Heat transfer in materials with a disordered structure

L A Marushin and D A Tikhonova
Moscow Polytechnic University, 16 Avtozavodskaya street, Moscow, 115280, Russia

E-mail: dashuta155@yandex.ru

Abstract. The article discusses the issue of the heat transfer in amorphous materials with an expressed crystal structure in detail. Based on the accumulated amount of experimental data on the processes of heat transfer in materials, the authors analysed the thermophysical mechanisms of heat transfer in non-ferrous metal alloys: aluminium alloys (AD-1; D 16, etc.), Constantan copper alloy and titanium alloys. The temperature dependences of the thermal conductivity of materials, in which heat transfer is determined by conduction electrons, are shown graphically.

1. Introduction
Experimental temperature dependence of thermal conductivity of conductive materials (figure 1), where for various known materials temperature $T_{\text{MAX}}$ corresponds to the maximum value of thermal conductivity $\lambda_{\text{MAX}}$, the values of which are from $\approx 2$ to $\approx 50$ K.

It was established experimentally that in cleaner and more advanced materials, the maximum thermal conductivity value $\lambda_{\text{MAX}}$ is higher and corresponds to lower temperatures $T_{\text{MAX}}$. On the contrary, with the deterioration of the quality of the material, its maximum thermal conductivity decreases, and the corresponding temperature $T_{\text{MAX}}$ shifts towards higher temperatures.

When melting, the thermal conductivity values usually undergo a discontinuous change caused by structural changes. In electrically conductive materials during their melting, the thermal conductivity usually decreases and with a subsequent increase in temperature varies slightly. It should be noted that the data on the thermal conductivity of this class of substances (as a rule, metals) in the liquid state are
very contradictory: for the same material, according to one data, the thermal conductivity increase
with increasing temperature, according to others it decreases, [1]. This is due to the great difficulty of
measuring the thermal conductivity of the melts and its rather high error. The magnitude of the error (± 15–20%) most often exceeds the limits of the temperature variation of the thermal conductivity of
liquid electrically conductive materials. Therefore, in Figure 1 the dependence of thermal conductivity
in this area is shown conditionally.

The authors had a problem in the theoretical description of the dependence shown in figure 1 for
materials, heat transfer in which is determined by conduction electrons. Comparison of theoretical
calculations with the thermal conductivity values and the parameters defining it was carried out on such
characteristic chemical elements, the required set of properties of which was well enough studied
experimentally [2], [3].

In metals, electron melts and semiconductors, heat carriers are free electrons (in semiconductors this
is only a part of the heat transferred, the so-called electronic heat conductivity). The analysis of the
mechanisms of scattering and transfer should be carried out in this case on the basis of the following
dependencies [4]:

\[ \lambda = \frac{1}{3} c \rho \bar{v}_s I_s \]  \hspace{1cm} (1)
\[ u_e = \frac{a}{kT} e \]  \hspace{1cm} (2)

It is known that in metals \( I_s \) the electron mean free path is \( 10^8 < I_s < 10^{-3} \), which is caused by violations
of the periodic field of the ionic core of the crystal caused by dynamic and statistical imperfections [5].
The thermal speed of electrons \( \langle \bar{v} \rangle \) in metals is a value of the \( 10^8 \) m/s order and varies little with
the temperature. The average wavelength of free electrons in metals is of the \( 5 \times 10^{-10} \) m order (i.e., is equal
to the interatomic distances). Considering that in metals \( I_s \sim u_e \) and theory it was shown that at
temperatures \( T < \theta \); \( I_s \sim u_e \sim T^{-3} \), and for \( T > \theta \); \( I_s \sim u_e \sim T^{-1} \). When scattering by ionized impurities \( u_e \)
\( \sim T^{0.2} \), and when scattering by the acoustic branch of grid vibrations \( u_e \sim T^{-3/2} \) [4]. It is shown that for
impurity semiconductors, the temperature dependence of the mobility can be represented as:

\[ u_e = AT^{-1.5} + BT^{-1.5} \]  \hspace{1cm} (3)

where: \( A \) and \( B \) are constants, whereas \( A \) at \( T < 300 \) K, and \( B \) at \( T > 300 \) K.

When the concentration of electrons and holes is more than \( 10^{26} \) m\(^{-3} \), their mutual scattering occurs,
at which the temperature change in the mobility is \( u_e \sim T^{-3.5} \). In cases where the effective mass of
electrons and holes increases sharply with temperature (for example, in narrow-gap semiconductors),
the magnitude of mobility with temperature varies as \( u_e \sim T^{-2.5} \).

Everything said about the theoretical prerequisites for the transfer of heat by electrons allows us to
establish the following order of analysis of the electron and phonon thermal conductivity. The
temperature dependences of thermal conductivity, heat capacity, density [4] were used to determine the
values of thermal diffusivity and mobility. Based on these data, the degrees of temperature variation of
thermal conductivity \( x_l (\lambda \sim T^{x_l}) \), thermal diffusivity \( x_a (a \sim T^{x_a}) \), thermal mobility of electrons \( x_e (u_e \sim T^{x_e}) \), as well as the values of \( n - \) the fraction of scattering acts affecting the process of energy
transfer - are calculated.

The following alloys of non-ferrous metals were considered:

- aluminum alloys: AD-1, AMg5, AMg6, AMg3, D16;
- Constantan copper alloy;
- titanium alloys: VT5-1, VT6, VT14.

For the above materials, the laws of thermal conductivity $\lambda=f(T)$ and mobility $U=f(T)$, as well as the values of $n$ - the fraction of scattering acts affecting the process of energy transfer - were obtained using a computer program.

2. Analysis of electron heat transfer in metals

2.1. Aluminum alloys

The studied alloys based on aluminum have an average density in the range of 2,600 - 2,800 kg/m$^3$. The temperature dependences of thermal conductivity and mobility of the considered aluminum alloys are shown in figure 2 and 3 respectively. On the basis of the calculations performed, the degrees of the temperature change of the thermal conductivity and mobility of these materials are obtained. In addition, the calculated values of the carrier scattering probability $n$. The temperature dependences of $n$ for the studied group of alloys were constructed (figure 4).

The analysis of the dependences shown in Figure 3 shows that for the group of aluminum-based alloys, AD1, AMg5, AMg6, AMg3 and D16 in the temperature range under consideration, the electron mobility decreases according to a law determined by the theoretical value of degree (-1), and a smaller value of degree (AMg5, AMg6 alloys) indicates the presence of slight additional inelastic scattering. The larger degree (compared to AD1, AMg3, D16) is due to the additional elastic scattering of transfer carriers. The thermal conductivity of these alloys (figure 2) increases according to the law, determined by the theoretical value of the degree (0.5). A slight deviation of the degree from the theoretical value indicates that in addition to the main electron-phonon scattering, there are also additional scattering mechanisms due to the presence of impurities. The growth of thermal conductivity of these materials in the temperature range under study is apparently explained by the non-uniform chemical composition of these elements, bringing their structure closer to the disordered one [5].

![Figure 2. Temperature dependence of thermal conductivity of aluminum alloys.](image-url)
2.2. Copper alloys
The studied Constantan copper alloy has an average density of 8,900 kg/m$^3$. The temperature dependences of thermal conductivity and mobility for this material are shown in figure 5 and 6, respectively. On the basis of the calculations performed, the degrees of the temperature change in the thermal conductivity and mobility of the Constantan alloy are also presented, which are presented in table 1. The temperature dependence of the probability of carrier scattering is shown in figure 7.

| Material        | Temperature range | $X_\lambda$ | $X_U$ |
|-----------------|-------------------|-------------|-------|
| Constantan alloy| 150-300 K         | 0.37        | -0.96 |

From the graphs presented in figure 6 it is seen that at temperatures of 150 ÷ 300 K, the mobility of the Constantan alloy decreases according to the law, determined by the theoretical value of degree (-1), and a small deviation to a smaller, compared to theoretical, value of the degree is due to additional inelastic scattering besides the main scattering on grid vibrations. The calculated value of the degree of thermal conductivity of this alloy (figure 5) substantially deviates from the theoretical value (0.5), which is explained by a significant fraction of carrier scattering on foreign impurities [5], [6].

2.3. Titanium alloys
The studied titanium alloys VT5-1, VT6 and VT14 have a density in the range of 4430 ÷ 4510 kg/m$^3$. The temperature dependences of the thermal conductivity and mobility of these alloys are shown in figure 8 and 9. On the basis of the calculations performed, the degrees of the temperature change of the thermal conductivity and mobility of these materials are obtained, presented in table 2. The dependence of the probability of carrier scattering $n$ for a group of titanium-based alloys is shown in figure 10.
Figure 4. Temperature dependencies aluminum alloys $n$.

Figure 5. Temperature dependence of thermal conductivity Constantan alloy.
Figure 6. Temperature dependence of mobility of the Constantan alloy.

Figure 7. Temperature dependences of the Constantan alloy $n$. 
Figure 8. Temperature dependence of thermal conductivity of titanium alloys.

Figure 9. Temperature dependence of mobility of titanium alloys.

Table 2. VT5-1, VT6 and VT14 alloy.

| Material     | Temperature range | $X_\lambda$ | $X_U$   |
|--------------|-------------------|-------------|---------|
| VT5-1 alloy  | 200-1073 K        | 0.61        | -0.58   |
| VT6 alloy    | 200-873 K         | 0.63        | -0.71   |
| VT14 alloy   | 200-973 K         | 0.55        | -0.71   |
Analysis of the graphs presented in figure 10 shows that for a group of alloys based on titanium VT5-1, VT6 and VT14, in the temperature ranges under consideration, the electron mobility decreases according to a law determined by the theoretical value of the degree (-1). A significant deviation from this theoretical value indicates the presence of significant additional inelastic scattering, as well as scattering on impurity ions. The thermal conductivity of the studied titanium alloys (figure 8) increases according to the law, determined by the theoretical value of the degree (0.5). A slight deviation of the degree from the theoretical one in a large direction indicates that in addition to the main electron-phonon scattering there are also additional scattering mechanisms [5], [6]. The growth of thermal conductivity of these materials in the temperature range under study is explained by the inhomogeneous chemical composition of these elements, bringing their structure closer to disordered.

3. Conclusions

Thus, in real bodies at very low temperatures \((T<50-70 \text{ K})\), when the thermal vibrations of atoms are practically frozen, the decisive process of electron scattering is their interaction with the sample boundaries, since at such low temperatures the mean free path is comparable to the body size. In this case, the dependence of the mobility of \(U\) on temperature is proportional to \(U^{-3}\), with a smaller degree corresponding to inelastic scattering at the sample boundaries, and a larger one corresponding to elastic scattering at the sample boundaries [7], [8], [9].

At high temperatures \((T>50-70 \text{ K})\), the motion of electrons is determined by their scattering on thermal grid vibrations, i.e. on phonons. In this case, the dependence of the mobility of \(U\) on temperature is proportional to \(U^{-1.5}\) [8]. However, in addition to the basic electron-phonon scattering, there are also additional scattering mechanisms due to the presence of impurities, which leads to a deviation of the value of the degree "\(\chi_U\)" from the indicated −1.5 [7], [8], [9].

References

[1] Aliyev M I 1963 Thermal conductivity of semiconductors (Baku)
[2] Meilikhov E Z and Lazarev S D 1987 Electrophysical properties of semiconductors (Moscow: CRI of Inform. and tech.-econ. researches for atom. science and technology)
[3] Kikoin A K and Kikoin I 1976 Molecular physics (Moscow: Science)
[4] Kolesnikov K S, Rumyantsev V V, Leontyev A I and Polezhaev Yu V et al. 1999 Mechanical Engineering (Moscow: Mechanical Engineering)

[5] Okhotin A S, Marushin L A and Zhmakin L I 2000 Thermal conductivity: Models, mechanisms, experimental data (Moscow: Science)

[6] Tikhonov B S 2000 Heavy non-ferrous metals and alloys (Moscow: Federal State Unitary Enterprise TSNIIIEItsvetmet)

[7] Marushin L A and Tikhonova D A 2019 Quantitative analysis of thermophysical properties of chalcogenide materials for thermoelectric transducers Topical Issues of Modern Science pp 97-104

[8] Marushin L A and Tikhonova D A 2019 Analysis of thermophysical properties of cooling elements IOP Conf. Series: Mater. Sci. Eng. 537 062023

[9] Uvdiev J Y, Marushin L A and Treshchalina D A 2016 Analyse der thermophysikalischen eigenschaften amorpher Materialien für energetische Systeme mit direkter Energieumwandlung 6th Conf Europäische fachhochschule (Stuttgart) pp 95-9