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The use of a cluster-associate pattern for calculation of melt viscosity

The liquid state of the substance is the most complex for theoretical description. Modern ideas about the liquid and its viscosity are reduced to the following: in the structure of the liquid, the spatial arrangement of atoms is not fixed, as in a crystal, and is not in a free state, as in a gas. Therefore, liquid may approach its properties to gas near the boiling point or the solid state near the melting point. Thus, the structure of the liquid is characterized by the short-range order of the bond. The properties of liquid metals are obtained mainly from experimental studies. This article provides mathematical justification for the cluster-associate pattern. The purpose of the study is to show the possibility of applying a semi-empirical model to calculate the viscosity of liquid metals. The proposed model is developed using the concept of chaotized particles, which is based on the Boltzmann distribution. This model is developed based on the association degree of clusters of their crystal-moving particles. For many years, the viscosity of liquid metals has been studied only by experimental methods. The model enables to find melt viscosity values analytically. The calculated viscosity values of some metals are compared to experimental values in this model. It is established that in all cases the obtained values coincide with the experimental values. The correctness of the proposed model is confirmed by the correlation coefficient. The application of the proposed model has been shown previously on some metals. In this work, we also show the applicability of the cluster-associate pattern using the example of beryllium, since it can be correlated with semimetals by many physicochemical properties. The degree of novelty of the scientific results lies in the fact that the obtained high correlation coefficients for the analysed metals indicate their functionality.

Keywords: kinematic viscosity, cluster of crystal-moving particles, metallurgy, boiling point, melting point, melt, correlation coefficient, beryllium.

Introduction

Smelting and casting of metals and alloys are widely used in the national economy. Metallurgical processes in general and in the field of non-ferrous and rare earth metals in particular have been and still remain one of the most important factors affecting the development of the country's economy. In addition to meeting the needs of metallurgical production, liquid metals are used as fluids and heat carriers in heat engineering, nuclear and electronic technology, and other industries contributing to the development of new metallurgical technologies. However, the insufficient use of mathematical methods for calculating and modeling the state of complex polydisperse systems, for example, melts or liquid slags, and their manufacturing application for prediction of flow and industrial processing control significantly hinder the development progress of technologies in metallurgy. The most important direction in solving this problem is the improvement of existing and the creation of new high-efficiency technological schemes and processes for the production of import-substituting and export-oriented products.

The problem of developing theories and methods for modeling the processes of changing the physical properties of metal melts, such as viscosity, melting, ductility is complex and interesting. Therefore, it has been studied thoroughly by researchers all across the world. Despite the existence of numerous methods for studying the processes of measuring the physical properties of metal melts, today there are no single theoretical models for describing the viscosity of liquid metals.

The topological characteristics of the liquid phase are most clearly expressed in simple liquids, to which melts of most pure metals can be attributed, initial information about which appeared indirectly through the research results of the viscosity-temperature dependence, electrical conductivity, and other characteristics. Due to the development of quantum-statistical methods, including computer modeling, there is a certain understanding of the melt structure. However, direct experimental evidence of short-range order existence with non-crystalline coordination in metal melts was obtained using the neutron and X-ray scattering method, which made it possible to identify clusters with different geometries in melts of iron, nickel, and zirconium

in a wide temperature range from a value much higher than the melting point to a deeply supercooled state at a temperature less than the melting point.

Experimental

Earlier, scientists of the Chemical and Metallurgical Institute named after Zh. Abishev put forward the concept of chaotic particles based on the Boltzmann distribution for the study of the chemical properties of melts [1]. According to this concept, in each state of aggregation of matter, crystal-moving, liquid-moving and steam-moving particles are present. Depending on the state of the substance, the proportion of above particles varies. The proportion of three kinds of particles affects melt properties such as meltability, ductility and viscosity. Professors V.P. Malyshev and A.M. Turdukozhayeva (A.M. Mukasheva) proposed three models for calculating viscosity taking into account three types of particles. In particular, considering the proportion of crystal-moving particles, the following formula is proposed

$$\nu(1) = \nu_r T_r / T. \tag{1}$$

If the liquid fluidity, in addition to the inhibitory influence of the crystal-moving particles, is shown by the contributing effect of the liquid-moving particles, then the viscosity equation for the fraction of these particles will take the following form

$$\nu(2) = \frac{\nu_r T_r \left[\exp(-T_m / T_r) - \exp(-T_b / T_r)\right]}{T\left[\exp(-T_m / T) - \exp(-T_b / T)\right]}. \tag{2}$$

Under the influence of all three kinds of particles, the temperature dependence of viscosity will be described by the following formula

$$\nu(3) = \frac{\nu_r T_r}{T} \exp\left(\frac{T_m}{T} - \frac{T_m}{T_r}\right). \tag{3}$$

In these formulas, ν – a kinematic viscosity, T_m – a melting point, T_b – a boiling point, ν_r and T_r – kinematic viscosity and reference point temperature. As a reference point, we can take any reliably established observed point. Nevertheless, for more accurate calculations, it is advisable to choose a reference point near the melting point.

Kinematic viscosities for 28 metals were calculated from these formulas. However, not all formulas showed consistency of calculated data with experimental [1]. After the calculations, it became necessary to choose the most adequate model for a particular metal. Thus, the calculation procedure was complicated. Therefore, it became necessary to create a single model for calculating the viscosity of liquid metals. As a single model for calculating the kinematic viscosity of melts, we developed a semi-empirical model of viscosity [2, 3]

$$\nu(4) = \nu_r (T_r / T)^a. \tag{4}$$

In work [2], a formula was given by which the degree of cluster association is calculated. Obtained values of clusters association degree of analysed metals were tested for range uniformity on the Nalimov criterion according to the following equations:

$$r_{\substack{\max \\ \min}} = \frac{\left|\bar{x} - x_{\substack{\max \\ \min}}\right|}{S(x)\sqrt{\frac{n-1}{n}}} \le r_{cr},$$

$$S(x) = \sqrt{\frac{\sum (x_i - \bar{x})^2}{n-1}},$$

where $x_{\substack{\max \\ \min}}$ – the minimax value of the range, $\bar{X}$ – the average value, $S(x)$ – the mean-root-square error, and n – the volume of the range. Normative table values of Nalimov criterion for 5% of significance level are approximated with accuracy up to 5% to equation [4]

$$r_{cr} = 1{,}483 f^{0{,}187},$$

where $f = n - 2$ – the number of degrees of freedom of Nalimov criterion.

In this work, we will justify the proposed model using any melting energy barrier (RT_m) and melting heat (ΔH_m).

The use of quantum-chemical models of viscosity, as well as models based on activation energy of the process of transferring particles from one virtual cluster to another, will provide a reliable mathematical description of the temperature dependence of viscosity only for a narrow temperature range.

To extend a similar possibility is provided by the concept of chaotic particles, based on the application of the Boltzmann distribution to a single mapping of three aggregate states of the substance, taking into account the proportions of sub-barrier and over-barrier particles with respect to melting and boiling heats. In this case, the viscosity is compared with the proportion of sub-barrier melting heat particles called crystal-moving, which results in the following model

$$\eta = \eta_r (T_r / T)^{a_\eta}, \tag{5}$$

where η – a dynamic viscosity; T – an absolute temperature; η_r and T_r – the coordinates of reference point, experimental or theoretically found; a_η – clusters association degree of crystal-moving particles.

During the processing of experimental data on η_i and T_i according to converse equation (5)

$$a_i = \frac{\ln(\eta_i / \eta_r)}{\ln(T_r / T_i)}$$

it was found that this degree naturally decreases with increasing temperature, moreover the most adequate description will be obtained when the form of dependence is constant (5) relative to a_η, since the dynamics of association splitting is similar to that of the clusters splitting themselves in accordance with the concept of chaotic particles:

$$a_\eta = a_i (T_i / T)^b, \tag{6}$$

where b, for a given range a_i, T_i is a constant value that makes sense of the attenuation degree of the cluster association. In view of $a_i > 0$, the expression (6) guarantees the impossibility of obtaining absurd negative values of the clusters association degree and an asymptotic approximation $a_\eta \to 0$ with a distant extrapolation $T \to \infty$. The degree of attenuation of cluster association (b) is found by using an additional reference point a_j, T_j as

$$b = \frac{\ln(a_j / a_i)}{\ln(T_i / T_j)} \tag{7}$$

by enumerating and averaging all options i, j or by selecting the most reliable points a_i, T_i and a_j, T_j.

Thus, to build an adequate temperature dependence of viscosity based on the Boltzmann distribution and the concept of chaotic particles, only three experimental points are enough: η_r, T_r; a_i, T_i; a_j, T_j. In the most general form, this dependence, taking into account the formulae (5)-(7), will be expressed as

$$\eta = \eta_r (T_r / T)^{\frac{\ln(\eta_i / \eta_r)}{\ln(T_r / T_i)} \left(\frac{T_i}{T}\right)^{\ln \frac{\ln(\eta_j / \eta_r) \ln(T_r / T_i)}{\ln(T_r / T_j) \ln(\eta_i / \eta_r)}}}.$$

With the use of specific values of three reference points, this expression is simplified, reducing to the following view

$$\eta = \eta_r (T_r / T)^{a_i (T_i / T)^b}.$$

Selection of reference points from the experimental data array is advisable for η_r, T_r – at the beginning of temperature dependence, for a_i, T_i – in the middle and for a_j, T_j – at the end of it.

It is of interest to consider justification for derivation of temperature dependence of kinematic viscosity with independent consideration of another individual characteristic of the substance, that is, to consider the melting heat ΔH_m as an energy barrier.

Considering the melting heat as an energy barrier, the fraction of crystalline particles will be expressed

$$P_{crm} = 1 - \exp\left(-\frac{\Delta H_m}{RT}\right).$$

The range of the relative change in kinematic viscosity from ν_m at a melting point T_m to $\nu = 0$ at a infinitely high temperature, where the liquid can exist in the supercritical range of temperature and pressure in an indistinguishable state with the gas, will be as follows:

$$1 \geq \frac{\nu}{\nu_m} \geq 0. \tag{8}$$

The fraction of crystal-moving particles according to the formula with account of the melting heat in the same temperature range varies within the limits

$$1 - \exp\left(-\frac{\Delta H}{RT_m}\right) \geq 1 - \exp\left(-\frac{\Delta H}{RT}\right) \geq 0. \tag{9}$$

Using algebraic transformations, the obtained inequality leads to the form

$$\exp\left(-\frac{\Delta H}{RT_m}\right) \leq \exp\left(-\frac{\Delta H}{RT}\right) \leq 1.$$

After logarithmation we have

$$\frac{\Delta H}{RT_m} \geq \frac{\Delta H}{RT} \geq 0.$$

From where the original inequality (9) will take the following form

$$1 \geq \frac{T_m}{T} \geq 0,$$

that fully coincides with limits of relative changes of kinematic viscosity (8).

Thus, regardless of the choice of substance individual characteristic as an energy barrier, we come to the same equation of the basic formula (1).

Therefore, without changing the limits of changes in kinematic viscosity, it is possible to raise to any power the part $\frac{T_m}{T}$, that is,

$$1 \geq \left(\frac{T_m}{T}\right)^a \geq 0.$$

Therefore, based on the concept of chaotic particles, an additional justification is obtained for derivation of the basic model of kinematic viscosity with independent consideration of another individual characteristic of the substance. It has been shown that the normalization of the equation for the fraction of crystalline particles by melting heat or any other energy characteristic leads to the same model of viscosity (4), which justifies its base value.

Results and Discussion

In works [2, 3], we showed the possibility of applying model (4) to calculation of viscosity of liquid metals. We made calculations for many liquid metals. It was found that the proposed model most accurately describes the dependence of viscosity on temperature. This pattern was revealed in the process of comparing

experimental data [5, 6] and data calculated for model (4). As a result, we believe that this model can be used to calculate viscosity without conducting an experiment.

Let us consider the application of model (4) on beryllium, which can be correlated with semimetals according to physicochemical properties.

There are no data on kinematic viscosity of **beryllium** in work [5] and in reference book [6]. In reference book [6], melting points T_m = 1560 K and boiling point T_b = 2723 K are indicated.

The work [5] gives the formula for the dynamic viscosity of beryllium

$$\eta = 10^{-2} T^{0,2} \text{ , g/(sm·s)}$$

where $T = T_m + \Delta T$.

After analyzing this formula, the author [1] revealed a sharp increase in viscosity with temperature rise. Therefore, the author [1] proposes the following formula for calculating dynamic viscosity

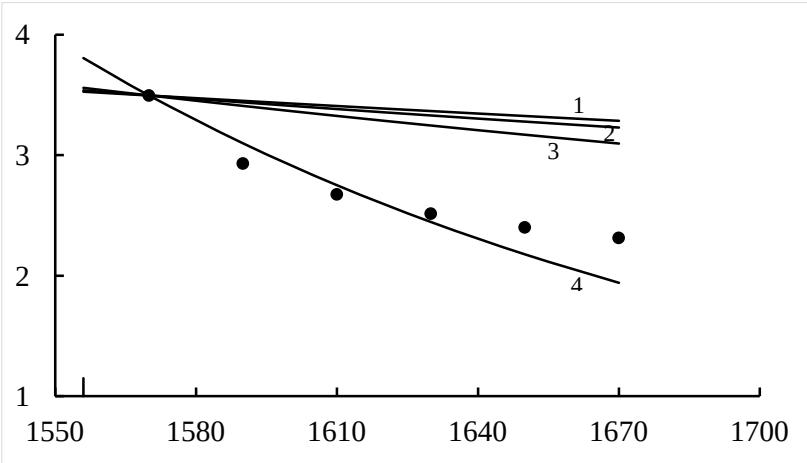
$$\eta = 10^{-2} \Delta T^{-0,2} \text{ , g/(sm·s)} \qquad (10)$$

here ΔT – the degree of superheat of the melt over the crystallization point of pure beryllium, which is equal to 1556 K. The kinematic viscosity of beryllium was estimated according to available data for the area 1560-1670 K through a leveled relationship (10). Point T_r = 1570 K and $\nu_r = 3{,}494 \cdot 10^{-7}$ m^2/s is taken as a reference point. Previously, in the work [1], it was found that the model (3) has an advantage in describing the relationship between viscosity and temperature. However, the results of the calculated viscosity values for four models [2], which are listed in Table 1 and shown in Figure 1, prove the most adequate description of this relationship with the help of the model (4).

Table 1

Comparison of data [1] with models calculated (1-4) on values of kinematic viscosity of beryllium, $\nu \cdot 10^7$, m^2/s

T	$\rho^*_{[6]}$, kg/m^3	$\eta^*_{[1]}$, mPa·s	ν(leveled relationship) $10^7 \cdot \nu = \eta^*/\rho^*$, m^2/s	ν(1)	ν(2)	ν(3)	a	ν(4)
T_m =1556	(1689,5)	(0,758)	-	3,52	3,52	3,54	-	3,71
1570	1688,4	0,590	3,494	3,49	3,49	3,49	-	3,49
1590	1686,1	0,494	2,930	3,45	3,44	3,41	13,91	3,10
1610	1683,8	0,450	2,674	3,41	3,38	3,32	10,63	2,75
1630	1681,5	0,423	2,514	3,37	3,33	3,24	8,78	2,45
1650	1679,2	0,403	2,4	3,32	3,28	3,17	7,56	2,18
1670	1676,9	0,388	2,313	3,28	3,23	3,10	6,68	1,94
R			-	< 0	< 0	0,51	-	0,84



ν – kinematic viscosity, T – temperature.
Points - data [1], 1 – on model (1),
2 – on model (2), 3 – on model (3), 4 – on model (4)

Figure 1. Dependence of kinematic viscosity of beryllium on temperature

The correlation coefficients for models (4) and (3) are equal to 0.84 and 0.51, respectively. Here there is a great difference in the values of correlation coefficients: for model (4), the value is higher. Therefore, the generalized model (4) is reasonable for describing the temperature dependence of viscosity.

The average value of $\bar{a}$ = 9,51 indicates that beryllium has a great tendency to associate clusters of metal atoms. This is because a higher ionization potential makes beryllium less electropositive, and all its compounds, at least partially, have covalent bonds. The tendency of beryllium to form a stronger metal bond due to the transition to the electron conduction zone is reflected in the strength of associates in metal melts, the destruction of which with an increase in temperature requires additional exposure to liquid- and vapor-moving particles.

The homogeneity of the obtained range for a according to Nalimov criterion is observed: $S(x)$ = 2,870; $r_{\min}^{\max}$ = 1,102 < r_{cr} = 1,821.

In this temperature range, considering the degree of cluster association, model (4) with reference point near the melting point can be used as a generalized model of melt viscosity T_r = 1570 K

$$\nu = (0{,}864 \cdot 10^{24} / T^{9{,}51}) \pm 0{,}2,\ \text{m}^2/\text{s}.$$

The activation energy is $E_a = 85231$ J/mol, and for the proposed model, the activation energy is $E_a^{/} = 128017$ J/mol.

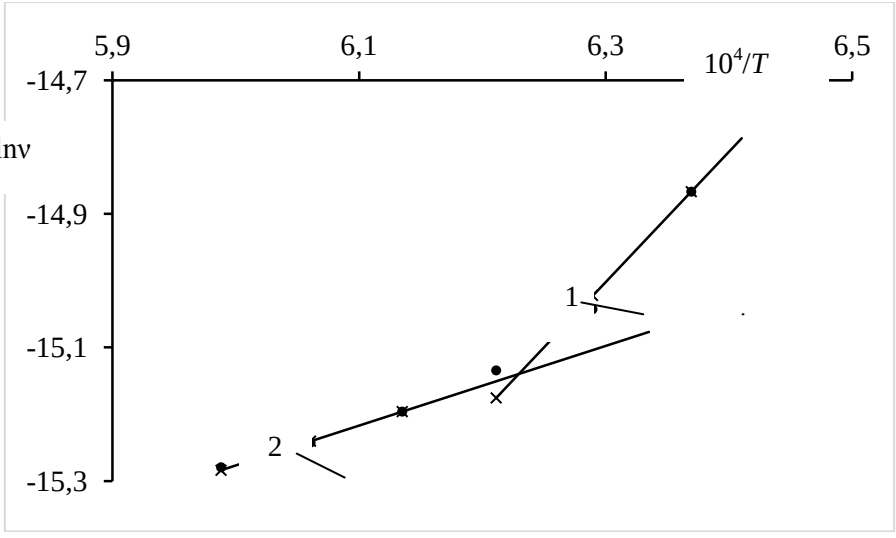
However, as it is shown in Figure 1, the processing of experimental data should be carried out for two areas: 1560-1610 K (low temperature) and 1630-1670 K (high temperature). For each of areas clusters association degrees $\bar{a}$ = 12,27 and $\bar{a}$ = 3,62 respectively were calculated.

Taking into account the obtained clusters association degrees for each of the areas, the temperature dependence of melt viscosity can be expressed by the equations:
for low-temperature area

$$\nu = (5{,}69 \cdot 10^{32} / T^{12{,}27}) \pm 7{,}52 \cdot 10^{-9},\ \text{m}^2/\text{s}, \quad (11)$$

for high-temperature area

$$\nu = (1{,}08 \cdot 10^{5} / T^{3{,}62}) \pm 2{,}69 \cdot 10^{-10},\ \text{m}^2/\text{s}. \quad (12)$$



ν – kinematic viscosity, T – temperature.
Points - experimental data, crosses - for models (11) and (12), straight lines - according to the equation $\ln\nu = \ln A' + E_a^{/}/(RT)$ for low-temperature and high-temperature areas

Figure 2. Logarithm dependence of beryllium kinematic viscosity on reciprocal temperature

The homogeneity of the obtained range for *a* according to Nalimov criterion in each area is observed: for low-temperature area $S(x)$ = 2,316; $r_{\min}^{\max}$ = 1,001< r_{cr} = 1,483, for high-temperature area $S(x)$ = 0,260; $r_{\min}^{\max}$ = 0,978< r_{cr} = 1,483.

Activation energy for each of areas is $E_a^{/} = 162181$ J/mol and $E_a^{/} = 49670$ J/mol respectively. The transition temperature from one area to another is 1605 K. The correlation coefficients for each area are equal to each other and $R_1 = R_2$ = 0,999.

This model was tested on 28 metals. In all cases, the viscosity values calculated from the proposed model were closest to the experimental data. Also, according to the proposed model, slag viscosity of the synthetic mixture of the system CaO-SiO_2-Al_2O_3-MgO-Cr_2O_3, obtained by members of the Chemical and Metallurgical Institute named after Zh. Abishev, laboratory of ferroalloys and restorative processes was calculated.

Conclusions

During the research, it was established that the given justification of the cluster-associate pattern makes it possible to judge its veracity and possibility of application for calculation of kinematic viscosity of melts from a mathematical point of view. The veracity of the results is also supported by the coincidence of some results obtained independently from other researchers with data available in the world literature [5–9]. We also assume that this model will allow conducting physical and chemical justification of chemical and metallurgical processes more reliably and will provide more reasonable requirements for their production technology. With the help of the proposed model, it is possible to calculate melt viscosity values at different temperature values, up to the highest values without conducting high-cost experiments. The model also provides prerequisites for calculation of viscosity of multicomponent systems.

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Балқымалардың тұтқырлығын есептеу үшін кластерлік-ассоциативті модельді қолдану

Белгілі болғандай, заттың сұйық күйін теориялық тұрғыдан сипаттау өте қиын. Сұйықтық пен оның тұтқырлығы туралы қазіргі заманауи ұғымдар мынаған саяды: сұйықтық құрылымында атомдардың кеңістіктік орналасуы кристалдағыдай бекітілмеген және газдағыдай еркін күйде емес. Сондықтан сұйықтық өзінің қасиеттері бойынша қайнау температурасына жақын газға немесе балқу температурасына жақын қатты денеге жақындауы мүмкін. Осылайша, сұйықтықтың құрылымы жақын байланыс тәртібімен сипатталады. Сұйық металдардың қасиеттері негізінен эксперименттік зерттеулерден алынады. Мақалада кластерлік-ассоциативті модельдің математикалық тұрғыдан негіздемесі келтірілген. Зерттеудің мақсаты — сұйық металдардың тұтқырлығын есептеу үшін жартылай эмпирикалық модельді қолдану мүмкіндігін көрсету. Ұсынылған модель Больцманның таратылуына негізделген ретсіз бөлшектер тұжырымдамасын қолдана отырып жасалған. Бұл модель ассоцирленген кластердің дәрежесін ескере отырып жасалған. Көптеген жылдар бойы сұйық металдардың тұтқырлығы тек эксперименттік әдіспен зерттелді. Ұсынылған модель балқымалардың тұтқырлық мәндерін аналитикалық түрде табуға мүмкіндік береді. Осы модель бойынша кейбір металдардың есептелген тұтқырлық мәндері эксперименттік мәндермен салыстырылды. Барлық жағдайларда алынған мәндердің эксперименталды мәндермен сәйкестігі анықталды. Ұсынылған модельдің дұрыстығы корреляция коэффициентімен расталады. Ұсынылған модельді қолдану бұрын кейбір металдарда көрсетілген. Сонымен қатар авторлар бериллий мысалында кластерлік-ассоциативті модельдің қолданылуын көрсеткен, өйткені оны көптеген физика-химиялық қасиеттері бойынша жарты металдармен байланыстыруға болады. Ғылыми нәтижелердің жаңашылдық дәрежесі ұсынылған модельдің негіздемесі оның сенімділігін дәлелдейді және зерттелген металдар үшін алынған жоғары корреляция коэффициенттері оның функционалдығын көрсетеді.

Кілт сөздер: кинематикалық тұтқырлық, ретсізделген бөлшектер, ассоцирленген кластердің дәрежесі, кластерлі-ассоциативті моделі, сұйық металдар, кристаллқозғалысты бөлшектер, тұтқырлықтың температураға тәуелдігі, бериллий.

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Применение кластерно-ассоциатной модели для расчета вязкости расплавов

Как известно, жидкое состояние вещества является наиболее сложным для теоретического описания. Современные представления о жидкости и ее вязкости сводятся к следующему: в структуре жидкости пространственное расположение атомов не закреплено, как в кристалле, они не находятся в свободном состоянии, как в газе. Поэтому жидкость по своим свойствам может приближаться к газу вблизи температуры кипения или к твердому телу вблизи температуры плавления. Тем самым структуре жидкости характерен ближний порядок связи. Свойства жидких металлов получены в основном из экспериментальных исследований. В статье приведено обоснование кластерно-ассоциатной модели с математической точки зрения. Цель исследования — показать возможность применения полуэмпирической модели для расчета вязкости жидких металлов. Предлагаемая модель разработана с помощью концепции хаотизированных частиц, в основе которой лежит распределение Больцмана. Данная модель разработана с учетом степени ассоциации кластеров их кристаллоподвижных частиц. Многие годы вязкость жидких металлов исследовалась только экспериментальным методом. Предлагаемая модель позволяет аналитически найти значения вязкости расплавов. Рассчитанные значения вязкости некоторых металлов по данной модели были сравнены с экспериментальными значениями, во всех случаях было выявлено их совпадение. Корректность предлагаемой модели подтверждается коэффициентом корреляции. Применение такой модели было показано ранее на некоторых металлах. Кроме того, авторами статьи показана применимость кластерно-ассоциатной модели на примере бериллия, так как его по многим физико-химическим свойствам можно соотнести к полуметаллам. Степень новизны научных результатов состоит в том, что полученные высокие коэффициенты корреляции для исследованных металлов указывают на ее функциональность.

Ключевые слова: кинематическая вязкость, кластер из кристаллоподвижных частиц, степень ассоциации, температура кипения, температура плавления, расплав, коэффициент корреляции, бериллий.

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