DOI: 10.63527/1607-8829-2021-3-44-50

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COMPUTER METHOD OF DESCRIPTION OF THE TECHNOLOGIES AND PROPERTIES OF Bi_2-Te_3 -BASED THERMOELECTRIC MATERIALS OBTAINED BY THE BRIDGMAN METHOD

This paper presents the results of the study of literary sources describing the technologies and properties of thermoelectric materials obtained by the Bridgman method. The results of one of the stages of creating a software product for the description of the production technologies and properties of a thermoelectric material based on Bi-Te compounds are given.Bibl.8, Fig.2, Table 1.
Key words: Bridgman method, interpolation, bismuth telluride.

Introduction

Thermoelectric materials are in high demand due to their use in power generation and refrigeration applications. They are an excellent solution in active cooling devices in military, telecommunication equipment and temperature control systems.

Bismuth telluride (Bi_2Te_3) is one of the best thermoelectric materials with the highest thermoelectric figure of merit (Z), which in turn is related to thermal conductivity (κ) and electric conductivity (σ), as represented in formula 1

$$Z = \frac{\alpha^2 \sigma}{\kappa}, \quad (1)$$

where α is the Seebeck coefficient.

Traditional methods of manufacturing bismuth telluride compounds include the Bridgman, Czochralski, and zone melting methods, as well as powder metallurgy methods such as hot pressing and hot extrusion [1].

The purpose of this work is to study the thermoelectric characteristics of solid solutions based on bismuth telluride obtained by the Bridgman method, as well as application of a modified computer program with the study of Bridgman's method and characteristics of thermoelectric materials based on *Bi-Te* compounds.

Dependence of the thermoelectric characteristics of Bi_2-Te_3-based materials obtained by the Bridgman method

When obtaining samples of Bi_2Te_3 and its solid solutions by the Bridgman method, the material is synthesized by fusing the initial components in the same ampoule in which the material will be

grown later [2]. The Bridgman method consists in the fact that an ampoule with a crystallizing substance moves in the furnace from the upper part with a temperature exceeding the melting temperature to the lower part, the temperature of which is lower than the melting temperature. Bridgman-produced ingots of Bi_2Te_3 consist of one or more crystalline grains large enough to be cut into single-crystal samples.

Table 1 shows the thermoelectric characteristics of *Bi-Te*-based materials obtained by the Bridgman method.

Table 1

Thermoelectric characteristics of Bi-Te-based materials obtained by the Bridgman method.

Working temperature, K	Z, 10^{-3},K^{-1}	α, mV/K	σ, $Ohm^{-1}cm^{-1}$	κ, W/m·K	Material type:	Material composition	Ingot length, mm	Melt temperature, K	Annealing temperature, K	Annealing duration, h	Literary source:
308	4.57	-	-	1.21	P	$(Bi_{0,25}Sb_{0,75})_2Te_3$	15	686	473-673	2-5	[3]
308	3.67	-	-	-	N	$Bi_2(Te_{0,94}Se_{0,06})_3$	15				[3]
298	1.27	-	-	1.38	P	$(Bi_{0.25}Sb_{0.75})_2Te_3$	-	-	-	-	[4]
298	1.25	-	-	1.36	N	$Bi_2(Te_{0.94}Se_{0.06})_3$	-	-	-	-	[4]
298	0.91	221	-	1.36	P	$(Bi_{0,25}Sb_{0,75})_2Te_3$	15	-	673	5	[5]
298	1.09	223	-	1.65	N	$Bi_2(Te_{0,94}Se_{0,06})_3$	15	-	673	5	[5]
473	-	-	-	-	P	$Bi_{0,5}Sb_{1,5}Te_{3,0}$	-	923	-	-	[6]
300	2.8	171	1910	10.2	N	$Bi_2Te_{1.5}Se_{1.5}$	-	-	600	1200	[7]
300	2.7	161	2120	9.5	N	$Bi_{1.9998}Sn_{0.0002}Te_{1.5}Se_{1.5}$	-	-	600	1200	[7]
300	3	163	2320	8.9	N	$Bi_{1.9996}Sn_{0.0004}Te_{1.5}Se_{1.5}$	-	-	600	1200	[7]

All the data in the table were implemented in the software product to describe the technologies and properties of *Bi-Te* -based thermoelectric material. Updating the software product database will be described in future papers.

Theory of linear interpolation

Interpolation in the general sense is a method of calculating certain intermediate values of any studied quantity based on a set of known values.

If the investigated process can be described by a linear function, the procedure for calculating unknown parameters can be significantly simplified compared to other calculation cases. Mathematical modeling of various production situations of engineering and scientific practicality by methods of linear interpolation suggests the possibility of mathematical forecasting by identifying the value of the interpolated coordinate *Y* by a given parameter of the *X* coordinate with known coordinates of two points of a linear function [8].

For successful management, it is necessary to foresee how this or that system will behave within the framework of the existing process described by the corresponding linear function. The first point of the linear function has coordinates X0,Y0, the second - X1,Y1, the resulting interpolated Y coordinate, which is calculated, based on the given value of the X coordinate, is calculated according to formula 2:

$$Y = \left(\left(X - X_0\right) \times \left(Y_1 - Y_0\right) \div \left(X_1 - X_0\right)\right) + Y_0, \qquad (2)$$

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

The function of theoretical calculation of unknown values of α and δ using interpolation was introduced into the software product for describing the production technologies and characteristics of thermoelectric material based on *Bi-Te* compounds. The general algorithm of this function is as follows.

- Calling the interpolation function by the user.
- Creation of a dynamic form and all its components for interpolation.
- After the user enters the required working temperature, the program searches the database for a material whose performance range may include the desired value. To do this, the following algorithm is implemented (Fig.1).
- After selecting the optimal material, the program calculates the value of the coefficient α using a linear interpolation formula.
- Based on the result obtained, the program plots the dependence of α on temperature.
- After receiving the results of α, the program calculates the value of δ using a linear interpolation formula.
- Based on the result obtained, the program plots the dependence of δ on temperature.
- The results are also displayed in Label.
- After the user terminates, the program deletes all form components and the form itself. The general view of the value interpolation window is shown in Fig.1.

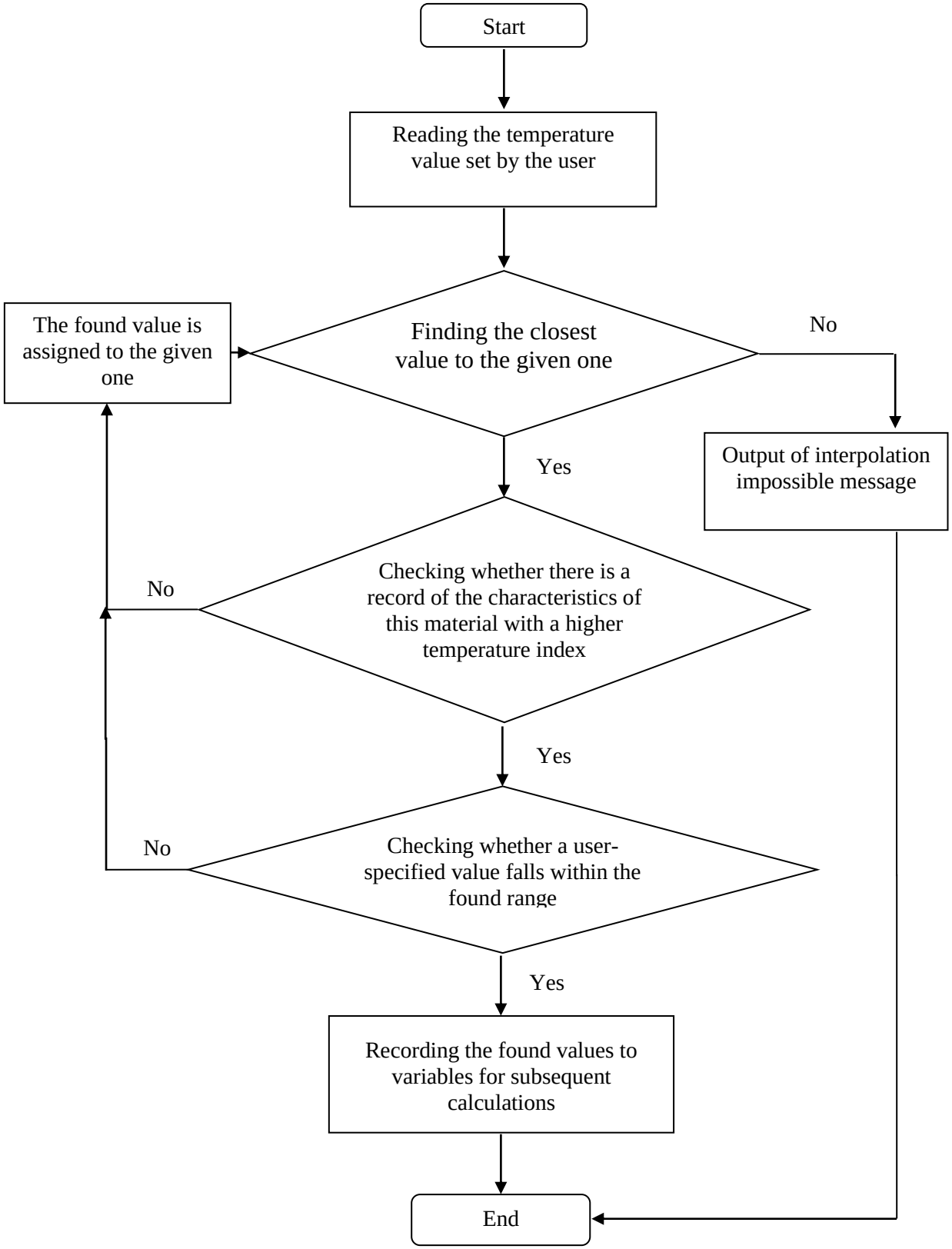

Fig. 1. Algorithm of finding optimal material for interpolation

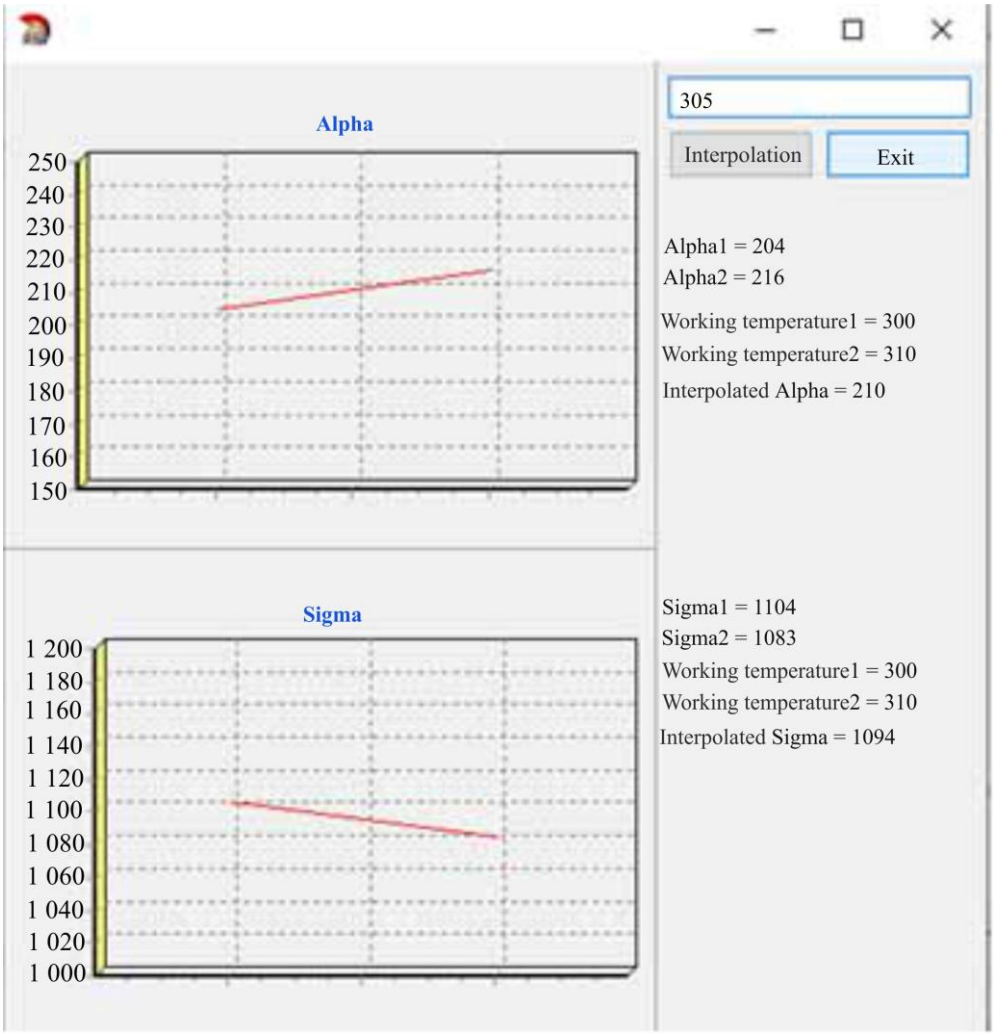

Fig. 2. General view of the value interpolation window
Interpolation; output; working temperature; interpolated Alpha; interpolated Sigma

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

Conclusions

A study of literary sources describing *Bi-Te*-based thermoelectric materials obtained by the Bridgman method was carried out.

1. The research data were added to the database of the software product to describe the technologies and properties of obtaining *Bi-Te*-based thermoelectric material.
2. The interpolation function is implemented in the software product to describe the technologies and properties of obtaining *Bi-Te*-based thermoelectric material.
3. Further versions of the software product will be described in subsequent papers.

The authors express their gratitude to Anatychuk Lukyan Ivanovych, academician of the National Academy of Sciences, for the suggested topic of the paper.

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Submitted 12.07.2021

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

У даній роботі наводяться результати дослідження літературних джерел в яких описуються технології та властивості термоелектричних матеріалів отриманих методом Бріджмена. Наводяться результати одного з етапів створення програмного продукту для опису технологій отримання та властивостей термоелектричного матеріалу на основі сполук Bi-Te. Бібл. 8. рис. 2. табл. 1.

Ключові слова: метод Бріджмена, інтерполяція, телурид вісмуту.

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КОМПЬЮТЕРНЫЙ МЕТОД ОПИСАНИЯ ТЕХНОЛОГИЙ И СВОЙСТВ ТЕРМОЭЛЕКТРИЧЕСКИХ МАТЕРИАЛОВ НА ОСНОВЕ Bi_2-Te_3, ПОЛУЧЕННЫХ МЕТОДОМ БРИДЖМЕНА

В данной работе приводятся результаты анализа литературных источников, в которых описываются технологии и свойства термоэлектрических материалов, полученных методом Бриджмена. Приводятся результаты одного из этапов создания программного продукта для описания технологий производства и свойств термоэлектрического материала на основе соединения Bi-Te. Библ. 8. рис. 2. табл. 1.
Ключевые слова: метод Бриджмена, интерполяция, теллурид висмута.

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