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On the Problem of Determining the Density of the Metallic Phase of the Periodic Table Elements

Feliks F. Gorbatsevich,
Kola Science Centre of The Russian Academy of Sciences, Apatity, Russian Federation.

Abstract
Based on the analysis of the relationship between the metals density and the parameters of atoms, a prediction was made of the density values of metal phase substances of the Periodic Table. The densities of substances such as hydrogen, oxygen, nitrogen, fluorine, and others in the metal phase can acquire high values comparable to the densities of metals. The predicted values of the metal phase density of substances can reduce the search for the necessary experimental parameters to obtain such a state.
Keywords*: atom, metal, volume, density, phase, element, nucleus.*

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Density is one of the most important parameters of a substance. It depends on the state of the substance aggregation. In the gaseous state, when atoms (molecules) are separated, it has low values. During the transition to the liquid state, the density of the substance is higher than in the gas phase. In the solid state, the density is usually higher than in the liquid phase. Under normal conditions (at atmospheric pressure and a temperature of 0°C), metals have the highest density. Previously, a rather close relationship was found between the density of metals and semimetals (as elements of the Periodic Table of D.I. Mendeleev) with the parameters of atoms and their nuclei [1, 2]. At the same time, metals represent the metallic phase of the substance state.

It was found in [1, 2] that one of the factors influencing the density is the size of an atom, which is determined by the diameter of the orbits of the outermost electrons, which are farthest from the nucleus. Another factor is that the bulk of the mass of an element atom is concentrated in its nucleus. The masses of the nuclei of elements increase in proportion to the atomic number of the element. Along with this, a strict dependence of the substance density on the atomic number and its atomic weight (mass) is not observed. Probably, this dependence is influenced by the ratios of the atom parts. For the analysis of this influence in Table 1 a summary of the parameters of elements - metals, including the name of the element, its formula, atomic number, atomic weight (A), density (ρ_m), diameter of the atom (D_a) and diameter of the nucleus (D_n) is presented.

The atomic weights of the elements are presented in [3]. Density (ρ_m), of metals has been repeatedly measured and given in a large number of publications [4-7]. The value of the radius (diameter) of an atom to a certain extent depends on whether the atom is isolated, covalently bound in molecules in a condensed medium, or in an ionized and excited state. The value of the diameter varies both from the state of the atom and also from the environment.

The atomic diameters (D_a) given in the table refer to isolated free atoms. They were calculated by the Hartree-Fock calculation method and taken from [8]. According to the author of the work, the Hartree-Fock method is currently the most efficient of the available methods for calculating the size of the electron shells of atoms.

Table 1. Parameters of the metal group of the Periodic Table.

Element	For-mula	Atomic number	Atomic weight, A	Atom diameter, $D_a \cdot 10^{10}$, m	Nucleus diame-ter, $D_n \cdot 10^{15}$, m	$V_n/V_a \cdot 10^{15}$	Density, (ρ_m), g/cm^3
Lithium	Li	3	6.94	2.90	4.96	5.11	0.53
Beryllium	Be	4	9.012	2.24	5.41	14.1	1.848
Natrium	Na	11	22.99	3.80	7.39	7.35	0.971
Magnesium	Mg	12	24.31	3.20	7.53	13.02	1.736
Aluminum	Al	13	26.98	2.86	7.79	20.33	2.70
Kalium	K	19	39.10	4.70	8.82	6.61	0.856
Calcium	Ca	20	40.08	3.94	8.90	11.52	1.55
Scandium	Sc	21	44.96	3.24	9.24	23.19	2.99
Titanium	Ti	22	47.87	2.94	9.44	33.09	4.54
Vanadium	V	23	50.94	2.68	9.64	46.53	6.11

Chromium	Cr	24	51.99	2.60	9.70	52.0	7.19
Manganum	Mn	25	54.94	2.54	9.88	58.85	7.21
Ferrum	Fe	26	55.84	2.52	9.94	61.36	7.87
Cobaltum	Co	27	58.93	2.50	10.12	66.34	8.90
Niccolum	Ni	28	58.69	2.48	10.10	67.52	8.90
Cuprum	Cu	29	63.55	2.56	10.38	66.69	8.92
Zincum	Zn	30	65.38	2.76	10.47	54.65	7.13
Rubidium	Rb	37	85.47	4.96	11.45	12.30	1.532
Strontium	Sr	38	87.62	4.30	11.55	19.38	2.54
Yttrium	Y	39	88.90	3.56	11.60	34.60	4.47
Zirconium	Zr	40	91.22	3.20	11.70	48.86	6.51
Niobium	Nb	41	92.90	2.92	11.77	63.71	8.57
Molybdaenum	Mo	42	95.95	2.76	11.90	80.14	10.22
Technetium	Tc	43	98	2.72	11.99	85.63	11.5
Ruthenium	Ru	44	101.1	2.68	12.11	92.25	12.4
Rhodium	Rh	45	102.90	2.68	12.18	93.86	12.4
Palladium	Pd	46	106.42	2.74	12.32	90.91	12.0
Argentum	Ag	47	107.86	2.88	12.38	79.41	10.5
Cadmium	Kd	48	112.41	3.08	12.55	67.65	8.65
Indium	In	49	114.81	3.32	12.64	55.19	7.31
Stannum	Sn	50	118.71	3.24	12.78	61.37	7.31
Caesium	Cs	55	132.90	5.34	13.26	15.31	1.873
Barium	Ba	56	137.32	4.44	13.41	27.55	3.50
Lanthanum	La	57	138.90	3.74	13.46	46.62	6.17
Cerium	Ce	58	140.11	3.62	13.50	51.88	6.76
Praseodymium	Pr	59	140.90	3.64	13.53	51.36	6.77
Neodymium	Nd	60	144.24	3.64	13.64	52.62	7.01
Promethium	Pm	61	145	3.66	13.66	51.99	7.26
Samarium	Sm	62	150.36	3.62	13.83	55.76	7.52
Europium	Eu	63	151.96	3.98	13.87	42.32	5.24
Gadolinium	Gd	64	157.25	3.58	14.03	60.20	7.90
Terbium	Tb	65	158.92	3.60	14.08	59.83	8.23
Dysprosium	Dy	66	162.50	3.60	14.19	61.24	8.55
Holmium	Ho	67	164.93	3.58	14.26	63.20	8.79
Erbium	Er	68	167.25	3.56	14.32	65.10	9.06
Thulium	Tm	69	168.93	3.54	14.37	66.88	9.32
Ytterbium	Yb	70	173.05	3.88	14.49	52.09	6.97
Lutetium	Lu	71	174.96	3.50	14.54	71.72	9.84
Hafnium	Hf	72	178.48	3.34	14.64	84.21	13.3
Tantalum	Ta	73	180.94	2.98	14.71	120.2	16.65
Wolframium	W	74	183.84	2.74	14.78	157.0	19.25
Rhenium	Re	75	186.20	2.74	14.85	159.2	21.0
Osmium	Os	76	190.23	2.70	14.95	169.7	22.6
Iridium	Ir	77	192.21	2.72	15.00	167.7	22.6
Platinum	Pt	78	195.08	2.78	15.08	159.6	21.3
Aurum	Au	79	196.96	2.88	15.13	144.9	19.3
Thallium	Tl	81	204.38	3.42	15.32	89.80	11.85
Plumbum	Pb	82	207.2	3.50	15.38	84.85	11.34
Bismuthum	Bi	83	208.98	3.40	15.43	93.49	9.79

The dimensions of atomic nuclei are primarily related to the radius of nuclear forces action. Different methods give different sizes of atomic nuclei. The work, which is specially devoted to the theory of the atomic nucleus, lists the methods by which the sizes of the nucleus of atoms are determined [9]. For example, according to the method of determining the cross section of nuclear reactions, the radius of the nucleus is

$$R_n = \mathrm{a}_0 \sqrt[3]{\mathrm{A}} \cdot 10^{-15}\ m, \tag{1}$$

where $a_0 = 1.4$.

According to the method of measuring the electrostatic interaction of protons in the nucleus, it was found that $a_0 = 1.5$. The method of electron scattering by atomic nuclei made it possible to estimate the coefficient $a_0 = 1.2$. Using the X-ray energy of μ mesons, it was found that $a_0 = 1.2$. The approach that makes it possible to represent the nucleus as a uniformly charged Coulomb sphere gave the value $a_0 = 1.23$.

A detailed analysis of different methods for calculating the radii of nuclei is presented in [10]. For heavy nuclei, somewhat different results have been obtained by different methods. They all lie within

$$R_n = (1.2 - 1.5) \sqrt[3]{\mathrm{A}} \cdot 10^{-15}\ m. \tag{2}$$

Similar estimates are given in [11]. Summing up the above results, we can obtain the average $a_0 = 1.3$. Thus, the average core diameter is

$$D_n = 2.6\sqrt[3]{\mathrm{A}} \cdot 10^{-15}\ m. \quad (3)$$

It should be noted that the mass of the nucleus also determines its volume [9, 10]. According to Table 1, the density of the metals group varies from 0.53 g/cm^3 (lithium) to 22.6 g/cm^3(osmium, iridium). The atomic size range is $2.48 \cdot 10^{-10}\ m$ (nickel) – $5.34 \cdot 10^{-10}\ m$ (cesium). Changes in core diameters are within $4.96 \cdot 10^{-15}\ m$ (lithium) – $15.43 \cdot 10^{-15}\ m$ (bismuth).

It is known that the main mass of an atom is concentrated in its nucleus [9-11]. The ratio of the nucleus mass to the sum of the atom electrons masses is approximately 2000:1 and may, as a first approximation, not be taken into account. In addition to the mass of the atom nuclei, the density of a substance depends on the distance between its atoms (molecules). This distance is determined by the size of the atom electron shells. The data in Table 1 show that alkali metals have the largest sizes of outermost electron shells at a relatively low density.

In order to take into account the effect of the distance between the atoms of an element in the substance, the ratio of the nucleus volume to the atom volume, V_n/V_a, was calculated. Assuming the shape of the nucleus in the form of a right sphere, its volume is

$$V_n = \frac{1}{6}\pi {D_n}^3.$$

Taking a similar condition regarding the shape of the isolated atom, we obtain

$$\frac{V_n}{V_a} = \frac{D_n^3}{D_a^3}.$$

This ratio compensates the influence of the differing volume of the nucleus and the volume of the electron shell of the atom substance. Table 1 shows the calculated values of V_n/V_a for the group of metals. The plot (Fig.) shows the field of points ρ_m vs V_n/V_a. A review of the plot reveals a high correlation between the values of ρ_m and V_n/V_a. The linear correlation coefficient for 58 metals, from lithium to lead, is $R^2 = 0.989$. The mathematical formula that reflects this ratio is:

$$\rho_m = 1.33 \cdot (V_n/V_a) \cdot 10^{14},\quad g/cm^3 \quad (4)$$

Dependence (4) indicates a close packing of metal atoms. This is practically a strict dependence, showing that the density of a substance directly depends on the mass (volume) of the nucleus and the volume occupies in space by the outermost electron shells of atoms.

In addition to metals, the Periodic Table also contains elements that, under normal conditions, are in a different state of aggregation, for example, gaseous and liquid. Also in this group there are solids that cannot be attributed to metals, including semimetals. The parameters of such substances is given in Table. 2.

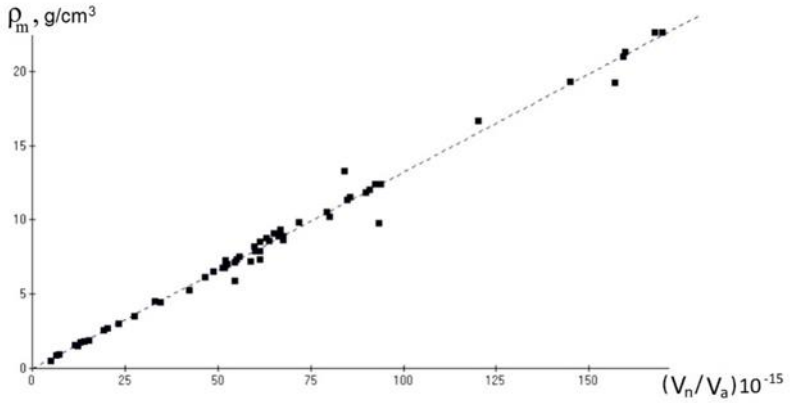

Fig. Distribution of the ratio V_n/V_a and the corresponding values of the density ρ_m of metals.

It can be assumed that all elements of the Periodic Table, which under normal conditions (n.c. - at atmospheric pressure and a temperature of 0^0C) are gaseous, liquid or are in a solid, non-metallic phase, under other *PT* conditions can pass into metallic phase of the substance state. The resulting dependence (4) makes it possible to predict at what element density such transition is possible.

According to the data, hydrogen has the lowest density under normal conditions (otherwise, the monatomic gas protium, $\rho_n = 8.99\ 10^{-5}\ g/cm^3$). Hydrogen is the most abundant element in the universe. In the temperature range 20.28–14.01^{0}K, hydrogen is in the liquid phase. It is a very light colorless liquid with a density of 0.0708 g/cm^3 (at 20^{0}K). Below 14.01^{0}K, it is in a solid state and is a snow-like mass. Solid hydrogen also has a very low density ($\rho_n = 0.08667\ g/cm^3$, at 14.1^{0}K) [6-7].

The production of liquid and solid hydrogen is achieved in a relatively easy way in cryogenic apparatures. Metallic hydrogen can be produced at very high pressures. In 1935, the first publication appeared, in which it was suggested that at high pressures, hydrogen from a gas with dielectric properties should turn into a conducting metal [12]. However, this could happen at pressures exceeding 25 GPa. Equipment capable of creating such pressure did not yet exist in those years.

Soviet theoretical physicists suggested that metallic hydrogen could be in a metastable state [13, 14]. In 2017 a report appeared that in an experiment at an even higher pressure, a possible transition of hydrogen to a metallic state was observed [15]. There are later reports of experiments with metallic hydrogen. For example, French physicists reported in 2020 that they had observed metallic hydrogen at pressure of 4.18 million *atm*.

Interest in this substance is explained by the fact that it should exhibit superconductivity at high temperatures [16, 17]. On the other hand, obtaining a substance in a stable state opened up new prospects for its application. It would be an ultra-light, very energy-intensive fuel. Together with metallic oxygen, this metal would present attractive prospects for their use as propellant components.

Table 2. Parameters of non-metallic group of the Periodic Table.

Element	For-mula	Ato-mic num-ber	Atomic weight, A	Atom diameter, $D_a \cdot 10^{10}$, m	Nucleus diame-ter, $D_n \cdot 10^{15}$, m	$V_n/V_a \cdot 10^{15}$	Density, ρ_n, g/cm^3	Den-sity, ρ_c, g/cm^3	ρ_c / ρ_n
Hidrogenium	H	1	1.008	1.06	2.60	14.8	$8.99 \cdot 10^{-5}$ (n.c.) 0.086 (solid)	1.96	22.7
Borum	B	5	10.81	1.96	5.75	25.25	2.34	3.34	1.43
Carboneum	C	6	12.01	1.40	5.95	76.9	3.51 (dia-mond)	10.2	2.91
Nitrogenium	N	7	14.01	1.50	6.27	72.9	$1.25 \cdot 10^{-3}$ (n.c.) 1.026 (solid)	9.71	9.46
Oxygen	O	8	15.99	1.20	6.55	162.6	$1.43 \cdot 10^{-3}$ (n.c.) 1.33 (solid)	21.6	16.2
Fluorum	F	9	18.99	1.46	6.94	107.4	$1.696 \cdot 10^{-3}$ (n.c.) 1.7 (solid, β-phase)	14.3	8.41
Silicium	Si	14	28.08	2.64	7.90	26.8	2.33	3.56	1.53
Phosphorus	P	15	30.97	2.56	8.16	32.39	1.82	4.31	2.37
Sulfur	S	16	32.06	2.54	8.26	34.39	2.07	4.57	2.21
Chlorum	Cl	17	35.45	1.98	8.54	80.24	$3.21 \cdot 10^{-3}$ (n.c.) 2.13 (solid)	10.7	3.33
Gallium	Ga	31	69.72	2.82	10.70	54.63	5.91	7.27	1.23
Germanium	Ge	32	72.63	2.44	10.85	87.9	5.32	11.7	2.20
Arsenicum	As	33	74.92	2.76	10.96	62.6	5.73	8.33	1.45
Selenium	Se	34	78.96	2.80	11.15	63.1	4.79	8.40	1.75
Bromum	Br	35	79.91	2.38	11.20	104.2	3.10 (n.c.) 4.07 (solid)	13.8	3.39
Stibium	Sb	51	121.76	3.18	12.89	66.6	6.69	8,86	1.32
Tellurium	Te	52	127.60	3.20	13.09	68.4	6.24	9.10	1.46
Iodum	I	53	126.90	2.72	13.07	110.9	4.93	14.6	2.96
Hydrargyru m	Hg	80	200.59	3.14	15.22	113.9	13.55 (n.c.) 14.2 (solid)	15.1	1.06
Polonium	Po	84	209	3.52	15.43	84.2	9.20	11.2	1.22
Astatium	At	85	210	2.90	15.45	151.2	6.40	20.1	3.14

Notes:

1. The elements in the Periodic Table with an atomic mass higher than Astatine are subject to radioactive decay in large numbers. They are present in the earth's crust in very small quantities and are not given here. Also, the

data of noble gases are not given in Table 2 due to the inaccuracy of the indicated values of their atoms radii in the sources;

2. For hydrogen and all subsequent elements, the density ρ_n is indicated under normal conditions (n.c.- at 1 atm. and 0°C). Density data of the gaseous, liquid and solid phases of nitrogen, hydrogen, oxygen, fluorine and other elements are given from the Big Chemical Encyclopedia et al. [4-7];
3. For carbon, the density of diamond is indicated;
4. Table 2 shows the density of white phosphorus (n.c.).

Attempts to obtain metallic oxygen were also made by applying super high pressures. A strong shock wave was created in a small chamber with liquid oxygen, which, reflected from the walls of the chamber, repeatedly passed through the liquid. As a result, a pressure of 132 GPa and a temperature of about 4500^0K were created in the chamber for 100–200 *ns* [18]. The presence of a metallic phase was recorded by measuring the electrical resistance of oxygen.

Experiments were carried out with the aim of obtaining the metallic phase of other elements that are in a gaseous state under normal conditions, and in particular nitrogen. The diffraction method was used to study the structural transition of molecular nitrogen to a singly bound state at pressures up to 170 GPa [19]. There is evidence that employees of the Department of Solid State Physics of the Hefei Institute of Materials Science of the Chinese Academy of Sciences managed to successfully synthesize metallic nitrogen in the laboratory. The metallic phase of nitrogen opens up prospects for obtaining a super-powerful explosive. Normally gaseous fluorine can also, in principle, be obtained in the metallic phase. It is the strongest oxidizing agent and its compounds are used in rocket fuels.

Publications on the production of metallic phase of hydrogen, oxygen, nitrogen, and fluorine do not provide information on the substance density in this state, since the volume of the substance used in these experiments was calculated in micrograms. For example, to obtain stable metallic hydrogen, diamond anvils are most often used, which compress a sample with a thickness of less than a hundredth of a millimeter [18]. Under such conditions, it is not possible to measure the density of the sample.

The dependence found above (Fig.) makes it possible to predict the density of the substance that it will acquire upon transition to the metallic state. Applying formula (4) and using the values of V_n/V_a, the calculation of the expected density (ρ_c) that a substance in the metal phase would have was performed. The calculated values of ρ_c are given in Table 2. Table 2 also shows the ratio of the substance density in the metal phase to the density in the solid phase (ρ_c/ρ_n).

According to the data in Table 2, it was found for hydrogen that the density of this substance in the metal phase will be $\rho_c = 1.95$ *g/cm*^{3}, and the ratio of the density of the metal phase to the solid phase is 22.7. The metallic phase of oxygen will have the highest density $\rho_c = 22.7$ *g/cm*^{3} at the ratio $\rho_c/\rho_n = 16.2$. As an oxidizing agent, oxygen in this phase will have the highest energy intensity. In the metallic phase, nitrogen will have a density of $\rho_c = 9.71$ *g/cm*^{3} at a ratio of $\rho_c/\rho_n = 9.46$, and fluorine $\rho_c = 14.3$ *g/cm*^{3} ($\rho_c/\rho_n = 8.41$).

Apparently, through the coefficient of solid compressibility, it is possible to calculate the necessary pressure, which should be applied in order to transfer the elements listed in Table 2 to the metallic state. In this respect, the lowest pressure (comprehensive) will need to be applied for mercury ($\rho_c = 15.1$ *g/cm*^{3}, $\rho_c/\rho_n = 1.06$). As is known, in its normal state (n.c.) mercury is a semimetal. All values given in Table 2 of ρ_c are predictive. However, they can suggest the conditions for setting up an experiment to obtain one or another substance in the metallic state.

I. Conclusion

Hydrogen, together with oxygen, is the most environmentally friendly fuel, harmless to the environment. The receiving of a metastable metallic phase of hydrogen would make it possible to reduce the volume of the tank containing this element by a factor of 10^3-10^4. The same prospects open up for the metallic phase of oxygen. Accordingly, the volume of tanks containing fuel, for example, aircraft and rockets, would be so reduced. Application of the dependence obtained for metals makes it possible to predict the density of the metal phase of hydrogen and oxygen. Prediction of the density of the metal phase of other substances listed in Table 2 will shorten the search for the necessary experimental parameters to obtain such a state.

Conflict of interest: None.
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Data availability: The data that support the findings of this study are available upon reasonable request.

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