Study of Thermophysical Properties of Materials on the Basis of Periodic Law

Mohammed M. Meteab*, Ashraf Abdullah Ahmed

Department of Mechanical, College Engineering, Tikrit University, Tikrit, Iraq.

*Corresponding author E-mail: muh.muhana@tu.edu.iq

ABSTRACT

In this article the problems associated with the thermophysical properties of various materials are considered. The general thermal properties of various solids and materials listed in the periodic table are presented. A new approach to analyzing the thermophysical properties of materials (substances) on the basis of the periodic table is studied. An integral characteristic of the thermal properties of materials reflecting their ability to grow and accumulate energy in the form of transport calorific values is proposed. The results of processing experimental data based on generalizing thermal properties showed the presence of a correlation relationship between the heat capacity of a solid from the periodic table and the number of the chemical element in this table.

KEYWORDS

Thermophysical properties, periodic table, temperature expansion, linear thermal expansion coefficient, heat capacity

INTRODUCTION

The development of new materials and the change in approaches to the design of various objects (construction, engineering, etc.) increases the value of reliable knowledge about the behavior of various structural materials with their temperature changes. Data about the thermophysical properties of materials can be taken from standards, reference books, regulatory documents. But unfortunately, not all materials have information. This is due to, on the one hand, the rapid changes taking place in materials science, on the other hand, theoretical studies should be confirmed by experiments, and vice versa, the experiments should be supported by theoretical studies. When conducting experimental studies, it is necessary to ensure high accuracy of measurement of thermal quantities to ensure the measurement legitimacy. An interesting approach is to study the thermophysical properties of materials (substances) on the basis of the periodic table. The goal of this paper is to propose an integral characteristic of the thermal properties of materials reflecting their ability to grow and accumulate energy in the form of transport calorific values.

MATERIALS AND METHODS

With a change in temperature, the sizes of solids change. Expansion under the temperature exposure is characterized by a linear thermal expansion coefficient [1].

The change in the linear dimensions of the body is described by the formula (1)

\[ l = l_0 (1 + \alpha \cdot \Delta T) \]  \hspace{1cm} (1)

where

- \( l \) — body length;
- \( l_0 \) — initial body length;
- \( \alpha \) — a linear thermal expansion coefficient;
- \( \Delta T \) — temperature difference.

A linear thermal expansion coefficient shows, how which part of the original length or width will change the size of the body, if its temperature rises by 1 degree.

Examples of the expansion of some materials are shown in Fig. 1.
The main tool in the study of thermal properties of materials, obtaining numerical values of the thermal conductivity coefficient \(\lambda\), the specific heat capacity at constant pressure \(c_p\) at a known density \(\rho\) is the thermophysical experiment [2]. Thermophysical experiment (TPE) is one of the main means of improving the quality and efficiency of thermal research. TPE includes various experimental studies of the thermophysical properties of substances and thermal processes, conducting industrial tests of heat engines. It’s known that, the normal conditions for both operation and experimentation are room temperature 20 ± 5 °C [3]. It is obvious that industrial equipment is not always operated in “ideal” conditions, and therefore it is important to know how this or that structural material behaves when the temperature changes. Moreover, the temperature can not only rise, but also fall below zero.

It is difficult to obtain high reproducibility of results and the ability to measure in a wide range, purposefully change variables. Improvements and installations used in the measurements are expensive [4]. The thermophysical experiment has a high degree of a priori information, i.e. processes with varying degrees of accuracy are described by a system of differential equations. In a thermophysical experiment, it is possible to preliminarily identify dependent and independent variables by methods of generalized variables or local modeling. Chemical elements, according to the Periodic Table, have the dependence of their various properties on their charge of the atomic nucleus. Substances with clear periodic trends are combined into groups. Inside the group, a regularity is seen in the change in properties as the atomic number increases. It was proposed to consider the thermophysical properties of simple solids, in terms of blockiness and periodicity. For the experiment, single crystals and high-purity monocrystals were selected.

RESULTS AND ITS DISCUSSION

Let’s consider a brief method for calculating thermal properties through integral characteristics. Let us consider the surface of the material, which is affected by thermal radiation. The thermal flux has thermal conductivity \(q_x\) and radiation \(q_e\). Denote the change in temperature inside the object (material) by \(\Delta T_s\). The distance at which the temperature changes inside the object, denoted by \(\Delta l_s\). index s denotes the parameters associated with the translational motion toward the surface, and the index (c) from the surface. Simply, amount of thermal flux is determined by the formula (2)

\[
q_x = \lambda \frac{\Delta T_s}{\Delta l_s} = \lambda T_s \frac{1}{\Delta l_s * n_s}
\]  

(2)

Where \(n_s\) - a number of temperature ranges of \(\Delta T_s\).

The reflected thermal flux, according to the Stefan-Boltzmann law, is determined by the formula (3)

\[
q_s = \sigma * T_s^4
\]  

(3)
where $\sigma$ - Stefan-Boltzmann constant.

Taking into account (3), we correct the heat balance equation (2)

$$\lambda T_s \frac{1}{\Delta l_s n_s} = \sigma * T_s^4$$

or

$$\lambda = \sigma * \Delta l_s * n_s * T_s^3$$

Convert equation (5) by extracting the cubic root and multiplying by the volumetric heat capacity $c_p * \rho$. We obtain a complex of thermophysical characteristics of the substance.

$$K = \lambda^{1/3} * c_p * \rho = (\sigma * \Delta l_s * n_s) * T * c_p * \rho$$

Formula (6) is an integral characteristic of the thermal properties of a substance [5].

There are two approaches to the consideration of thermal properties. The first approach involves the use of a mathematical model in the form of a boundary problem of heat conductivity. In this case, the parameters of the model are selected in such a way as to ensure the coincidence of the temperature field of the object and the model. In assessing the reliability of these fields, the zero function of the error between temperatures at the selected point and the model is used. That allows obtaining simpler calculation formulas for determining the desired values. In the second approach, to describe the model, a system of equations is used that describes the integral law of heat conservation over a given time interval and at the desired point of the field. For the selection of parameters in this case, the error functions of this equation in a given region are equated to zero. Both approaches ensure high adequacy of the temperature fields. But at the same time, analytical expressions for temperature fields have a complex structure and a large number of assumptions and boundary conditions.

A positive point is the consideration of specific conditions that can be used in the creation of experimental facilities for conducting thermophysical studies. The main feature of thermophysical measurements is a large variety of methods, most of which are universal, therefore the results obtained are relatively inaccurate, the performance is low, the measurement technique is complex. The difficulty is related to the fact that a dynamic system with distributed parameters is being studied. The main direction in the development of a thermophysical experiment follows the path of simplifying the mathematical apparatus, which in turn will not only simplify the experiment, but also increase its accuracy. To obtain a mathematical model in integral form, the principle of superposition of temperature fields caused by the action of point heat sources is used. The integral parameter included in the integral forms of the heat conductivity equation: a repeated and one-time integral, is the only source of error in their adequacy, which can be reduced by imposing certain conditions on the performance of heat exposure and measurement.

The definition of a measurable quantity (in our case, a thermophysical quantity) includes the adoption of a certain model of the measurement object, in which the true value is represented by a certain parameter. The choice of a mathematical model of an object is determined by a specific measurement task, which consists in determining the value of a quantity by measuring it with the required accuracy under the specified measurement conditions. This presupposes the existence of an established permissible measurement error and imposes certain requirements on the non-measurable properties of an object, for example, its geometry and size. This should take into account such factors as the degree of complexity of the development and technical implementation of the measurement method, the time and complexity of preparation and measurement. For the study of the periodicity of thermophysical properties, fifty-six simple solids were selected from the periodic table. Experimental studies were conducted, showing the presence of a relationship between them. The resulting analytical expression (7)

$$c_{pp} = 23,96 + (4,581 + 1,457 * z) * \frac{T}{T_{cl}}$$

where $T$ – thermodynamic temperature;

$T_{cl}$ - crystallization temperature;

$z$ – place in the periodic table.

insert in the formula (7) the crystallization temperature
where $T_{cl}^{1/2} = 3.1 \times 10^{-3} \times (2 \times n^2 + 1) \times \theta_g$ \hspace{1cm} (8)

$n$ – an integer number showing possible energy values of the studied solid.

Analytical expression (7) shows that there is a correlation between the heat capacity of the chemical element of the periodic system and his place in it. The relationship between the generalized thermophysical characteristic of a solid body $k_\mu$ and the place of the element in the Periodic table.

$k_\mu = \lambda^{3/3} \rho \left[ 23.96 + (4.581 + 1.457z) \frac{T}{9.61 \times 10^{-3} (2n^2 + 1)^2 \theta_g^2} \right] \hspace{1cm} (9)$

Table 1 shows the results of tests and calculations of $k_\mu$ for some solid materials [6]. Measurements were carried out in the range from 20 °C to 100 °C. The same data (but already based on one mole of the substance) in the coordinates $k_\mu - tg\alpha$ is shown in Fig. 2.

Table 1. The results of the experimental determination of the complex thermophysical properties $k_\mu$

<table>
<thead>
<tr>
<th>Element</th>
<th>Ti</th>
<th>V</th>
<th>Cr</th>
<th>Zr</th>
<th>Nb</th>
<th>Mo</th>
<th>Hf</th>
<th>Ta</th>
<th>W</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n$</td>
<td>20</td>
<td>23</td>
<td>24</td>
<td>40</td>
<td>41</td>
<td>42</td>
<td>72</td>
<td>73</td>
<td>74</td>
</tr>
<tr>
<td>$k_\mu$, 10^6</td>
<td>6.60</td>
<td>9.58</td>
<td>14.74</td>
<td>5.29</td>
<td>8.71</td>
<td>13.21</td>
<td>5.47</td>
<td>10.0</td>
<td>14.86</td>
</tr>
</tbody>
</table>

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**Figure 2.** Dependence of the complex of metals properties $k_\mu$ on the universal parameter $tg\alpha$ at a temperature of 20 °C.

Here, the universal parameter $tg\alpha$ [7] reflects the structural features of the outer electron shells of atoms. For similar elements, the values of the complex property $k_\mu$ are almost a linear function of the parameter $tg\alpha$ in the series of the periodic table. The extensive properties of chemical elements are also characterized by their volume, heat capacity, and entropy. Strong bonded crystals have partial molar entropy. Molar entropy is determined by the ratio of entropy to the amount of a substance. Thermodynamic entropy is understood as a function that depends only on the equilibrium state of the thermodynamic system. It does not depend on the specific type of thermodynamic process that brought the system to the specified state. Fig. 3 shows the results of processing of experimental data for some elements of the periodic table in the form of dependences $k_\mu l = \varphi (S_\mu l)$, corresponding to the temperature T01 = 300K.
Figure 3. Experimental data and property diagram

The point with coordinates $[\delta \mu_0 = 23.6 \text{ J} / (\text{mol} \ast \text{R}) ; \ k_\mu 0 = 0]$ adopted for the original. The obtained values of $k_\mu$ corresponding to $s_\mu$ formed a triangle, in the other two vertices of which are located chemical elements tungsten W (period 6, row 8, VI element group, element number 74) and cesium Cs (period 6, row 8, group I, element number 55). The formed triangle is divided into geometric shapes at the vertices of which the following chemical elements are located: chromium Cr (number 24), molybdenum Mo (42), series Y (39), titanium Ti (22), scandium Sc (21), calcium Ca (20), niobium Nb (41), zirconium Zr (40), potassium K (19), strontium Sr (38), rubidium Rb (37), hafnium Hf (72), lanthanum La (57), and barium Ba (56).

Correlation dependence is found between the elements belonging to one periodic group (they lie on one straight line):

- for group VI between Cr - Mo - W;
- for group III between Y - Nb - Ta and Sc - La;
- for group IV between Ti - Zr - Hf;
- for group II between Ca - Sr - Ba;
- for group I between K - Rb - Cs.

The greater the number of atoms in the external energy level, the tighter the angle of the correlation segments relative to the $s_\mu$ axis.

For the temperature $T02 = 1000K$ (segment 4 in Fig. 3) and $T03 = 1500K$ (segment 5 in Fig. 3), additional studies of three chemical elements: Cr - Mo - W were carried out. The radius of these elements increases with their atomic number, decreases the ionization energy, increase metallic properties. With increasing temperature, the segment (Cr - Mo - W) shifts to the right while maintaining the periodicity of thermophysical properties. The presence of 4 and 5 fractures on the segment is due to the measurement and calculation error. Under ideal conditions, these segments are parallel. Parallelism indicates that the thermophysical properties of these elements change simultaneously with all of them with a known discrete step.

CONCLUSIONS

The reliable knowledge about the behavior of various structural materials with their temperature changes is very important for development of new materials and design of various objects. Due to the rapid changes in materials science not all materials have information about their thermophysical properties in standards, reference books, regulatory documents. A new approach to analyzing the thermophysical properties of materials (substances) on
the basis of the periodic table is studied. An integral characteristic of the thermal properties of materials reflecting their ability to grow and accumulate energy in the form of transport calorific values is proposed. The results of processing experimental data based on generalizing thermal properties showed the presence of a correlation relationship between the heat capacity of a solid from the periodic table and the number of the chemical element in this table.

REFERENCES


