atoms of disordered crystalline bodies occupy the correct position in the nodes of the crystal lattice, but the order of arrangement of atoms of various kinds is not observed. In addition, lattice defects and block boundaries have a significant impact. All these reasons lead to the complex nature of the heat transfer process in multicomponent structures with complex and variable ordering. Nevertheless, in the general case, as shown in recent works (see, for example, [3, 4], as well as references in these publications), the temperature dependence of the effective thermal conductivity for most natural and artificial heterogeneous materials at a fixed pressure is fairly well described by the power law:

\[
\lambda(T) \propto \left(T\right)^n.
\]

(1.1)
Most of the papers aimed at studying the thermal conductivity of rocks, including recent ones [5-7], concentrates on the effect of temperature without consideration of the pressure. However, pressure has a significant effect on many physical parameters. In particular, internal stresses arise with the pressure, and it lead to a decrease in the inter-atomic distance and the amplitude of atomic vibrations, and increase their maximum frequency [8–10] changing the Debye temperature. According to theoretical calculations carried out by the authors of [9–11] based on the Leibfried–Sheiman equation, the lattice thermal conductivity should linear increase with pressure following the increase in the maximum frequency of atomic vibrations. This linear approximation can be used after some pressure (~ 100 MPa) and in isolation from the temperature dependence [12], nevertheless it is not entirely adequate for the initial near-zero region, where the kinetics of grain boundary processes can be significantly changed due to the increasing the maximum vibration frequency of defects.

The present work is devoted to the construction of a model of thermal conductivity of rocks and artificial heterogeneous materials in the region of 0.1–400 MPa based on an analysis of experimental dependences.

2. Experiment
For a detailed analysis of the experimental temperature and pressure dependences of thermal conductivity, we took the following rock data: granite (Republic of Dagestan, occurrence depth about 3 km, porosity 1%, density $\rho = 3.2$ g/cc) of fine-grained sandstone (Republic of Dagestan, occurrence depth about 4.9 km, open porosity 7%, density $\rho = 2.28$ g/cc) and marl (Sukhokumskoye oil and gas field, well No. 22, occurrence depth about 3.8 km, porosity 11.3% and density $\rho = 2.57$ g/cc).

We carried out the measurements in the pressure range from 0.1 to 400 MPa and the temperature range of 273–523 K by the absolute stationary method, the error of which doesn’t exceed 3-4%. Tables of the obtained values of thermal conductivity were published in our recent works [3, 4].

For the studied granite and sandstone samples, the sign of $n$ is negative (-0.72 and -0.32 at atmospheric pressure, respectively), for the marl, it is positive (0.368 at atmospheric pressure). Thus, we considered heterogeneous materials with different degrees of ordering: from close to polycrystalline (studied granite), to close to amorphous (marl).

3. Results and discussion
Applying the equation (1.1) to the variable $(T)$ and to the fixed $(T_0)$ temperatures, we obtain:

$$\lambda(T, P) = \lambda(T_0,0) \cdot f_{T_0}(P) \cdot \left(\frac{T}{T_0}\right)^{n(P)}, \quad (3.1)$$

where $\lambda(T_0, P)$ is the baric dependence of thermal conductivity at a fixed temperature $T_0$ and

$$f_{T_0}(P) = \frac{\lambda(T_0, P)}{\lambda(T_0,0)}. \quad (3.2)$$

If to determine the functions $\delta_{T_0}(P)$ and $\nu(P)$ as:

$$\delta_{T_0}(P) = f_{T_0}(P) - 1 \quad (3.3)$$

and

$$\nu(P) = 1 - \frac{n(P)}{n_0}, \quad (3.4)$$

accordantly, then the equation (3.1) can be rewritten as:
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\[ \lambda(T,P) = \lambda(T_0,0) \cdot \left[ 1 + \delta(T_0) \left( \frac{T}{T_0} \right)^{\nu(P)} \right]^{n_0(1-\nu(P))}. \] (3.5)

The value \( n_0 \) and the function \( \nu(P) \) are independent of the choice of a fixed temperature \( T_0 \) and are therefore objective parameters, while the function \( \delta(T_0) \) parametrically depends on \( T_0 \), and since its choice is subjective, the physical meaning of the empirical coefficients describing this function is rather arbitrary and requires additional research. Nevertheless, from equation (3.5) it is easy to find that the dependences \( \delta(T_0) \) for two fixed temperatures \( T_0^* \) and \( T_0 \) are correlated as:

\[ \delta(T_0^*) = \left[ 1 + \delta(T_0) \left( \frac{T_0^*}{T_0} \right)^{\nu(P)} \right]^{-n_0(1-\nu(P))}. \] (3.6)

Equation (3.5) is convenient for comparative analysis, where the absolute values of thermal conductivity differ greatly. About the physical meaning of the quantities included this equation, first of all, the absolute value and the sign of \( n_0 \) determine the degree of ordering for zero pressure (the atmospheric pressure for our pressure ranges 0.1 - 400 MPa can be considered very close to zero): the value \( \leq -1 \) The change in the nature of the temperature dependence (and, therefore, the ordering) with the pressure is determined by the function \( \nu(P) \), which is determined by equation (3.4). As a rule this function has a positive sign and the absolute value \( \ll 1 \) over the entire pressure diapason (at least up to 400 MPa, see figure 1 (a) ).

The pressure dependence of the effective thermal conductivity for the fixed temperature \( T_0 \), as it is clear from equation (3.4)-(3.5), is completely determined by \( \lambda(T_0,0) \) and \( \delta(T_0) \). The functions \( \nu(P) \) and \( \delta(T_0) \) (for two selected reference temperatures) for marl, sandstone, and granite are shown in figure 1.

\[ \nu(P) \]
\[ \delta(T_0=273K) \]
\[ \delta(T_0=473K) \]

Figure 1. The functions \( \nu(P) \) (a) \( \delta(T_0=273K) \) (b) \( \delta(T_0=473K) \) (c) for: (1) granite; (2) sandstone and (3) marl.
Figure 2. The result of the calculation of thermal conductivity according to equation (3.1) with experimental values $\lambda(T_0, P)$ and $\mu(P)$ (solid lines) and according to equation (3.5) with parameters $\delta_{T_0}(P)$ and $\nu(P)$ calculated by (3.7)-(3.8) (dotted lines) together with the initial experimental data (symbols): (a) granite, (b) sandstone.

For all our materials we can see a significant weakening of the temperature dependence of effective thermal conductivity with pressure, which is characterized by the function $\nu(P)$. At the same time, we can see the increase of the thermal conductivity with pressure ($\delta_{T_0}(P)$, see figure 1 (b),(c) ).

Figure 2 shows the result of calculating the effective thermal conductivity of granite and sandstone, respectively, according to equation (3.1) (solid lines, $T_0=273$ K) and according to equation (3.5) (dotted lines) using the empirical estimates

$$\nu(P) = \delta_{473K}(P) = (P(MPa)/3500)^{0.56}$$

(3.7)

for granite and

$$\nu(P) = \delta_{1700K}(P) = (P(MPa)/6.021 \cdot 10^4)^{0.67}$$

(3.8)

for sandstone. In the latter case, an additional recalculation of $\delta_{1700K}(P)$ was done according to equation (3.6).

Thus, with a certain choice of a fixed temperature $T_0$, both pressure dependences $\nu(P)$ and $\delta_{T_0}(P)$ can be described in one simple approximation, which reduces the number of parameters of the general temperature-pressure description while maintaining a sufficiently high accuracy.

4. Conclusion
The temperature-pressure dependence of the effective thermal conductivity of rocks as natural inhomogeneous materials has been investigated on the example of samples of granite, sandstone and marl. It was found that an increase in pressure, as a rule, leads to a decrease in the temperature dependence of the effective thermal conductivity and a certain increase in thermal conductivity.

A low-parameter description of the $PT$-dependence of the effective thermal conductivity is proposed using one temperature and two baric components, one of which describes the behaviour of
the power-law coefficient of the temperature dependence, and the other describes the isothermal pressure dependence.

5. References

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