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Research article

Determining the density of metals based on their atomic construction using the theoretical model

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Abstract: The article is a discussion and analysis of research related to the development of a theoretical model for the determination of physical properties of metals, as well as common semimetals and non-metals occurring in the form of a solid under normal conditions. This is the basis for further consideration in this direction because the presented discourse is limited to the analysis of pure elements. The innovation of the presented approach is an attempt to use only information on the physical atomic structure of elements in relation to their physical properties. The article attempts to link one of the basic physical properties that are the density of metal with its atomic structure. The study involved 75 different chemical elements. The theoretical calculation results determined by means of the presented model remain in correlation with experimental values for 61 chemical elements, not exceeding the calculation error of 6%. This can be considered a satisfactory result of the model in comparison with other models, for example, to determine viscosity, whose differences in computational results, often very much different from experimental values, as well as were directed to a narrow group of materials tested. In addition, other models are often semi-empirical, where in comparison with the theoretical model based only on the atomic structure puts it in a very interesting light.

Keywords: physicochemical properties; density; atomic structure; theoretical model

1. Introduction

The physicochemical properties of metals and alloys are a determinant of their usefulness and application for specific purposes, as they will directly affect their technological and mechanical

properties, which are the basis for industrial applications. The physicochemical properties of the extraction coatings will be particularly important, including protection of the liquid metal mirror against the atmosphere, reducing the negative effect on the furnace lining, and entrapment of reaction products in liquid metal [1]. The extraction coatings, due to their refining effect, will significantly affect the possibilities of obtaining ultra pure metals. Although metal alloys, among others due to higher hardness and strength compared to pure products, are more frequently used in industry [2], this very high purity metals are beginning to gain significance in today's world [3,4].

The basic physicochemical properties of extraction coatings, metals and alloys in the liquid state are viscosity, surface tension, wettability, electrical conductivity, melting point, chemical activity, acidity or alkalinity. In the context of refining coatings, do not forget about refining properties. The determination of the properties listed herein is well known and described in the literature. Conducting research for a given material or material arrangement is tedious, time-consuming and expensive. However, knowledge of these values is the basis for improving the technological process and further production. Finding the dependence that allows linking the structure of metals, alloys, or oxides, chlorides and fluorides with their physicochemical properties would be a milestone in the field of chemistry, physics and materials science, because with the appropriate calculations you could get all kinds of information about the interesting system. You can approach this concept in three ways:

1) Determining properties using a given theoretical model
2) Determining device properties using a semi-empirical model
3) Determining properties using experimental analysis

The characteristics of materials used in the metallurgical industry can be considered in terms of physical, chemical, refining and technological properties. Undoubtedly, the first two groups (physical and chemical properties) are determinants of other properties of a given material. The basic physical properties of the substance are density, melting point, viscosity, electrical conductivity, etc. Determination of individual physical properties of materials are well known and described in the literature; however, the development of an algorithm that would link the atomic structure of the element with its physical properties could form the basis for further considerations on the mathematical model for determining the physical properties of substances.

2. Determining density using a theoretical model

Looking at the contemporary periodic table of elements, one can conclude that the basic distinguishing feature between atoms of elements is their belonging to different groups and periods. The location of the elements in the system is not accidental, and depends first of all on the atomic mass of the element. In simplified form, a relative atomic mass is used, which determines how many times the mass of a given element is greater or smaller than the weight of the carbon atom of the 12C isotope. As you know, the whole mass of the atom is concentrated mainly in its nucleus. The nucleus has inside neutrons with neutral electric charge and protons, which are electrically charged positive. Outside, there are electrons that have a negative charge. The fact that electrons "do not bump into" protons, in spite of their opposite charges, is explained by centrifugal force balancing the attractive force of the atomic nucleus. Other features related to the construction of atoms are the number of electron shells on which negatively charged particles can move as well as the radius of the atom. The

valence of a given element that is the number of valence electrons present in the last electron shell will also be significant.

How would we already link the listed building elements of atoms at this stage. The number of protons in atoms is equal to the number of electrons. The more protons there are, the more electrons there are, and their number is always in correlation with each other. It can also be noted that the more electrons within a given group of elements, the more their radius increases. At the same time, it can be seen that as the number of protons attracting electrons in the atom increases, the atomic radius decreases. This applies to a specific period and the same number of atomic shells. Additionally, to refer to the real mass of the atom, the concept of absolute atomic mass was used in the analyzes. It is equal to the atomic mass ratio relative to the Avogadro number.

The classic calculation of material density is reduced to determine its mass by weighing the material and determining its volume. The basic unit of density is a kg/m^3, which means that in a cube measuring 1 ×1 × 1 m made of one material. There is a certain mass of substance. It can determine the function showing the mathematical relationship between density of materials, and atomic structure with quite high accuracy. This is possible thanks to the use of numerical methods and the approximation process. For this purpose, the absolute atomic mass of the element related to the number of electrons in the atom, the number of atoms in a given volume and the atomic radius was introduced to the proposed mathematical relationship.

During the research, the authors assumed that there must be a logical connection between the density of the element and its features related to atomic structure. Various properties related to atomic rays, electron configuration, coating filling, electronegativity, ionization potentials or even cohesion energy were taken into account. On the basis of many analyzes, it was possible to determine that the density of elements is related to the number of electrons of the non-ionized atom (atomic number), absolute atomic mass and atomic radius. The relationship shown is described in Eq 1. To increase accuracy, the mathematical relationship was subjected to the process of approximation, and the polynomial function of grade 7 was chosen, especially of the 4th periodiec Mendeleev system. The analysis covered substances present in the modern periodic table, which occur in a natural form (they were not created artificially by laboratory) and exist in a solid form.

It was noted that for all of the above elements from the second, third and seventh period of the Mendeleev system, can determine a pattern that determines the density of the material with an accuracy of 0.0000%. The main assumption referring to such a formula (Eq 1 below) is the necessity of the relationship between the density of an element and its atomic structure. This applies in particular to such parameters as electrical configuration, degree of coating filling, atom radius, electronegativity, ionization potential or cohesion energy. The formula for the density of the extracted material can be described as follows:

$$\rho_{STP} = \left(\frac{Az^5 + Bz^4 + Cz^3 + Dz^2 + Ez + F}{r_{at}}\right)^3 m_A \quad (1)$$

where: *ρstp*—density of substances under normal conditions (STP—standard conditions for temperature and pressure—temperature: 0 ℃; pressure: 1000 hPa)
A, *B*, *C*, etc.—polynomial coefficients
z—atomic number
rat—atom radius (empirical value)
mA—absolute atomic mass

In the case of IV, V and VI period of the periodic table, there are already slightly larger discrepancies. In spite of everything in this group, over 3/4 of all analyzed elements had a computational error not exceeding 6%. Only in the case of 14 elements, there were larger errors from the range from 7 to even 39%. It should also be noted that in the case of the analysis of the fourth, fifth and sixth periods of the Mendeleev system. A 7th order polynomial should be used to more accurately analyze the calculations, then we obtain 7 polynomial coefficients and 8 free expression. The Table 1 presents the values of polynomial coefficients (A to F) depending on the analyzed period for Eq 1.

Table 1. Values of polynomial coefficients depending on the analyzed period in the system of periodic elements.

Period number	The number of the polynomial coefficient							
	Numeral value	1	2	3	4	5	6	7
II	−0.717544527	0.8642958585	−0.1862270005	0.011919791	0	0	0	0
III	254.568778866997	−93.7422457685665	13.68042430375	−0.98595032954166	0.03505997175	$-4.91892391666665 \times 10^{-4}$	0	0
IV	−95.8071560895088	33.09122555702	−4.66450647828032	0.35501400368175	−0.015907030024395	0.000422142170896459	$-6.16424670551513 \times 10^{-6}$	$3.82563839391743 \times 10^{-8}$
V	8979.39412093296	−1249.89223615025	72.2930050018278	−2.22377495488247	0.038367454559976	−0.000352019045373507	$1.34172286909084 \times 10^{-6}$	0
VI	−2560.94730829028	223.803181139243	−8.11942707717231	0.156557833637046	−0.0016920993969052	$9.71940359429707 \times 10^{-6}$	$-2.31787597226639 \times 10^{-8}$	0
VII	4703253.57396151	−257389.906797486	5633.72216414025	61.6482869037425	0.33726334890277	$-7.37956290277771 \times 10^{-4}$	0	0

3. Results and discussion

On the basis of assumptions adopted above, it was possible to perform calculations for the adopted group of elements in the periodic table. The following tables (Tables 2–7) below show calculation density values based on the proposed Eq 1, comparing them with values determined empirically for subsequent periods of the Mendeleev system. In addition, the last column shows the error occurring in the calculation in relation to the actual value. The actual value is the official value read from the physical tables, which was determined experimentally using sensitive laboratory scales in normal conditions.

Table 2. Density values determined for elements from period II.

Calculation result (g/m^3)	Experimental densities (g/m^3)	The name of the element	Error (%)
535000.0003	535000.0000	Li	0.00000
1848000	1848000.000	Be	0.00000
2460000.005	2460000.000	B	0.00000
2260000.004	2260000.000	C	0.00000

Table 3. Density values determined for elements from period III.

Calculation result (g/m^3)	Experimental densities (g/m^3)	The name of the element	Error (%)
968000.0027	968000.000	Na	0.00000
1738000.004	1738000.000	Mg	0.00000
2700000.003	2700000.00	Al	0.00000
2329999.999	2330000.000	Si	0.00000
1823000.007	1823000.0000	P	0.00000
1960000.007	1960000.000	S	0.00000

Table 4. Density values determined for elements from period IV.

Calculation result (g/m^3)	Experimental densities (g/m^3)	The name of the element	Error (%)
857191.5786	856000.0000	K	0.13901
1543470.141	1550000.00	Ca	0.42128
2587461.756	2985000.00	Sc	13.31786
4545297.355	4507000.000	Ti	0.84257
6092222.783	6110000.000	V	0.29095
6287251.578	7140000.000	Cr	11.94326
7350083.178	7470000.000	Mn	1.60531
7989039.467	7874000.000	Fe	1.43997
9570005.903	8900000.000	Co	7.00110
9083920.833	8908000.000	Ni	1.93662
8631707.491	8920000.0000	Cu	3.23198
7087377.675	7140000.000	Zn	0.73701
6179405.842	5904000.000	Ga	4.45683
5153063.273	5323000.000	Ge	3.19250
5768137.989	5727000.000	As	0.71319

Table 5. Density values determined for elements from period V.

Calculation result (g/m^3)	Experimental densities (g/m^3)	The name of the element	Error (%)
1534995.969	1532000.000	Rb	0.19518
2613439.357	2630000.000	Sr	0.62968
3897872.278	4472000.000	Y	12.83828
6616336.088	6511000.000	Zr	1.59206
8472717.312	8570000.000	Nb	1.13515
8874037.271	10280000.000	Mo	13.67668
11398704.51	11500000.0	Tc	0.88083
13496857.9	12370000.0	Ru	8.34904
12663674.22	12450000.00	Rh	1.68730
11994280.32	12023000.00	Pd	0.23887
8024626.75	10490000.00	Ag	23.50213
8500796.681	8650000.000	Cd	1.72489
7382922.377	7310000.000	In	0.98772
7358744.698	7310000.000	Sn	0.66241
6659511.391	6697000.000	Sb	0.55978
6244265.339	6240000.000	Te	0.06831

Table 6. Density values determined for elements from period VI.

Calculation result (g/m^3)	Experimental densities (g/m^3)	The name of the element	Error (%)
1809976.662	1879000.000	Cs	3.67341
3860077.636	3510000.000	Ba	9.06919
5647609.827	6146000.000	La	8.10918
6868088.942	6689000.0000	Ce	2.60755
6921392.8	7010000.0000	Pr	1.26401
7005037.943	7010000.000	Nd	0.07079
7078619.281	7353000.000	Sm	3.73155
7071188.447	5244000.000	Eu	25.83991
7885991.371	7901000.000	Gd	0.18996
8641167.365	8219000.000	Tb	4.88554
8822579.456	8551000.00	Dy	3.07823
8946321.747	8795000.00	Ho	1.69144
9054241.792	9066000.000	Er	0.12970
9104331.983	9321000.000	Tm	2.32451
9257061.194	6570000.000	Yb	29.02715
9262540	9841000.000	Lu	5.87806
13428499.85	13310000.00	Hf	0.88245
16410791.17	16650000.00	Ta	1.43669
20419959.75	19250000.0	W	5.72949
20527305.74	21020000.00	Re	2.34393
23462445.65	22610000.00	Os	3.63323
21335825.38	22650000.00	Ir	5.80210
22038465.3	21090000.00	Pt	4.30368
22859539.97	19300000.00	Au	15.57135
9105950.517	11850000.00	Tl	23.15654
11146000.37	11340000.00	Pb	1.71076
16080904.41	9780000.00	Bi	39.18253
9261126.119	9196000.000	Po	0.70322

Table 7. Density values determined for elements from period VII.

Calculation result (g/m^3)	Experimental densities (g/m^3)	The name of the element	Error (%)
5000002.293	5000000	Ra	0.0000
11724003.95	11724000	Th	0.0000
15370004.16	15370000	Pa	0.0000
19050004.62	19050000	U	0.0000
20450004.1	20450000	Np	0.0000
19816003.21	19816000	Pu	0.0000

Based on the research, it can be concluded that there is a large correlation between the atomic structure of the elements and their physicochemical properties in this case the density. Thanks to the proposed formula, their density can be determined with high accuracy. For more than 80% of the selected group of elements, the result error did not exceed 6%. The selected group contains 14 elements with a higher error value. For cobalt Co is 7%, and for bismuth Bi as much as 39%. It is noteworthy that higher errors begin to appear in elements with more than 3 atomic coatings: 3

elements with 4 coatings, 4 elements with 5 coatings, and up to 7 elements with 6 coatings. In addition, there is a tendency to increase the computational error as the number of atomic shells increases. For elements with 4 coatings the error is from 7 to 13%, for elements with 5 coatings is from 12 to 23%, and for elements with 6 coatings from 8 to 39%. No influence of the number of electrons, including valence electrons, on the result error is observed.

Returning to the presented model, it is also worth noting that for the simplest set of two atomic shells. The polynomial achieves only 3 degrees, and only for the next elements with more coatings it increases its value. In addition, high accuracy of polynomial coefficients can be noted, which in some cases are recorded with an accuracy of 22 decimal places. The research indicates relatively large deviations of calculations from real values with reduced accuracy of writing coefficients; hence, it would be very difficult to omit calculations computer programs to determine above values of coefficients.

4. Conclusion

In the study, it's worth looking at a group of elements called lanthanides. These elements are very similar. Meanwhile, for the two elements shown, there is a big difference in the calculated and actual value. These include the Europium Eu (25% error) and Ytterbium Yb (29% error). Looking at this group of elements, it can be said that such a large computational error is affected by electron orbitals, where each of them has its own energy level and properties. Orbitals are described by the principal quantum number (n), the magnetic quantum number (m) and the orbital angular momentum quantum (e). It turns out that only these two elements from the lanthanide group have the same properties, i.e., e = 3, m = 3 and n = 4. This may indicate that the electronic configuration of atomic orbitals will have an additional effect on the density.

Based on the above analyzes, it can be concluded that the theoretical model presented can accurately determine the density of materials for a large group of pure elements. Comparing it with many other models, especially to assess other physical properties, for example, viscosity which are often semi-empirical models, it achieves quite satisfactory results. Many other models are directed only to a specific group of materials, with considerable deviations from the actual values [5–7]. The presented model is also directed to a relatively narrow group of materials as it relates to elements of metals, semi-metals or non-metals in the solid state in a pure form. However, it should be noted that this model uses only and exclusively information on the structure of the atomic elements such as the atomic number, atomic shellsnumber, atomic radius or absolute atomic mass. The author is convinced that one can attempt to determine theoretical models based on the atomic properties of elements for other compounds, for example, oxides or alloys. Taking up the presented course of thinking, one could attempt to determine other physical properties, for example, melting temperatures based on similar assumptions. Finally, the logic suggests that it is the structure and atomic properties of the elements that influence their physicochemical properties as materials used in science and industry.

It is also worth mentioning that the authors attempted to create a theoretical model for determining the melting point of materials. The research using, the Bohr atom model, the so-called the improved atom model as well as the cohesion energy give very interesting results. However, research in this area has not yet been completed and works are still under way.

Conflict of interests

All authors declare no conflicts of interest in this paper.

Reference

1. Bydałek AW (1998) *Slag Carbon Dioxide Systems in the Melting Processes of Copper and its Alloys*, Zielona Góra: Politechniki Zielonogórskiej, 186.
2. Głowacka M (1996) *Metallography*, Gdańsk: Politechnika Gdańska, 383.
3. Kisza A, Urbanowicz J (1981) A method of purifying metals to high purity. PL Patent 106967 B1.
4. Herszkiewicz A, Krasoń Z, Kuniewicz M, et al. (2000) A method of recovering palladium and platinum in the form of compounds of high purity of these metals from post-production materials containing activated carbon in the form of a paste. PL Patent 189680 B1.
5. Han C (2017) Viscosity studies of high-temperature metallurgical slags relevant to ironmakingprocess [PhD's thesis]. The University of Queensland, Australia.
6. Yakymovych A, Sklyarchuk V, Plevachuk Yu, et al. (2016) Viscosity and electrical conductivity of the liquid Sn-3.8Ag-0.7Cu alloy with minor Co admixtures. *J Mater Eng Perform* 25: 4437–4443.
7. Gąsior W (2014) Viscosity modeling of binary alloys: comparative studies. *Calphad* 44: 119–128.

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