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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. 7, 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 Bi₂-Te₃ 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:	Extrusion temperature, K
280	2.39	225	567	1.2	P	Bi _{0.4} Sb _{1.6} Te ₃	753
328	2.44	239	512	1.2	P	Bi _{0.4} Sb _{1.6} Te ₃	753
400	1.75	230	406	1.23	P	Bi _{0.4} Sb _{1.6} Te ₃	753
475	0.90	200	332	1.47	P	Bi _{0.4} Sb _{1.6} Te ₃	753
280	2.50	230	525	1.11	P	Bi _{0.4} Sb _{1.6} Te ₃	753
328	2.50	241	469	1.09	P	Bi _{0.4} Sb _{1.6} Te ₃	753
400	1.75	236	377	1.2	P	Bi _{0.4} Sb _{1.6} Te ₃	753
475	0.93	205	295	1.34	P	Bi _{0.4} Sb _{1.6} Te ₃	753
280	2.96	240	669	1.3	P	Bi _{0.4} Sb _{1.6} Te ₃	753
328	2.74	247	809	1.8	P	Bi _{0.4} Sb _{1.6} Te ₃	753
400	2	245	439	1.32	P	Bi _{0.4} Sb _{1.6} Te ₃	753
475	1.16	206	422	1.55	P	Bi _{0.4} Sb _{1.6} Te ₃	753
280	2.96	243	627	1.25	P	Bi _{0.4} Sb _{1.6} Te ₃	753
328	2.89	252	556	1.22	P	Bi _{0.4} Sb _{1.6} Te ₃	753
400	2.05	250	419	1.28	P	Bi _{0.4} Sb _{1.6} Te ₃	753
475	1.22	207	421	1.48	P	Bi _{0.4} Sb _{1.6} Te ₃	753
294	1.06	191	369	1.27	P	Bi _{0.5} Sb _{1.5} Te ₃	613
294	2.17	229	438	1.06	P	Bi _{0.5} Sb _{1.5} Te ₃	653
294	2.78	237	529	1.07	P	Bi _{0.5} Sb _{1.5} Te ₃	693
294	2.72	241	568	1.21	P	Bi _{0.5} Sb _{1.5} Te ₃	733
294	1.11	176	444	1.24	P	Bi _{0.5} Sb _{1.5} Te ₃	593
294	1.94	177	879	1.42	P	Bi _{0.5} Sb _{1.5} Te ₃	623
294	1.56	194	497	1.41	P	Bi _{0.5} Sb _{1.5} Te ₃	613
294	1.71	197	564	1.29	P	Bi _{0.5} Sb _{1.5} Te ₃	653
294	2.44	215	621	1.18	P	Bi _{0.5} Sb _{1.5} Te ₃	693
294	2.70	225	675	1.27	P	Bi _{0.5} Sb _{1.5} Te ₃	733
294	0.67	145	144	0.46	P	Bi _{0.5} Sb _{1.5} Te ₃	573
294	1.63	207	263	0.69	P	Bi _{0.5} Sb _{1.5} Te ₃	643
294	2.94	231	540	0.98	P	Bi _{0.5} Sb _{1.5} Te ₃	713
300	2.7	150	1844	1.5	P	(Bi _{0.3} Sb _{0.6})Te ₃	673
350	2.5	170	1423	1.6	P	(Bi _{0.3} Sb _{0.6})Te ₃	673
400	2.1	180	1114	1.7	P	(Bi _{0.3} Sb _{0.6})Te ₃	673
450	1.7	185	934	1.8	P	(Bi _{0.3} Sb _{0.6})Te ₃	673
300	3.3	200	1083	1.3	P	(Bi _{0.4} Sb _{0.8})Te ₃	673
350	2.85	215	834	1.35	P	(Bi _{0.4} Sb _{0.8})Te ₃	673
400	2.4	210	761	1.4	P	(Bi _{0.4} Sb _{0.8})Te ₃	673
450	1.7	212	573	1.45	P	(Bi _{0.4} Sb _{0.8})Te ₃	673
300	3.16	250	658	1.3	P	(Bi _{0.5} Sb ₁)Te ₃	673
350	2.28	245	495	1.3	P	(Bi _{0.5} Sb ₁)Te ₃	673

Continuation of table

400	1.62	240	366	1.3	<i>P</i>	$(\text{Bi}_{0.5}\text{Sb}_1)\text{Te}_3$	673
450	1	215	281	1.3	<i>P</i>	$(\text{Bi}_{0.5}\text{Sb}_1)\text{Te}_3$	673
240	3.2	193	1350	1.57	<i>P</i>	$\text{Bi}_{0.4}\text{Sb}_{1.6}\text{Te}_3$	673-723
260	3.28	202	1180	1.47	<i>P</i>	$\text{Bi}_{0.4}\text{Sb}_{1.6}\text{Te}_3$	673-723
280	3.3	210	1010	1.35	<i>P</i>	$\text{Bi}_{0.4}\text{Sb}_{1.6}\text{Te}_3$	673-723
300	3.25	220	900	1.34	<i>P</i>	$\text{Bi}_{0.4}\text{Sb}_{1.6}\text{Te}_3$	673-723
320	3.19	225	800	1.27	<i>P</i>	$\text{Bi}_{0.4}\text{Sb}_{1.6}\text{Te}_3$	673-723
340	3.05	230	700	1.21	<i>P</i>	$\text{Bi}_{0.4}\text{Sb}_{1.6}\text{Te}_3$	673-723
360	2.78	235	675	1.34	<i>P</i>	$\text{Bi}_{0.4}\text{Sb}_{1.6}\text{Te}_3$	673-723
240	2.79	205	1195	1.80	<i>N</i>	$\text{Bi}_2\text{Te}_{2.82}\text{Se}_{0.18}$	673-723
260	2.83	215	1090	1.78	<i>N</i>	$\text{Bi}_2\text{Te}_{2.82}\text{Se}_{0.18}$	723-773
280	2.84	220	990	1.69	<i>N</i>	$\text{Bi}_2\text{Te}_{2.82}\text{Se}_{0.18}$	723-773
300	2.82	222	900	1.57	<i>N</i>	$\text{Bi}_2\text{Te}_{2.82}\text{Se}_{0.18}$	723-773
320	2.7	230	800	1.57	<i>N</i>	$\text{Bi}_2\text{Te}_{2.82}\text{Se}_{0.18}$	723-773
340	2.6	231	750	1.54	<i>N</i>	$\text{Bi}_2\text{Te}_{2.82}\text{Se}_{0.18}$	723-773
360	2.4	230	700	1.54	<i>N</i>	$\text{Bi}_2\text{Te}_{2.82}\text{Se}_{0.18}$	723-773
240	3.18	193	1300	1.52	<i>P</i>	$\text{Bi}_{0.4}\text{Sb}_{1.6}\text{Te}_3$	673-723
260	3.26	201	1130	1.40	<i>P</i>	$\text{Bi}_{0.4}\text{Sb}_{1.6}\text{Te}_3$	673-723
280	3.29	205	960	1.23	<i>P</i>	$\text{Bi}_{0.4}\text{Sb}_{1.6}\text{Te}_3$	673-723
300	3.25	209	850	1.14	<i>P</i>	$\text{Bi}_{0.4}\text{Sb}_{1.6}\text{Te}_3$	673-723
320	3.18	218	750	1.12	<i>P</i>	$\text{Bi}_{0.4}\text{Sb}_{1.6}\text{Te}_3$	673-723
340	3.04	220	670	1.07	<i>P</i>	$\text{Bi}_{0.4}\text{Sb}_{1.6}\text{Te}_3$	673-723
360	2.76	230	650	1.25	<i>P</i>	$\text{Bi}_{0.4}\text{Sb}_{1.6}\text{Te}_3$	673-723
240	2.74	193	1250	1.70	<i>N</i>	$\text{Bi}_2\text{Te}_{2.82}\text{Se}_{0.18}$	673-723
260	2.78	200	1145	1.65	<i>N</i>	$\text{Bi}_2\text{Te}_{2.82}\text{Se}_{0.18}$	723-773
280	2.80	205	1045	1.57	<i>N</i>	$\text{Bi}_2\text{Te}_{2.82}\text{Se}_{0.18}$	723-773
300	2.82	207	955	1.45	<i>N</i>	$\text{Bi}_2\text{Te}_{2.82}\text{Se}_{0.18}$	723-773
320	2.71	208	855	1.36	<i>N</i>	$\text{Bi}_2\text{Te}_{2.82}\text{Se}_{0.18}$	723-773
340	2.62	209	805	1.34	<i>N</i>	$\text{Bi}_2\text{Te}_{2.82}\text{Se}_{0.18}$	723-773
360	2.43	210	755	1.37	<i>N</i>	$\text{Bi}_2\text{Te}_{2.82}\text{Se}_{0.18}$	723-773
240	3.1	182	1600	1.71	<i>P</i>	$\text{Bi}_{0.4}\text{Sb}_{1.6}\text{Te}_3$	673-723
260	3.2	193	1400	1.63	<i>P</i>	$\text{Bi}_{0.4}\text{Sb}_{1.6}\text{Te}_3$	673-723
280	3.23	195	1200	1.41	<i>P</i>	$\text{Bi}_{0.4}\text{Sb}_{1.6}\text{Te}_3$	673-723
300	3.25	200	1100	1.35	<i>P</i>	$\text{Bi}_{0.4}\text{Sb}_{1.6}\text{Te}_3$	673-723
320	3.19	203	1000	1.29	<i>P</i>	$\text{Bi}_{0.4}\text{Sb}_{1.6}\text{Te}_3$	673-723
340	3.05	205	900	1.24	<i>P</i>	$\text{Bi}_{0.4}\text{Sb}_{1.6}\text{Te}_3$	673-723
360	2.83	207	800	1.21	<i>P</i>	$\text{Bi}_{0.4}\text{Sb}_{1.6}\text{Te}_3$	673-723
240	2.7	170	1450	1.55	<i>N</i>	$\text{Bi}_2\text{Te}_{2.82}\text{Se}_{0.18}$	673-723
260	2.73	180	1350	1.60	<i>N</i>	$\text{Bi}_2\text{Te}_{2.82}\text{Se}_{0.18}$	723-773
280	2.78	185	1250	1.54	<i>N</i>	$\text{Bi}_2\text{Te}_{2.82}\text{Se}_{0.18}$	723-773
300	2.8	195	1150	1.56	<i>N</i>	$\text{Bi}_2\text{Te}_{2.82}\text{Se}_{0.18}$	723-773
320	2.78	200	1050	1.51	<i>N</i>	$\text{Bi}_2\text{Te}_{2.82}\text{Se}_{0.18}$	723-773
340	2.7	203	1000	1.53	<i>N</i>	$\text{Bi}_2\text{Te}_{2.82}\text{Se}_{0.18}$	723-773
360	2.6	204	950	1.52	<i>N</i>	$\text{Bi}_2\text{Te}_{2.82}\text{Se}_{0.18}$	723-773
294	2.92	166	1600	1.51	<i>P</i>	$\text{Bi}_{0.3}\text{Te}_{1.7}\text{Se}_3$	-
294	3.25	208	960	1.28	<i>P</i>	$\text{Bi}_{0.6}\text{Te}_{1.4}\text{Se}_3$	-

Continuation of table

294	3.2	205	1020	1.34	<i>P</i>	<i>Bi</i> _{0.6} <i>Te</i> _{1.4} <i>Se</i> ₃	-
294	1.62	296	168	0.91	<i>P</i>	<i>Bi</i> _{0.6} <i>Te</i> _{1.4} <i>Se</i> ₃	-
294	3	215	1030	1.59	<i>N</i>	<i>Bi</i> ₂ <i>Te</i> _{2.82} <i>Se</i> _{0.18}	-
294	2	295	225	0.98	<i>N</i>	<i>Bi</i> ₂ <i>Te</i> _{2.82} <i>Se</i> _{0.18}	-
294	1.9	245	325	1.03	<i>N</i>	<i>Bi</i> ₂ <i>Te</i> _{2.1} <i>Se</i> _{0.9}	-
294	1.7	240	323	1.09	<i>N</i>	<i>Bi</i> ₂ <i>Te</i> _{1.8} <i>Se</i> _{1.2}	-
300	3.2	208	960	1.30	<i>P</i>	<i>Bi</i> _{0.6} <i>Te</i> _{1.4} <i>Se</i> ₃	-
300	2.2	260	310	0.95	<i>P</i>	<i>Bi</i> _{0.6} <i>Te</i> _{1.4} <i>Se</i> ₃	-
300	1.6	295	170	0.92	<i>P</i>	<i>Bi</i> _{0.6} <i>Te</i> _{1.4} <i>Se</i> ₃	-
300	3.2	205	776	1.02	<i>P</i>	<i>Bi</i> _{0.6} <i>Te</i> _{1.4} <i>Se</i> _{0.12} <i>Te</i> _{2.88}	-
300	3.1	213	1055	1.54	<i>N</i>	<i>Bi</i> ₂ <i>Te</i> _{2.82} <i>Se</i> _{0.18}	-
300	2.9	240	655	1.30	<i>N</i>	<i>Bi</i> ₂ <i>Te</i> _{2.82} <i>Se</i> _{0.18}	-
300	2	295	260	1.13	<i>N</i>	<i>Bi</i> ₂ <i>Te</i> _{2.82} <i>Se</i> _{0.18}	-
300	3.2	208	960	1.30	<i>P</i>	<i>Bi</i> _{0.5} <i>Te</i> _{1.5} <i>Se</i> ₃	-
300	2.92	163	1166	1.06	<i>N</i>	<i>Bi</i> ₂ <i>Te</i> _{2.7} <i>Se</i> _{0.3}	660
300	2.62	171	1059	1.18	<i>N</i>	<i>Bi</i> ₂ <i>Te</i> _{2.7} <i>Se</i> _{0.3}	660
300	2.55	157	1407	1.36	<i>N</i>	<i>Bi</i> ₂ <i>Te</i> _{2.7} <i>Se</i> _{0.3}	660
300	1.40	165	1308	2.53	<i>N</i>	<i>Bi</i> ₂ <i>Te</i> _{2.7} <i>Se</i> _{0.3}	660
300	1.73	175	1197	2.12	<i>N</i>	<i>Bi</i> ₂ <i>Te</i> _{2.7} <i>Se</i> _{0.3}	660
300	1.80	196	1975	2.34	<i>N</i>	<i>Bi</i> ₂ <i>Te</i> _{2.7} <i>Se</i> _{0.3}	660
300	2.03	214	846	1.91	<i>N</i>	<i>Bi</i> ₂ <i>Te</i> _{2.7} <i>Se</i> _{0.3}	660
300	2.10	202	940	1.83	<i>N</i>	<i>Bi</i> ₂ <i>Te</i> _{2.7} <i>Se</i> _{0.3}	660
300	2.50	207	978	1.69	<i>N</i>	<i>Bi</i> ₂ <i>Te</i> _{2.7} <i>Se</i> _{0.3}	660
300	2.33	222	741	1.57	<i>N</i>	<i>Bi</i> ₂ <i>Te</i> _{2.7} <i>Se</i> _{0.3}	660

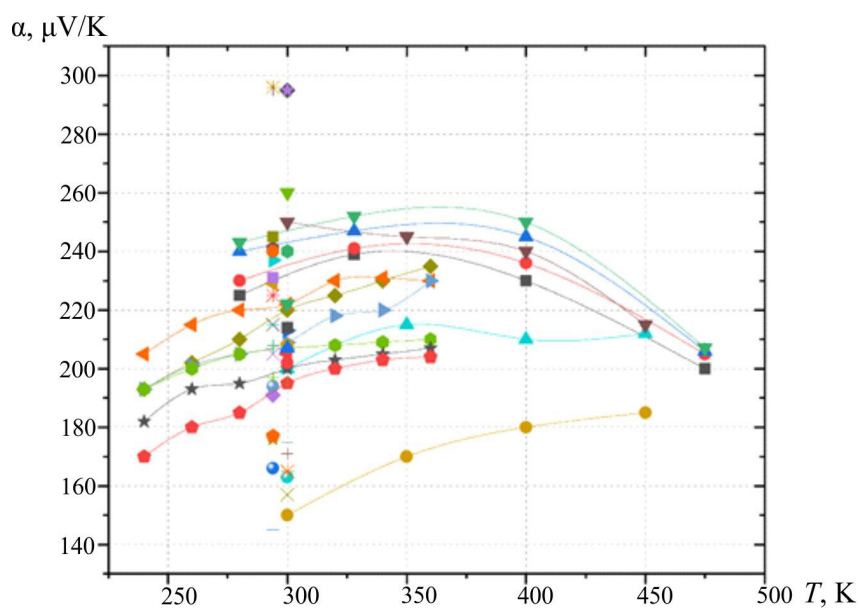


Fig. 1. Graph of dependence of thermoEMF
on temperature

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.

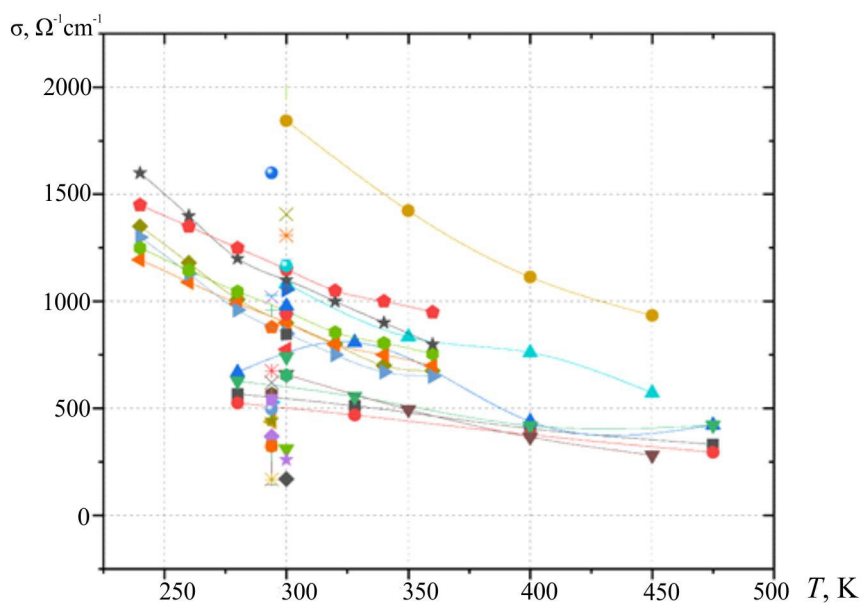


Fig. 2. Graph of dependence of electrical conductivity on temperature

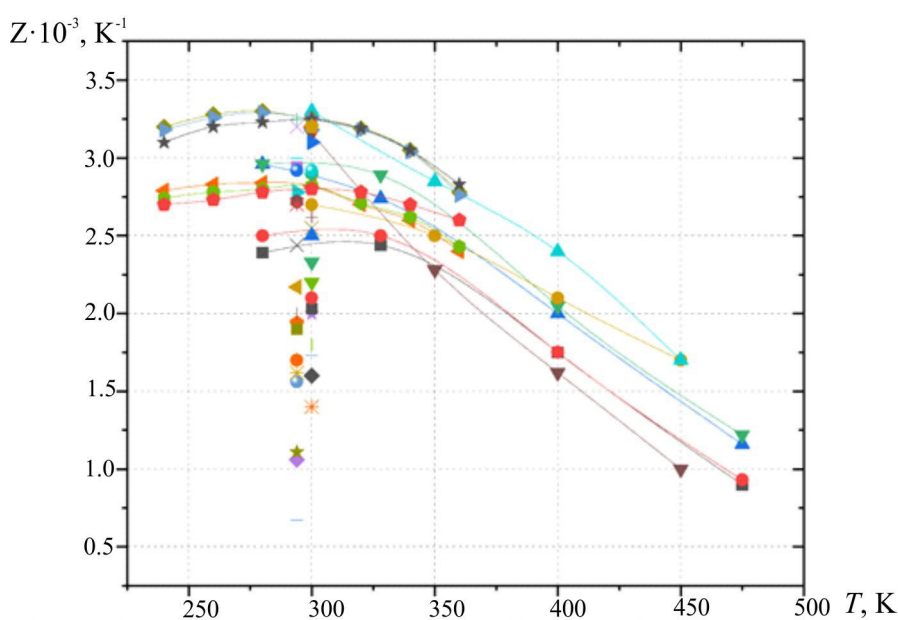


Fig. 3. Graph of dependence of the figure of merit on temperature

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:

$$Y = Y_0 + ((Y_1 - Y_0) \div (X_1 - X_0)) \times (X - X_0) \quad (1)$$

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.

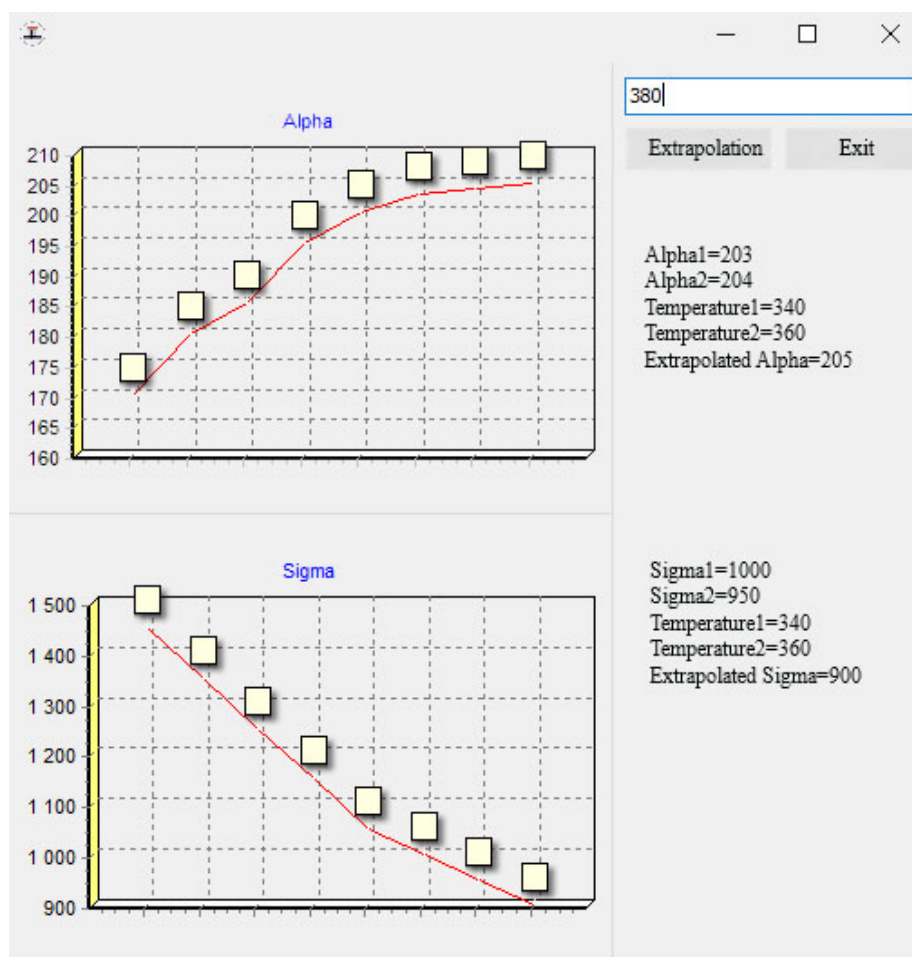


Fig. 4. General view of the value extrapolation window

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. 7. рис. 4. табл. 1.

Ключові слова: метод екструзії, екстраполяція, телурид вісмуту.

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