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# COMPUTER METHOD OF DESCRIPTION OF TECHNOLOGIES AND PROPERTIES OF THERMOELECTRIC $Bi_2$-$Te_3$ BASED MATERIAL BY EXTRUSION METHOD

*This paper presents the results of a study of literature sources which describe the technology and properties of thermoelectric materials obtained by extrusion method. The result of one of the stages of creating a software product to describe the technologies for obtaining of a thermoelectric materials based on Bi-Te compounds and their properties are presented. Bibl. 9, Fig.4, Tabl.1.*

**Key words:** extrusion method, extrapolation, bismuth telluride.

## Introduction

Thermoelectric materials science is the most promising trend in thermoelectricity, covering such aspects as the development of methods for optimizing the parameters of thermoelectric materials (TEMs), the study of the properties of semiconductors traditionally used in thermoelectric conversion, and the improvement of technology for manufacturing TEMs for thermoelectric generators, refrigerators and measuring instruments, development of high-precision methods for measuring and monitoring material parameters.

The optimization of TEM properties is one of the most important issues in materials science. It is a well- known fact that thermoelectric materials must satisfy a number of requirements, often contradicting each other: have high values of figure of merit in a wide temperature range, have a high thermoEMF coefficient at low values of the resistivity and thermal conductivity coefficients, and be characterized by high mechanical strength. The mechanical and thermoelectric properties of materials described above depend, in their turn, on the structure, composition of the initial components, impurities, and manufacturing method.

Traditional methods for producing bismuth telluride compounds include Bridgman, Czochralski and zone melting methods, alongside with the powder metallurgy methods such as hot pressing and hot extrusion [1].

The purpose of this work is to study the thermoelectric characteristics of bismuth telluride based solid solutions obtained by extrusion. Using a modified computer programme to study the extrusion method and characteristics of thermoelectric materials based on *Bi*-*Te* compounds.

## Dependence of thermoelectric characteristics of $Bi_2$-$Te_3$ based materials obtained by extrusion

When obtaining $Bi_2Te_3$ samples by extrusion, pre-formed pellets of thermoelectric material are pressed through a mold (die), during which the said pellet is heated to a temperature below the melting point [2]. Table 1 shows the thermoelectric characteristics of $Bi_2$-$Te_3$ based materials obtained by extrusion.

Table

*Thermoelectric characteristics of $Bi_2$-$Te_3$ based materials obtained by extrusion*

| Operating temperature, K | Z, $10^{-3}$,$K^{-1}$ | α, mV/K | σ, $Ohm^{-1}cm^{-1}$ | κ, W/m·K | Material type: | Material composition: | Ingot size, mm | Extrusion temperature, K | Source: |
|---|---|---|---|---|---|---|---|---|---|
| 280 | 2.39 | 225 | 567 | 1.2 | P | $Bi_{0.4}Sb_{1.6}Te_3$ | - | 753 | [3] |
| 328 | 2.44 | 239 | 512 | 1.2 | P | $Bi_{0.4}Sb_{1.6}Te_3$ | - | 753 | [3] |
| 400 | 1.75 | 230 | 406 | 1.23 | P | $Bi_{0.4}Sb_{1.6}Te_3$ | - | 753 | [3] |
| 475 | 0.90 | 200 | 332 | 1.47 | P | $Bi_{0.4}Sb_{1.6}Te_3$ | - | 753 | [3] |
| 280 | 2.50 | 230 | 525 | 1.11 | P | $Bi_{0.4}Sb_{1.6}Te_3$ | - | 753 | [3] |
| 328 | 2.50 | 241 | 469 | 1.09 | P | $Bi_{0.4}Sb_{1.6}Te_3$ | - | 753 | [3] |
| 400 | 1.75 | 236 | 377 | 1.2 | P | $Bi_{0.4}Sb_{1.6}Te_3$ | - | 753 | [3] |
| 475 | 0.93 | 205 | 295 | 1.34 | P | $Bi_{0.4}Sb_{1.6}Te_3$ | - | 753 | [3] |
| 280 | 2.96 | 240 | 669 | 1.3 | P | $Bi_{0.4}Sb_{1.6}Te_3$ | - | 753 | [3] |
| 328 | 2.74 | 247 | 809 | 1.8 | P | $Bi_{0.4}Sb_{1.6}Te_3$ | - | 753 | [3] |
| 400 | 2 | 245 | 439 | 1.32 | P | $Bi_{0.4}Sb_{1.6}Te_3$ | - | 753 | [3] |
| 475 | 1.16 | 206 | 422 | 1.55 | P | $Bi_{0.4}Sb_{1.6}Te_3$ | - | 753 | [3] |
| 280 | 2.96 | 243 | 627 | 1.25 | P | $Bi_{0.4}Sb_{1.6}Te_3$ | - | 753 | [3] |
| 328 | 2.89 | 252 | 556 | 1.22 | P | $Bi_{0.4}Sb_{1.6}Te_3$ | - | 753 | [3] |
| 400 | 2.05 | 250 | 419 | 1.28 | P | $Bi_{0.4}Sb_{1.6}Te_3$ | - | 753 | [3] |
| 475 | 1.22 | 207 | 421 | 1.48 | P | $Bi_{0.4}Sb_{1.6}Te_3$ | - | 753 | [3] |
| 294 | 1.06 | 191 | 369 | 1.27 | P | $Bi_{0.5}Sb_{1.5}Te_3$ | - | 613 | [4] |
| 294 | 2.17 | 229 | 438 | 1.06 | P | $Bi_{0.5}Sb_{1.5}Te_3$ | - | 653 | [4] |
| 294 | 2.78 | 237 | 529 | 1.07 | P | $Bi_{0.5}Sb_{1.5}Te_3$ | - | 693 | [4] |
| 294 | 2.72 | 241 | 568 | 1.21 | P | $Bi_{0.5}Sb_{1.5}Te_3$ | - | 733 | [4] |
| 294 | 1.11 | 176 | 444 | 1.24 | P | $Bi_{0.5}Sb_{1.5}Te_3$ | - | 593 | [4] |
| 294 | 1.94 | 177 | 879 | 1.42 | P | $Bi_{0.5}Sb_{1.5}Te_3$ | - | 623 | [4] |
| 294 | 1.56 | 194 | 497 | 1.41 | P | $Bi_{0.5}Sb_{1.5}Te_3$ | - | 613 | [5] |
| 294 | 1.71 | 197 | 564 | 1.29 | P | $Bi_{0.5}Sb_{1.5}Te_3$ | - | 653 | [5] |
| 294 | 2.44 | 215 | 621 | 1.18 | P | $Bi_{0.5}Sb_{1.5}Te_3$ | - | 693 | [5] |
| 294 | 2.70 | 225 | 675 | 1.27 | P | $Bi_{0.5}Sb_{1.5}Te_3$ | - | 733 | [5] |
| 294 | 0.67 | 145 | 144 | 0.46 | P | $Bi_{0.5}Sb_{1.5}Te_3$ | - | 573 | [6] |
| 294 | 1.63 | 207 | 263 | 0.69 | P | $Bi_{0.5}Sb_{1.5}Te_3$ | - | 643 | [6] |
| 294 | 2.94 | 231 | 540 | 0.98 | P | $Bi_{0.5}Sb_{1.5}Te_3$ | - | 713 | [6] |
| 300 | 2.7 | 150 | 1844 | 1.5 | P | $(Bi_{0.3}Sb_{0.6})Te_3$ | - | 673 | [7] |
| 350 | 2.5 | 170 | 1423 | 1.6 | P | $(Bi_{0.3}Sb_{0.6})Te_3$ | - | 673 | [7] |
| 400 | 2.1 | 180 | 1114 | 1.7 | P | $(Bi_{0.3}Sb_{0.6})Te_3$ | - | 673 | [7] |
| 450 | 1.7 | 185 | 934 | 1.8 | P | $(Bi_{0.3}Sb_{0.6})Te_3$ | - | 673 | [7] |
| 300 | 3.3 | 200 | 1083 | 1.3 | P | $(Bi_{0.4}Sb_{0.8})Te_3$ | - | 673 | [7] |
| 350 | 2.85 | 215 | 834 | 1.35 | P | $(Bi_{0.4}Sb_{0.8})Te_3$ | - | 673 | [7] |
| 400 | 2.4 | 210 | 761 | 1.4 | P | $(Bi_{0.4}Sb_{0.8})Te_3$ | - | 673 | [7] |
| 450 | 1.7 | 212 | 573 | 1.45 | P | $(Bi_{0.4}Sb_{0.8})Te_3$ | - | 673 | [7] |
| 300 | 3.16 | 250 | 658 | 1.3 | P | $(Bi_{0.5}Sb_1)Te_3$ | - | 673 | [7] |
| 350 | 2.28 | 245 | 495 | 1.3 | P | $(Bi_{0.5}Sb_1)Te_3$ | - | 673 | [7] |

*Continuation of table*

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 400 | 1.62 | 240 | 366 | 1.3 | *P* | $(Bi_{0.5}Sb_1)Te_3$ | - | 673 | [7] |
| 450 | 1 | 215 | 281 | 1.3 | *P* | $(Bi_{0.5}Sb_1)Te_3$ | - | 673 | [7] |
| 240 | 3.2 | 193 | 1350 | 1.57 | *P* | $Bi_{0.4}Sb_{1.6}Te_3$ | 65 | 673-723 | [8] |
| 260 | 3.28 | 202 | 1180 | 1.47 | *P* | $Bi_{0.4}Sb_{1.6}Te_3$ | 65 | 673-723 | [8] |
| 280 | 3.3 | 210 | 1010 | 1.35 | *P* | $Bi_{0.4}Sb_{1.6}Te_3$ | 65 | 673-723 | [8] |
| 300 | 3.25 | 220 | 900 | 1.34 | *P* | $Bi_{0.4}Sb_{1.6}Te_3$ | 65 | 673-723 | [8] |
| 320 | 3.19 | 225 | 800 | 1.27 | *P* | $Bi_{0.4}Sb_{1.6}Te_3$ | 65 | 673-723 | [8] |
| 340 | 3.05 | 230 | 700 | 1.21 | *P* | $Bi_{0.4}Sb_{1.6}Te_3$ | 65 | 673-723 | [8] |
| 360 | 2.78 | 235 | 675 | 1.34 | *P* | $Bi_{0.4}Sb_{1.6}Te_3$ | 65 | 673-723 | [8] |
| 240 | 2.79 | 205 | 1195 | 1.80 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 65 | 673-723 | [8] |
| 260 | 2.83 | 215 | 1090 | 1.78 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 65 | 723-773 | [8] |
| 280 | 2.84 | 220 | 990 | 1.69 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 65 | 723-773 | [8] |
| 300 | 2.82 | 222 | 900 | 1.57 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 65 | 723-773 | [8] |
| 320 | 2.7 | 230 | 800 | 1.57 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 65 | 723-773 | [8] |
| 340 | 2.6 | 231 | 750 | 1.54 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 65 | 723-773 | [8] |
| 360 | 2.4 | 230 | 700 | 1.54 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 65 | 723-773 | [8] |
| 240 | 3.18 | 193 | 1300 | 1.52 | *P* | $Bi_{0.4}Sb_{1.6}Te_3$ | 65 | 673-723 | [8] |
| 260 | 3.26 | 201 | 1130 | 1.40 | *P* | $Bi_{0.4}Sb_{1.6}Te_3$ | 65 | 673-723 | [8] |
| 280 | 3.29 | 205 | 960 | 1.23 | *P* | $Bi_{0.4}Sb_{1.6}Te_3$ | 65 | 673-723 | [8] |
| 300 | 3.25 | 209 | 850 | 1.14 | *P* | $Bi_{0.4}Sb_{1.6}Te_3$ | 65 | 673-723 | [8] |
| 320 | 3.18 | 218 | 750 | 1.12 | *P* | $Bi_{0.4}Sb_{1.6}Te_3$ | 65 | 673-723 | [8] |
| 340 | 3.04 | 220 | 670 | 1.07 | *P* | $Bi_{0.4}Sb_{1.6}Te_3$ | 65 | 673-723 | [8] |
| 360 | 2.76 | 230 | 650 | 1.25 | *P* | $Bi_{0.4}Sb_{1.6}Te_3$ | 65 | 673-723 | [8] |
| 240 | 2.74 | 193 | 1250 | 1.70 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 65 | 673-723 | [8] |
| 260 | 2.78 | 200 | 1145 | 1.65 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 65 | 723-773 | [8] |
| 280 | 2.80 | 205 | 1045 | 1.57 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 65 | 723-773 | [8] |
| 300 | 2.82 | 207 | 955 | 1.45 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 65 | 723-773 | [8] |
| 320 | 2.71 | 208 | 855 | 1.36 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 65 | 723-773 | [8] |
| 340 | 2.62 | 209 | 805 | 1.34 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 65 | 723-773 | [8] |
| 360 | 2.43 | 210 | 755 | 1.37 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 65 | 723-773 | [8] |
| 240 | 3.1 | 182 | 1600 | 1.71 | *P* | $Bi_{0.4}Sb_{1.6}Te_3$ | 65 | 673-723 | [8] |
| 260 | 3.2 | 193 | 1400 | 1.63 | *P* | $Bi_{0.4}Sb_{1.6}Te_3$ | 65 | 673-723 | [8] |
| 280 | 3.23 | 195 | 1200 | 1.41 | *P* | $Bi_{0.4}Sb_{1.6}Te_3$ | 65 | 673-723 | [8] |
| 300 | 3.25 | 200 | 1100 | 1.35 | *P* | $Bi_{0.4}Sb_{1.6}Te_3$ | 65 | 673-723 | [8] |
| 320 | 3.19 | 203 | 1000 | 1.29 | *P* | $Bi_{0.4}Sb_{1.6}Te_3$ | 65 | 673-723 | [8] |
| 340 | 3.05 | 205 | 900 | 1.24 | *P* | $Bi_{0.4}Sb_{1.6}Te_3$ | 65 | 673-723 | [8] |
| 360 | 2.83 | 207 | 800 | 1.21 | *P* | $Bi_{0.4}Sb_{1.6}Te_3$ | 65 | 673-723 | [8] |
| 240 | 2.7 | 170 | 1450 | 1.55 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 65 | 673-723 | [8] |
| 260 | 2.73 | 180 | 1350 | 1.60 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 65 | 723-773 | [8] |
| 280 | 2.78 | 185 | 1250 | 1.54 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 65 | 723-773 | [8] |
| 300 | 2.8 | 195 | 1150 | 1.56 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 65 | 723-773 | [8] |
| 320 | 2.78 | 200 | 1050 | 1.51 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 65 | 723-773 | [8] |
| 340 | 2.7 | 203 | 1000 | 1.53 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 65 | 723-773 | [8] |
| 360 | 2.6 | 204 | 950 | 1.52 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 65 | 723-773 | [8] |
| 294 | 2.92 | 166 | 1600 | 1.51 | *P* | $Bi_{0.3}Te_{1.7}Se_3$ | 10×120 | - | [9] |
| 294 | 3.25 | 208 | 960 | 1.28 | *P* | $Bi_{0.6}Te_{1.4}Se_3$ | 10×120 | - | [9] |

*Continuation of table*

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 294 | 3.2 | 205 | 1020 | 1.34 | *P* | $Bi_{0.6}Te_{1.4}Se_3$ | 10×120 | - | [9] |
| 294 | 1.62 | 296 | 168 | 0.91 | *P* | $Bi_{0.6}Te_{1.4}Se_3$ | 10×120 | - | [9] |
| 294 | 3 | 215 | 1030 | 1.59 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 10 | - | [10] |
| 294 | 2 | 295 | 225 | 0.98 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 10 | - | [10] |
| 294 | 1.9 | 245 | 325 | 1.03 | *N* | $Bi_2Te_{2.1}Se_{0.9}$ | 10 | - | [10] |
| 294 | 1.7 | 240 | 323 | 1.09 | *N* | $Bi_2Te_{1.8}Se_{1.2}$ | 10 | - | [10] |
| 300 | 3.2 | 208 | 960 | 1.30 | *P* | $Bi_{0,6}Te_{1.4}Se_3$ | 10 | - | [11] |
| 300 | 2.2 | 260 | 310 | 0.95 | *P* | $Bi_{0.6}Te_{1.4}Se_3$ | 10 | - | [11] |
| 300 | 1.6 | 295 | 170 | 0.92 | *P* | $Bi_{0.6}Te_{1.4}Se_3$ | 10 | - | [11] |
| 300 | 3.2 | 205 | 776 | 1.02 | *P* | $Bi_{0.6}Te_{1.4}Se_{0.12}Te_{2.88}$ | 10 | - | [11] |
| 300 | 3.1 | 213 | 1055 | 1.54 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 10 | - | [11] |
| 300 | 2.9 | 240 | 655 | 1.30 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 10 | - | [11] |
| 300 | 2 | 295 | 260 | 1.13 | *N* | $Bi_2Te_{2.82}Se_{0.18}$ | 10 | - | [11] |
| 300 | 3.2 | 208 | 960 | 1.30 | *P* | $Bi_{0.5}Te_{1.5}Se_3$ | - | - | [12] |
| 300 | 2.92 | 163 | 1166 | 1.06 | *N* | $Bi_2Te_{2.7}Se_{0.3}$ | - | 660 | [13] |
| 300 | 2.62 | 171 | 1059 | 1.18 | *N* | $Bi_2Te_{2.7}Se_{0.3}$ | - | 660 | [13] |
| 300 | 2.55 | 157 | 1407 | 1.36 | *N* | $Bi_2Te_{2.7}Se_{0.3}$ | - | 660 | [13] |
| 300 | 1.40 | 165 | 1308 | 2.53 | *N* | $Bi_2Te_{2.7}Se_{0.3}$ | - | 660 | [13] |
| 300 | 1.73 | 175 | 1197 | 2.12 | *N* | $Bi_2Te_{2.7}Se_{0.3}$ | - | 660 | [13] |
| 300 | 1.80 | 196 | 1975 | 2.34 | *N* | $Bi_2Te_{2.7}Se_{0.3}$ | - | 660 | [13] |
| 300 | 2.03 | 214 | 846 | 1.91 | *N* | $Bi_2Te_{2.7}Se_{0.3}$ | - | 660 | [13] |
| 300 | 2.10 | 202 | 940 | 1.83 | *N* | $Bi_2Te_{2.7}Se_{0.3}$ | - | 660 | [13] |
| 300 | 2.50 | 207 | 978 | 1.69 | *N* | $Bi_2Te_{2.7}Se_{0.3}$ | - | 660 | [13] |
| 300 | 2.33 | 222 | 741 | 1.57 | *N* | $Bi_2Te_{2.7}Se_{0.3}$ | - | 660 | [13] |

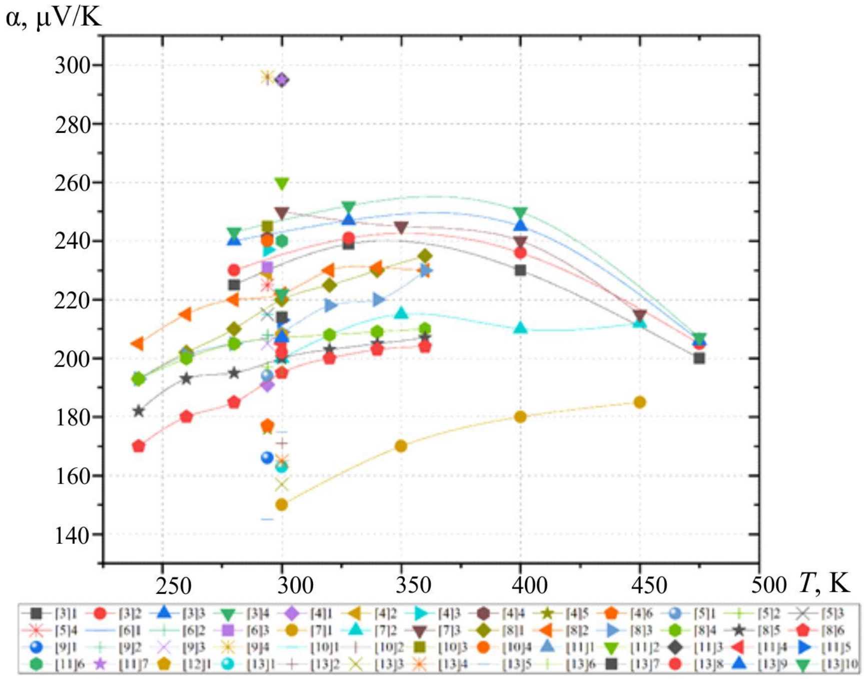


*Fig. 1. Graph of dependence of thermoEMF on temperature*

All data in the table were entered into a software product to describe the technologies and properties of *Bi*-*Te* based thermoelectric material. Updating the software product database will be described in the next articles. Based on the collected data, we will plot graphs of the dependence of electrical conductivity and thermoEMF on temperature fig. 1-3.

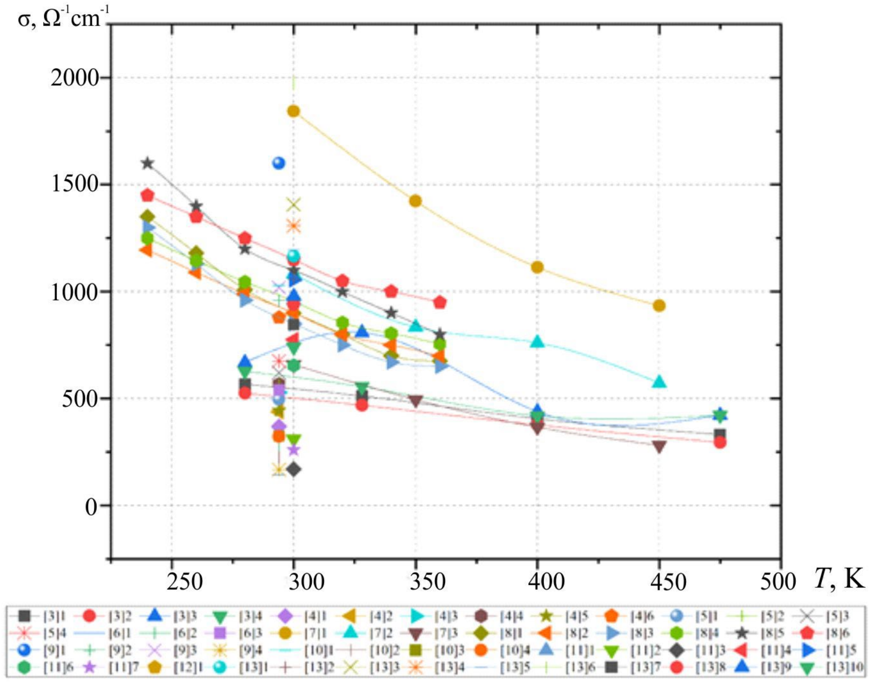


*Fig. 2. Graph of dependence of electrical conductivity on temperature*

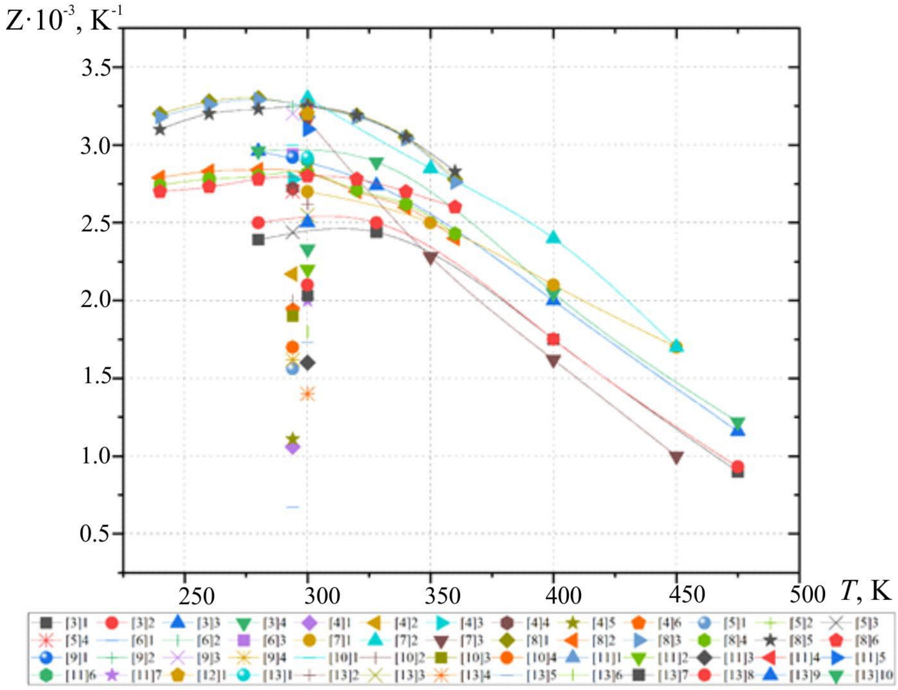


*Fig. 3. Graph of dependence of the figure of merit on temperature*

The given graphs not only clearly demonstrate the dependence of electrical conductivity, thermoEMF and figure of merit on temperature, but also allow introducing certain restrictions into the operation of the programme in order to bring the extrapolated values closer to the real ones.

## Theory of linear extrapolation

Extrapolation in the general sense is a method of calculating certain values beyond the known range of any studied value based on a set of known values.

Linear extrapolation means creating a tangent line at the end of known data and extending it beyond those. Linear extrapolation will only provide good results when used to extend the graph of an approximately linear function or not too far beyond the known data.

If the two data points are closest to the point to be extrapolated and, the linear extrapolation is calculated according to formula 1:

$$Y = Y_0 + \left((Y_1 - Y_0) \div (X_1 - X_0)\right) \times (X - X_0) \tag{1}$$

where $X_0$ is the abscissa of the first point, $X_1$ is the abscissa of the second point, and $X$ is the abscissa of the sought point, then $Y_0$ is the ordinate of the first point, $Y_1$ is the ordinate of the second point, and Y is the ordinate of the sought point.

(which is identical to linear interpolation if $X_{k-1} < X_* < X_k$). It is possible to include more than two points, and by averaging the slope of the linear interpolant, in regression-like techniques, on the data selected for inclusion. This is similar to linear prediction.[14].

The use of linear extrapolation in this work will allow predicting the behavior of materials, thus reducing the cost of resources and time to search for the optimal material for specific tasks.

## Further development of the software product for describing the technologies and properties of *Bi-Te* based thermoelectric material

Currently, a function for theoretical prediction of unknown values of α and σ using extrapolation has been introduced into the software product for describing the technologies for obtaining of thermoelectric material based on *Bi-Te* compounds and their characteristics. The general algorithm for this function is as follows.

• User call of extrapolation function.

• Creation of a dynamic form and all its components for extrapolation.

• After the user enters the required operating temperature, the program searches the database for a material with the closest operating temperature range.

• After selecting the optimal material, the program calculates the coefficient value using the linear extrapolation formula.

- Based on the obtained result, the programme builds a graph of temperature dependence.
- Having received the α results, the programme calculates the σ value using the linear extrapolation formula.
- Based on the obtained result, the programme builds a graph of temperature dependence.
- The results obtained are displayed in Label.
- When the user exits, the programme deletes all form components and the form.
- The general view of the value extrapolation window is shown in Fig. 4.

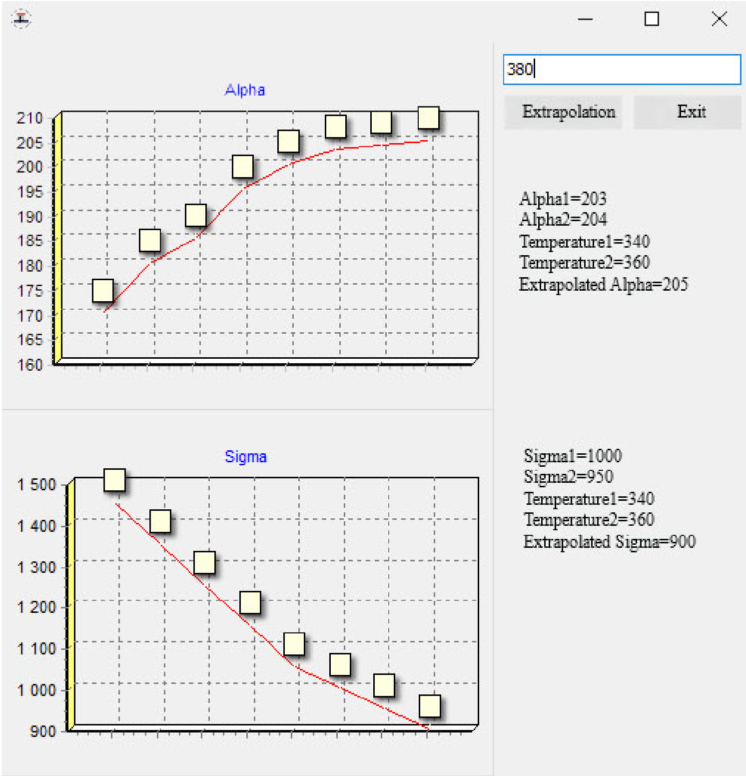


*Fig. 4. General view of the value extrapolation window*

Further development of the software product will be described in the articles in the future.

## Conclusions

1. A study of literary sources that describe *Bi-Te* based thermoelectric materials, obtained by extrusion, was carried out.
2. These studies were added to the software product database to describe the technologies and properties of obtaining *Bi-Te* based thermoelectric materials.
3. The function of extrapolation was introduced into a software product to describe the technologies and properties of obtaining *Bi-Te* based thermoelectric materials.
4. Further versions of the software will be described in the articles in the future.

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## КОМП'ЮТЕРНИЙ МЕТОД ОПИСУ ТЕХНОЛОГІЙ ТА ВЛАСТИВОСТЕЙ ТЕРМОЕЛЕКТРИЧНИХ МАТЕРІАЛІВ НА ОСНОВІ $Bi_2$-$Te_3$, ОТРИМАНИХ МЕТОДОМ ЕКСТРУЗІЇ

*У даній роботі наводяться результати дослідження літературних джерел в яких описуються технології та властивості термоелектричних матеріалів отриманих методом екструзії. Наводяться результати одного з етапів створення програмного продукту для опису технологій отримання та властивостей термоелектричного матеріалу на основі сполук Bi-Te. Бібл. 9. рис. 4. табл. 1.*

**Ключові слова:** метод екструзії, екстраполяція, телурид вісмуту.

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