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Araştırma Makalesi / Research Article

Determination of Boiling Temperatures from Elastic Constants

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Boiling temperatures; Cubic; Regression; MINITAB

Abstract

33 cubic and 11 hexagonal materials were selected to determine the boiling temperature of the materials by regression analysis. The boiling temperatures of these selected materials were estimated by regression analysis using the elastic constant and boiling temperature information in the literature. Variance and regression analyze were performed with MINITAB 17 software in 95% confidence interval. Regression coefficients were calculated with 98.9% determination coefficient. As a result of regression analysis, an empirical relationship between the elastic constants and the boiling temperature was obtained which predicts boiling temperatures for some cubic and hexagonal materials. The boiling temperatures calculated with the help of these relationships were compared with the literature data.

Elastik Sabitlerden Kaynama Sıcaklığının Belirlenmesi

Anahtar kelimeler
Kaynama sıcaklığı; Kübik; Regresyon; MINITAB

Öz

Regresyon analizi ile malzemelerin kaynama sıcaklığını belirlemek için 33 kübik ve 11 hekzagonal malzeme seçilmiştir. Bu seçilen malzemelerin kaynama sıcaklıkları, literatürdeki elastik sabit ve kaynama sıcaklığı bilgileri kullanılarak regresyon analizi ile tahmin edilmiştir. MINITAB 17 yazılımı ile %95 güven aralığında varyans ve regresyon analizi yapılmıştır. Regresyon katsayıları %98,9 tespit katsayısı ile hesaplanmıştır. Regresyon analizi sonucunda, elastik sabitler ile kaynama sıcaklığı arasında ampirik ilişki elde edilmiş ve bazı kübik ve hekzagonal malzemeler için kaynama sıcaklıkları öngörülmüştür. Bu ilişkilerin yardımıyla hesaplanan kaynama sıcaklıkları literatür verileri ile karşılaştırıldı.

1. Introduction

Since the existence of humanity, it has used the materials in nature to meet their needs according to their wishes. The use of materials in nature has sometimes taken place without any operation, and sometimes after various operations. The material has always been important for humanity and it still maintains its importance. Materials are critical to maintaining the current technological developments (Erdoğan 2007). The selection of suitable materials for the job is only possible by knowing the properties of the material. For example, it is desirable that the material used in the making of the boiling container is high melting temperature. The material used in the cutting and drilling tool must be very hardness. Nowadays, the physical properties of materials can be determined by theoretical and experimental studies. In cases where experimental measurements can be difficult or the cost may be high be able to be determined, it can be very easy and inexpensive to determine the properties of the material through a number of theoretical models (Arslan and Dogan 2019). There are many models and empirical relationships in the literature to determine each properties of the material, for example, evaluation of thermodynamic properties (Arslan et al. 2013, Arslan and Dogan 2015, Dogan and Arslan 2018), composition dependencies of thermodynamic properties (Dogan and Arslan 2016), estimation of excessive energies and activity coefficients (Dogan et al. 2015), determination of martensite conversion temperatures (Dogan and Ozer 2013), hardness of polycrystalline materials (Chen et al. 2011), etc. The computing power of computers is widely used in theoretical studies. Computer calculations help to you understand physical phenomena while also reducing research costs (Ozer 2016). As a result of the calculations, empirical relations can be established between the physical properties of the material.

As stated in many studies in the literature, the elastic properties of the solid are associated with physical properties such as heat capacity, melting point, inter-atom bond and Debye temperature (Liu 2011). Elastic constants of the material give interesting information about the mechanical and dynamic properties of the substance (Cabuk 2010). Also, the elastic constants are very important parameters for technological applications (Ozer and Cabuk 2018). The experimental determination of these quantities under high pressure is difficult because of the difficulty of the experimental conditions (Özer et al. 2017). Due to the relationship between the boiling temperature and the elastic constants, the boiling temperature of the material can be calculated by the help of elastic constants. The use of empirical relations in determining the boiling temperature will prevent the time and material consumption used in experimental studies. With empirical relations, the boiling temperature can be easily and quickly predicted.

Numerous experimental studies have been conducted to determine the boiling temperature of materials in the literature (Madelung 2004, Rumble 2018). There are empirical correlations in the literature for determining the melting temperatures of cubic, hexagonal and tetragonal materials (Özer 2018, Fine et al. 1984). However, we could not find any empirical relation to the determination of boiling points. In this sense, an empirical equation was proposed between the elastic constants and the boiling temperatures for the first time in solids. The proposed equation has a 95% confidence interval and a 98.9% coefficient of determination.

2. Materials and Methods

If the relationship between the variables is statistically significant, a statistical model can be created for this relationship. In constructing a statistical model, a variable is used as a dependent or as a response variable and other variable or variables are taken as explanatory variables. In this study, regression model was used. The purpose of the regression analysis is to explain the total change in the dependent or response variable using explanatory variable or variables. To explain the total change in the response variable, if the regression model uses an explanatory variable is called simple linear and if the regression model uses multiple explanatory variables is called as a multiple regression model.

Too many variables can come together and influence another a variable. Same time these explanatory variables can also affect each other among themselves. For example, if there is a linear relationship between the explanatory variable X_1 and the explanatory variable X_2, this causes the problem of multiple internal relations. These two explanatory variables do not need to be present in the model at the same time. One of the variables is enough to be in the model (Erol 2010). Scattering diagrams are plotted to easily visualize the relationship between variables. Scattering diagrams show the relationship and shape between variables.

The equation, which determines from the scattering diagrams functional form of the relationship between variables, is called the regression equation. In cases where a variable is used, a single regression analysis is performed. If using in the regression analysis multiple independent variables is called "multiple regression analysis".

The most common multiple regression equation; X_i explanatory variables or arguments, the e_i error term, and the Y response variable or dependent variable;

$$Y = a_0 + a_1 X_1 + a_2 X_2 + \cdots + a_k X_k + e_i \quad (1)$$

here, a_0 is the value Y when X = 0. a_1, a_2, a_k are the regression coefficient. When it is changed 1 unit in 's unit, it refers to the amount of change in X 's own unit in the Y. The term e_i error represents, in a way, the argument that is not included in the model. There are different methods (Gürsakal 2014) and software to solve the regression equations. In this study, we used the MINITAB software. In order to visually see the strength and direction of the relationship between two quantitative variables, a scattering diagram is drawn (Gürsakal 2014). If there is no relationship between variables, regression analysis cannot be applied. The scatter diagram drawn for this study is shown in Figure 2. The following figures (Figure-1) are given as examples for the scattering diagrams showing the shape and direction of the relationship.

It is not correct to make an estimate for an X value of outside the change range of the X values used in the calculation of the regression coefficient of the regression equation. If an X value outside this the range is used for estimating from the regression equation, the estimate may be inaccurate (Gürsakal 2014).

After the regression coefficients are calculated and regression estimation model is established, R_2 and corrected R_2 are calculated. The value of the R_2, variable or variables of the X, indicates the percentage of the total change in the variable Y. In the regression models with the same number of explanatory variables, R_2 uses the corrected R_2 value in regression models with a different number of explanatory variables (Erol 2010). Value of the coefficient of determination is $0 \leq R_2 \leq 1$. if the R_2 value is "0", it indicates that the variability in the dependent variable cannot be explained by the argument. if the R_2 value is "1", it indicates that the variability in the dependent variable is fully explained by the argument (Gürsakal 2014).

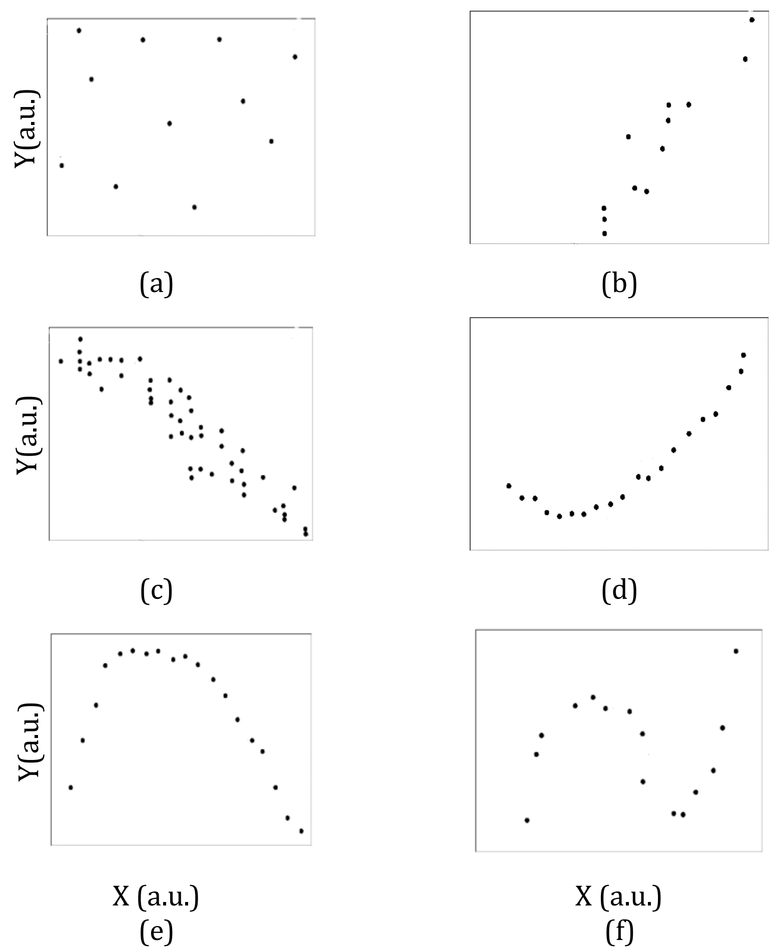

Figure 1: Examples of scattering diagrams, (a) There is no relationship between variables, (b) There is a positive linear relationship between variables, (c) There is a negative linear relationship between variables, (d) The relationship between variables is parabolic, (e) The relationship between the variables is parabolic in a negative direction, (f) The relationship between variables is curvilinear.

3. Results and Discussion

The boiling point and elastic constants of 33 cubic materials to be used in this study were obtained from the literature review and given in Table 1. The scattering diagrams of these materials showing the relationship between elastic constants and boiling temperatures are shown in Fig. 2. As seen from Figure 2, there is a positive linear relationship between the variables. For the cubic structures, variance and regression analyzes were performed with the MINITAB 17 (Minitab) software on the data shown in Table 1. As a result of the analyzes, it was seen that regression model and coefficients of the regression were statistically significant and the coefficient of determination of the model was 98.9%. According to this result, 98.9% of the variability in the boiling point of a cubic material can be explained by the elastic constants C_{11}, C_{12} and C_{44}, which cannot be explained by 1.1%. 1.1% depends on factors not included in the model. The empirical equation obtained in regression analysis is given below:

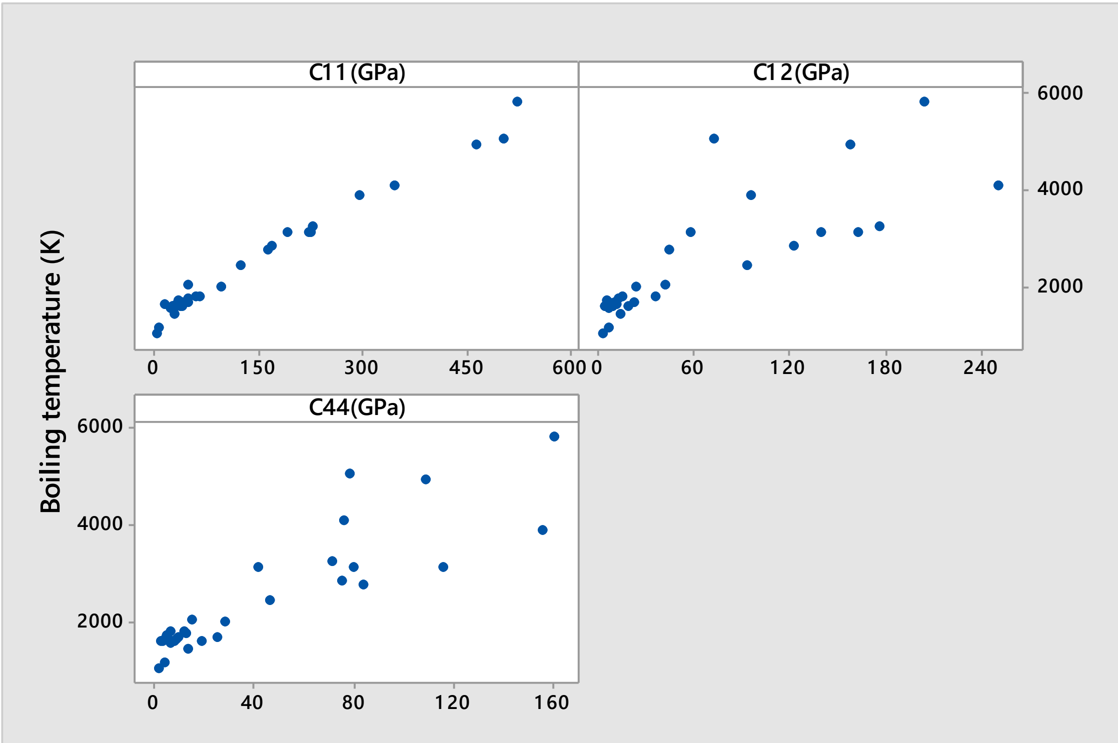

Figure 2: Scattering diagram for cubic structures.

$$b_t = 1312.5 + 7.019C_{11} + 1.221C_{12} + 2.26C_{44} \quad (2)$$

here, b_t is the boiling point in Kelvin (K) unit, C_{ij} is the elastic constants (GPa). As can be seen from this equation, the maximum contribution to boiling point comes from C_{11} constant. C_{12} and C_{44} contribute a little to the boiling point. The comparison of the boiling points obtained by using the proposed equation with this study is done in Table 1 and Table 2. As can be seen from Table 1, the values calculated using Equation (2) are quite consistent with experimental values. The maximum difference between the calculated value and the experimental values given in Table 1 is 30.48%, the smallest difference is 0.03% mean 5.05% difference.

In order to test the empirical equation (2), we applied to the materials in Table 2 which are not used in the analysis. Table 2 was compared with unused data in the analysis to test the predictive power of this equation. As can be seen from Table 2, the values calculated using Equation (2) are consistent with experimental data. The biggest difference between the calculated value and the experimental values given in Table 2 is 64.23%, the smallest difference is 2.32% and 25.95% difference.

Table 1: Comparison of boiling points for cubic structures (C_{ij} in GPa, Boiling point (b_t) in K)

Formula	C_{11}	C_{12}	C_{44}	b_t(expt.)	b_t (from eq.2)	Dif.
Ag [a]	123.99	93.67	46.12	2435.00	2401.39	1.38
AgBr [a]	59.20	36.40	6.16	1775.00	1786.39	0.64
Au [a]	192.44	162.98	42.00	3109.00	2957.15	4.88
CaF_2 [a]	164.20	43.98	84.06	2773.00	2708.69	2.32
CaO [a]	221.89	57.81	80.32	3123.00	3122.06	0.03
CsBr [a]	30.63	8.07	7.50	1573.00	1554.30	1.19
CsCl [a]	36.44	8.82	8.04	1570.00	1597.21	1.73
CsI [a]	24.46	6.61	6.29	1553.00	1506.47	3.00
Cu [a]	168.30	122.10	75.70	2833.00	2813.96	0.67
Fe [a]	226.00	140.00	116.00	3134.00	3331.89	6.31
K [a]	3.70	3.14	1.88	1032.00	1346.55	30.48
KBr [a]	34.68	5.80	5.07	1708.00	1574.46	7.82
KF [a]	64.90	15.20	12.32	1775.00	1814.44	2.22
KI [a]	27.10	4.50	3.64	1596.00	1516.44	4.99
Li [a]	13.50	11.44	8.78	1615.00	1441.07	10.77
LiBr [a]	39.40	18.80	19.10	1573.00	1655.17	5.22
LiCl [a]	49.27	23.10	24.95	1656.00	1742.92	5.25
LiI [a]	28.50	14.00	13.50	1444.00	1560.15	8.04
MgO [a]	297.08	95.36	156.13	3873.00	3866.99	0.16
Mo [a]	463.70	157.80	109.20	4912.00	5006.68	1.93
Na [a]	7.39	6.22	4.19	1155.94	1381.43	19.51
NaBr [a]	39.70	10.01	9.98	1663.00	1625.93	2.23
NaCl [a]	49.47	12.88	12.87	1738.00	1704.54	1.93
NaF [a]	97.00	23.80	28.22	1977.00	2086.18	5.52
NaI [a]	30.07	9.12	7.33	1577.00	1551.26	1.63
Pb [a]	49.66	42.31	14.98	2022.00	1746.58	13.62
Pd [a]	227.10	176.04	71.73	3236.00	3283.57	1.47
Pt [a]	346.70	250.70	76.50	4098.00	4224.98	3.10
RbBr [a]	31.52	5.00	3.80	1613.00	1548.43	4.00
RbCl [a]	36.24	6.12	4.68	1663.00	1584.92	4.70
RbI [a]	25.56	3.82	2.78	1573.00	1502.85	4.46
TaC [a]	505.00	73.00	79.00	5053.00	5124.77	1.42
W [a]	522.39	204.37	160.83	5828.00	5592.17	4.05
Max.	**522.39**	**250.70**	**160.83**	**5828.00**	**5592.17**	**30.48**
Min.	3.70	3.14	1.88	1032.00	1346.55	0.03
Mean.	128.40	56.15	39.50	2371.48	2371.58	5.05

[a] Rumble 2018

Table 2: Comparison of unused boiling points (in cubic structures) in regression analysis (C_{ij} in GPa, Boiling point (b_t) in K)

Formula	C_{11}	C_{12}	C_{44}	b_t(expt.)	b_t (from eq. 2)	Dif.
Al	106.75[a,b,c]	60.41	28.34	2792.00[a]	2199.59	21.22
CaF_2	164.20[a,b,d]	43.98	84.06	2773.00[a]	2708.69	2.32
Cr	339.80[a,b,e]	58.60	99.00	2944.00[a]	3992.85	35.63
Ge	128.35[a,b,f]	48.23	66.66	3106.00[a]	2422.93	21.99
LiF	113.97[a,b,g]	47.67	63.64	1946.00[a]	2314.49	18.94
MgO	297.10[o]	96.50	155.70	4070.00[o]	3867.55	4.97
Nb	246.50[a,b,h]	134.50	28.73	5014.00[a]	3271.84	34.75
Ni	248.10[a,b,i]	154.90	124.20	3186.00[a]	3523.74	10.60
Si	165.78[a,b,j]	63.94	79.62	3538.00[a]	2734.12	22.72
SrF_2	123.50[a,b, k]	43.05	31.28	2733.00[a]	2302.60	15.75
SrO	175.47[o]	49.08	55.87	3300.00[o]	2730.32	17.26
Ta	260.23[a,b,l]	154.46	82.55	5728.00[a]	3514.21	38.65
Th	75.30[a,b,m]	48.90	47.80	5058.00[a]	2008.77	60.29
ThO_2	367.00[a,b,n]	106.00	79.70	4673.00[a]	4198.02	10.16
TlBr	37.60[a]	14.58	7.57	1092.00[a]	1611.32	47.56
TlCl	40.15[o]	15.37	7.84	993.00[o]	1630.80	64.23
V	228.70[a,b,h]	119.00	43.20	3680.00[a]	3160.68	14.11
Max.	**367.00**	**154.90**	**155.70**	**5728.00**	**4198.02**	**64.23**
Min.	37.60	14.58	7.57	993.00	1611.32	2.32
Mean.	183.44	74.07	63.87	3330.94	2834.85	25.95

[a] Rumble 2018, [b] Simsons and Wang 1971, [c] Thomas 1968, [d] Wong and Schuele 1967, [e] Sumer and Smith 1963, [f] Bogardus 1965, [g] Drabble and Strathen1967, [h] Bolef 1961, [i] Epstein and Carlson 1965, [j] McSkimin and 1964, [k] Gerlich 1964, [l] Soga 1966, [m] Armstrong et al. 1959, [n] Macedo et al. 1964, [o] Madelung 2004,

For the hexagonal structures, elastic constant (C_{ij}) and boiling points are obtained from the literature and are shown in Table 3. A distribution graph shown in Figure 3 was obtained to form the empirical relationship between C_{ij} and the boiling point.

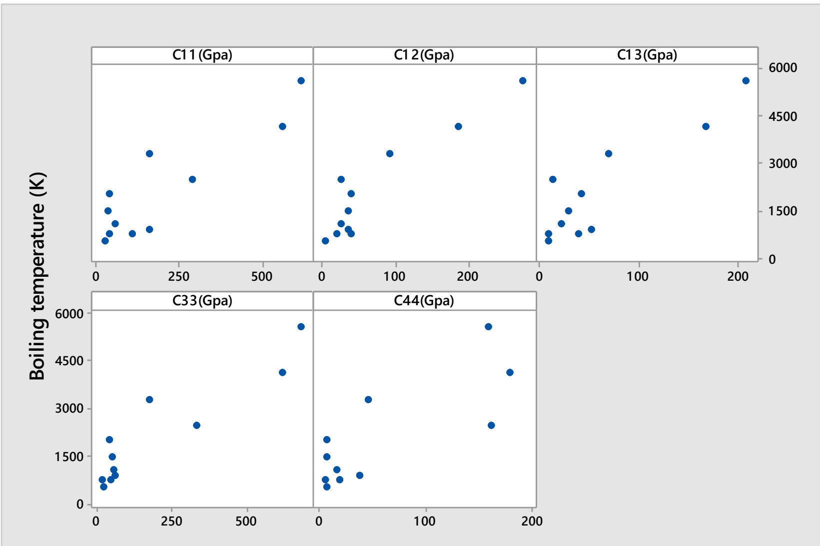

Figure 3: Scattering diagram for hexagonal structures.

Regression analysis was performed with MINITAB 17 software. It is seen that the proposed model explained the boiling point in 99.71%. Other factors that are not included in the model are 0.29% in determining the boiling point. The regression equation for hexagonal structures;

$$b_t = 555.4 - 25.94C_{11} + 44.88C_{12} + 16.05C_{13} - 7.48C_{33} + 65.14C_{44} \quad (3)$$

The boiling temperature values of 11 different materials calculated with the help of equation 3 are compared with the boiling points in the literature in Table 3. In the comparison, it is seen that the proposed model predicts the boiling point different by 6.9% on average.

Table 3: Determination of boiling point in hexagonal structure from elastic constants.

Formula	b_t **(expt.)**	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	b_t **(from eq.3)**	**Dif.**
Be	2468[a]	292.3[a,b,p]	26.7	14	336.4	162.5	2465.1	0.1
BiI_3	542[a]	29[o]	5	9	26	7	433.5	20.0
Cd	767[a]	114.5[a,b,r]	39.5	39.9	50.85	19.85	911.1	18.8
CdI_2	744[a]	43.1[o]	20.4	8.9	22.5	5.5	685.8	7.8
In	2027[a]	45.4[a,b,s]	40.06	41.51	45.15	6.51	1929.5	4.8
Mg	1090[a]	59.5[a,b,t]	26.12	21.8	61.55	16.35	1138.8	4.5
Ru	4147[a]	562.6[a]	187.8	168.2	624.2	180.6	4184.9	0.9
Ti	3287[a]	162.4[a,b,u]	92	69	180.7	46.7	3269.6	0.5
Tl	1473[a]	40.8[a,b,w]	35.4	29	52.8	7.26	1629.2	10.6
Zn	907[a]	163.68[a,b,y]	36.4	53	63.47	38.79	845.8	6.7
Re	5590[a]	618.2[a,b,z]	275.3	207.8	683.5	160.6	5558.9	0.6
Max.	5590	618.2	275.3	207.8	683.5	180.6	5558.9	20.0
Min.	542	29.0	5.0	8.9	22.5	5.5	433.5	0.1
Mean.	2095	193.8	71.3	60.2	195.2	59.2	2095.6	6.9

[a] Rumble 2018, [b] Simsons and Wang 1971, [o] Madelung 2004, [p] Smith and Arbogast 1960, [r] Chang and Himmel 1966, [s] Chandrasekhar and Rayne 1961, [t] Wazzan and Robinson 1967, [u] Fisher and Renken 1964, [w] Ferris et al. 1963, [y] Alers and Neighbours 1958, [z] Fisher and Ever 1967.

4. Conclusion

In this study, the scatter diagrams of some cubic and hexagonal structures in the literature have been drawn to find the relationship between their boiling points and their elastic constants. Regression analysis was applied on these distribution diagrams and empirical expressions were obtained. The boiling temperatures of some cubic and hexagonal materials were estimated using the equations obtained as a result of the regression analysis. The 50 boiling points calculated for cubic materials were found to be 12.12% different from the experimental value on average.

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