https://doi.org/10.15407/ujpe67.8.561

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DEPENDENCES OF THE INTERATOMIC QUASIELASTIC FORCE COEFFICIENT AND THE ROOT-MEAN-SQUARE AMPLITUDE OF THERMAL VIBRATIONS OF ATOMS ON THE CONFIGURATION OF VALENCE ELECTRONS

The interatomic quasielastic force coefficient f and the root-mean-square amplitude of thermal vibrations $\sqrt{\overline{u^2}}$ of atoms in s-, d-, and p-elements located in various groups of Mendeleev's Periodic Table are calculated. It is found that, with an increase in the atomic number of elements in the groups, the quasielastic force coefficient f and the amplitudes $\sqrt{\overline{u^2}}$ of thermal vibrations of atoms in the s-, d-, and p-elements change according to different patterns depending on the atomic number of the element in a group. The discovered regularities can be explained by the configurational model of the electronic structure of matter.

Keywords: Mendeleev Periodic Table of elements, s-, d-, and p-elements, configuration of valence electron orbitals, quasielastic force coefficient, root-mean-square (RMS) amplitude of thermal vibrations, Debye temperature, atomic number.

1. Introduction

The Mendeleev's Periodic table of chemical elements (MPTCE) plays an important role in science and particularly in material science which is developed and studies the properties of materials. In connection with the 150-th anniversary of the MPTCE discovery, the works [1,2] provided the extensive overview of how it has developed over the years. The acquaintance with these works allows one to conclude that the researchers over the years mainly focused on the atomic weight and valence. Indeed, these two parameters determine the entire spectrum of the MPTCE. The paper [3] emphasizes that the study of the Periodic table itself is not "fully completed," as it seems that it is necessary to pay attention to the search for special additional principles of symmetry in the MPTCE. Indeed, in the studies of inorganic materials, their relationship to the atomic weight and horizontal valence is considered [1, 2]. At present, there is no information on regularities in the dependence of quantities characterizing the thermal vibrations of atoms in a crystal lattice of elements on the atomic number by groups. Nevertheless, such consideration could provide a useful information about the nature of interatomic interaction forces for elements with the same electronic configuration, but with different principal quantum numbers. The aim of this work is to study the dependence of the quasielastic force coefficient and the root-mean-square (RMS) amplitude of thermal vibrations of atoms of the s-, d-, and p-elements of III–VIII groups of the MPTCE on the configuration of the orbitals of valence electrons n the groups.

2. Theoretical Analysis

According to works [4, 5], in addition to the atomic weight and valence, the configuration of outer electrons also plays an important role in the formation of the properties of elements. It is of interest that the configuration is diverse not only in chemical elements of different groups, but even in subgroups of one group.

In paper [6], it was shown that the Debye temperature θ in all groups of the Periodic table (that is, in elements with the same configuration of the outer electron shells of atoms) smoothly decreases with an increase in the atomic number of elements Z along a curve resembling hyperbolae. Note that the same conclusion was also made in paper [7] based on the experimental data from the investigations of the Debye temperature of rare-earth elements contained in a complex solid solution of rare-earth metal hexabarides. It is worth noting that this rule is fulfilled without exception for all elements in each group of MPTCE regardless of the difference in their crystal structure. For example, the B, Al, Ga, and Tl elements of IIIb group have a cubic, rhombic, tetragonal, and hexagonal crystal structures, respectively [8]. Nevertheless, for this group, a nonlinear smooth decrease in the Debye temperature can be also observed [6]. This indicates that, in the binding energies of elements with simple crystal structures, the dominant role is played by the outer electronic configuration, which is determined by the atomic number of the element. However, using the example of diamond and graphite modifications of carbon, one can see a sharp difference in their Debye temperatures (2230 K for diamond [6], and 1000 K for graphite [9]. This special case can be explained by the fact that, in the layered hexagonal structure of graphite, the layers are bound by weak van der Waals forces.

It is believed that the Debye temperature of a crystal θ can be a measure of the interaction of atoms in the lattice and the binding strength [6, 7]. If so, then, with a decrease in the Debye temperature, the binding strength decreases as well, and one should expect a decrease in the melting temperature of elements in all groups with an increase in the atomic number. In fact, according to [8, 10], the melting point of elements increases in some groups and decreases in another groups with the atomic number of the element in the group. Since the melting point depends on the binding strength in the crystal, one can assume that there is no direct relationship between the binding strength and the Debye temperature. The process of oscillation in a crystal is, in itself, a very complex process. However, due to the small amplitude of vibrations of its atoms compared to the lattice parameters, the vibrations of the atoms at room temperature can be assumed to be harmonic. By the way, the harmonic approximation for the vibrations of atoms in a crystal lattice is the basis for explaining many physical phenomena in solids [11]. Within the harmonic oscillation model, the expression for the interatomic quasielastic force coefficient f related to a one-component lattice [12]

$$f = \frac{k^2}{3\hbar^2}\ m\theta^2 \tag{1}$$

implies that the Debye temperature can be defined as

$$\theta = \sqrt{\frac{3\hbar^2}{k^2}\frac{f}{m}}, \tag{2}$$

where $\hbar = \frac{h}{2\pi}$, h is Planck's constant, k is Boltzmann's constant, and m is the mass of the atom. A smooth decrease in the Debye temperature, like a hyperbolic curve, with an increase in the atomic number of an element in the group indicates that the nature of its change is dominated by an increase in the mass of an atom in comparison with a change in the interatomic binding force in the group. This means that the change (increase) in the mass of an atom in a group from period to period occurs more strongly than the change in the interatomic binding force. Thus, the Debye temperature does not reflect the true nature of the change in the interatomic force and cannot serve as an unambiguous characteristic of the interatomic binding force. Obviously, the interatomic force in a crystal can be characterized by the quasielastic force coefficient f and the RMS amplitude of thermal vibrations of atoms ($\sqrt{\overline{u^2}}$). The quasielastic force coefficient f and a displacement of atoms from the ideal position in the harmonic approximation are related to the quasielastic force F between atoms in the crystal via the simplest expression $F = -fx$ [11].

3. Calculation Methodology and Discussion of Results

The value of the root-mean-square amplitude (RMSA) of atoms $\sqrt{\overline{u^2}}$ in the lattice is determined through the spectrum of lattice vibrations, which, in turn, is determined by the nature of the interatomic binding force. The RMSA of thermal vibrations of atoms in the lattice was calculated by using the formula connecting RMSA of atoms $\sqrt{\overline{u^2}}$ and the Debye

Table 1. **Debye temperature (in K) for the elements of Mendeleev's Periodic table [6, 8, 9, 12]**

Groups																		
No	Ia	IIa	IIIa	IVa	Va	VIa	VIIa	VIIIa			Ib	IIb	IIIb	IVb	Vb	VIb	VIIb	VIIIb
I	H																	He
II	Li 366	Be 1060											B 1150	C 2230	N	O	F	Ne
III	Na 164	Mg 386											Al 428	Si 645	P	S 180	Cl 109	Ar 82
IV	K 96	Ca 230	Sc 360	Ti 384	V 339	Cr 630	Mn 410	Fe 391	Co 454	Ni 357	Cu 347	Zn 313	Ga 240	Ge 371	As 285	Se 129	Br 84	Kr 72
V	Rb 55	Sr 129	Y 235	Zr 300	Nb 276	Mo 458	Tc 345	Ru 348	Rh 450	Pd 275	Ag 228	Cd 190	In 109	Sn 170	Sb 193	Te 129	I 81	Xe 64
VI	Cs 39	Ba 96	La 135	Hf 252	Ta 240	W 380	Re 281	Os 273	Ir 425	Pt 235	Au 162	Hg 72	Tl 79.6	Pb 92	Bi 117	Po	At	Rn
VII	Fr	Ra	Ac															

temperature established by the Debye theory of thermal vibrations of a lattice and experimentally confirmed by the X-ray diffraction and neutron diffraction methods [13–15]:

$$\bar{u}^2 = \frac{9\hbar^2}{k\,m\,\theta}\left[\frac{\Phi(x)}{x}+\frac{1}{4}\right], \tag{3}$$

where θ is the Debye temperature, $\bar{u}^2$ is RMSA of thermal vibrations of atoms, $\hbar = \frac{h}{2\pi}$, h is Planck's constant, k is Boltzmann's constant, m is the mass of an atom of the element, $x = \frac{\theta}{T}$ is the ratio of the Debye temperature to the measured temperature T (in K), $\Phi(x)$ is the-tabulated Debye function [14]:

$$\Phi(x) = \frac{1}{x}\int\limits_0^x \frac{\xi d\xi}{e^{\xi}-1}, \tag{4}$$

where $\xi = \frac{h\omega}{kT}$, ω is the frequency of the normal harmonic oscillations. To calculate the quasielastic force coefficient f and RMSA of thermal vibrations of atoms ($\sqrt{u^2}$), formulas (1) and (3), respectively, can be used. For the calculation, the Debye temperature values were mainly taken from the data given in work [6], which are reliable and very close to the data in [8, 9]. The missing data in [6] were taken from [8–10] (Table 1). When selecting data on the Debye temperature θ, we have used its decrease with an increase in the atomic number of elements Z in groups along a nonlinear curve resembling a hyperbola [6].

The results of calculations of the quasielastic force coefficient f and the RMSA $\sqrt{u^2}$ for the elements of the MPTCE are obtained by using formulas (1) and (3), respectively, and are presented in Table 2.

As is seen from Table 2, in s- and some p-elements, the quasielastic force coefficient f decreases, and RMSA $\sqrt{u^2}$ increases with an increase in the atomic number of the element, that is, with an increase in the principal quantum number of valence electrons. Figure 1 shows the dependences of values of f and $\sqrt{u^2}$ on the atomic number of s-elements in group Ia. One can see that these dependences in Fig. 1 are nonlinear. For other s-elements, as well as for p-elements of groups IIIb–Vb, the same form of dependence of f and $\sqrt{u^2}$ on the atomic number in the corresponding groups can be also observed. Such a decrease in f and, accordingly, an increase in RMSA $\sqrt{u^2}$ in these elements with an increase in their atomic number can be explained as follows. According to [4, 5], in s-elements, the bonds occur by means of valence s-electrons. With an increase in the principal quantum number (atomic number), the binding energy of valence s-electrons de-

Table 2. **Atomic number, configuration of outer valence electrons (1-st row in cells), quasielastic force coefficient (in N/m, 2-nd row in cells), and the RMS amplitude of thermal vibrations (in Å, 3-rd row)**

	Groups																	
No.	Ia	IIa	IIIa	IVa	Va	VIa	VIIa	VIIIa			Ib	IIb	IIIb	IVb	Vb	VIb	VIIb	VIIIb
I	**1 H** $1s^1$																	**2 He** $1s^2$
II	**3 Li** $2s^1$ 26.45 0.38	**4 Be** $2s^2$ 288.03 0.130											**5 B** $2s^22p^1$ 406.74 0.115	**6 C** $2s^22p^2$ 1699.22 0.067	**7 N** $2s^22p^3$	**8 O** $2s^22p^4$	**9 F** $2s^22p^5$	**10 Ne** $2s^22p^6$
III	**11 Na** $3s^1$ 17.59 0.459	**12 Mg** $3s^2$ 103.01 0.194											**13 Al** $3s^23p^1$ 140.61 0.167	**14 Si** $3s^23p^2$ 332.36 0.112	**15 P** $3s^23p^3$	**16 S** $3s^23p^4$ 29.55 0.355	**17 Cl** $3s^23p^5$ 11.98 0.556	**18 Ar** $3s^23p^6$ 7.64 0.695
IV	**19 K** $4s^1$ 10.25 0.601	**20 Ca** $4s^2$ 60.31 0.249	**21 Sc** $3d^14s^2$ 165.74 0.151	**22 Ti** $3d^24s^2$ 206.05 0.137	**23 V** $3d^34s^2$ 166.55 0.151	**24 Cr** $3d^54s^1$ 550.40 0.084	**25 Mn** $3d^54s^2$ 262.76 0.122	**26 Fe** $3d^64s^2$ 242.88 0.126	**27 Co** $3d^74s^2$ 345.58 0.106	**28 Ni** $3d^84s^2$ 212.81 0.134	**29 Cu** $3d^{10}4s^1$ 217.67 0.132	**30 Zn** $3d^{10}4s^2$ 182.23 0.145	**31 Ga** $4s^24p^1$ 114.26 0.182	**32 Ge** $4s^24p^2$ 284.42 0.125	**33 As** $4s^24p^3$ 173.14 0.148	**34 Se** $4s^24p^4$ 37.38 0.314	**35 Br** $4s^24p^5$ 16.04 0.480	**36 Kr** $4s^24p^6$ 12.36 0.547
V	**37 Rb** $5s^1$ 7.36 0.707	**38 Sr** $5s^2$ 41.48 0.299	**39 Y** $4d^15s^2$ 139.68 0.164	**40 Zr** $4d^25s^2$ 233.58 0.128	**41 Nb** $4d^45s^1$ 201.34 0.137	**42 Mo** $4d^55s^1$ 572.69 0.080	**43 Tc** $4d^55s^2$ 331.56 0.119	**44 Ru** $4d^75s^1$ 348.24 0.105	**45 Rh** $4d^85s^1$ 592.84 0.081	**46 Pd** $4d^{10}5s^0$ 228.31 0.128	**47 Ag** $4d^{10}5s^1$ 159.54 0.153	**48 Cd** $4d^{10}5s^2$ 115.45 0.180	**49 In** $5s^25p^1$ 38.81 0.309	**50 Sn** $5s^25p^2$ 97.61 0.196	**51 Sb** $5s^25p^3$ 129.04 0.17	**52 Te** $5s^25p^4$ 60.41 0.248	**53 I** $5s^25p^5$ 23.69 0.395	**54 Xe** $5s^25p^6$ 15.3 0.492
VI	**55 Cs** $6s^1$ 5.75 0.799	**56 Ba** $6s^2$ 36.01 0.320	**57 La** $5d^16s^2$ 72.02 0.227	**72 Hf** $5d^26s^2$ 322.49 0.108	**73 Ta** $5d^36s^2$ 296.52 0.113	**74 W** $5d^46s^2$ 755.27 0.072	**75 Re** $5d^56s^2$ 418.32 0.095	**76 Os** $5d^66s^2$ 403.37 0.097	**77 Ir** $5d^76s^2$ 987.81 0.063	**78 Pt** $5d^96s^1$ 306.51 0.111	**79 Au** $5d^{10}6s^1$ 147.06 0.159	**80 Hg** $5d^{10}6s^2$ 29.59 0.354	**81 Tl** $6s^26p^1$ 36.84 0.316	**82 Pb** $6s^26p^2$ 49.9 0.272	**83 Bi** $6s^26p^3$ 81.39 0.214	**84 Po** $6s^26p^4$	**85 At** $6s^26p^5$	**86 Rn** $6s^26p^6$
VII	**87 Fr** $7s^1$	**88 Ra** $7s^2$	**89 Ac** $6d^17s^2$															

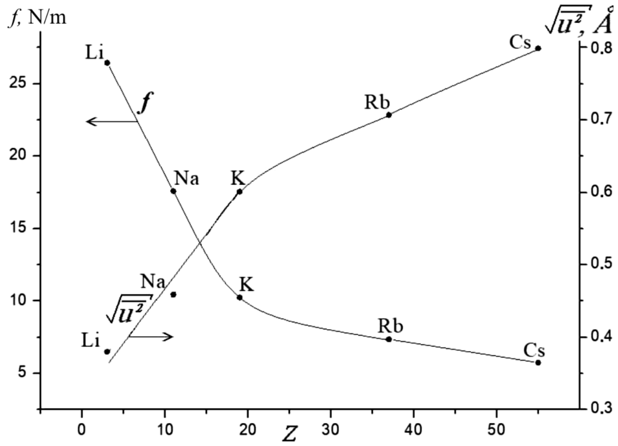

Fig. 1. Dependence of the quasielastic force coefficient and the root-mean-square amplitude $\sqrt{\overline{u^2}}$ for s-elements of the group Ia (Li–Cs) on the atomic number

creases due to an increase in the distance from the atomic nucleus. In addition, with an increase in the atomic number of an element, the degree of screening of nuclear charges by internal electrons increases which also leads to a weakening of the binding energy of valence s-electrons.

Consequently, in s-elements, an increase in the atomic number of elements within a group leads to the weakening of interatomic force. In this case, a decrease in the quasielastic force coefficient f and, respectively, an increase in RMSA of thermal vibrations $\sqrt{\overline{u^2}}$ are observed in the elements under consideration of an increase in their atomic number in groups.

The regularity discovered for p-elements of groups IIIb–Vb can be explained by the fact that, according to the configurational model of the electronic structure of matter [4, 5], in p-elements, the outer adjacent electron shells of s^xp^y-configurations participate in the interatomic interaction, while the connecting stability of these configurations decreases with an increase in their principal quantum number. Consequently, in these elements, with an increase in the atomic number in the groups, their interatomic binding force decreases, respectively, whereas RMSA of thermal vibrations of atoms $\sqrt{\overline{u^2}}$ increases. Interestingly, in p-elements in groups from oxygen to inert gases (in metastable crystals of inert gases), the dependence of the quasielastic force coefficient f and RMSA of thermal vibrations $\sqrt{\overline{u^2}}$ on the atomic number in groups demonstrate opposite character than in other previously mentioned p-elements. Such dependence cannot be explained basing on the available literature data on outer electronic configurations of elements. Apparently, an increase in the number of p-electrons from the left side of the groups of these elements to the right one ($ns^2np^1 \to ns^2np^4$) leads to an increase in the degree of overlap of s- and p-electrons, which increases with an increase in their principal quantum number and leads to an increase in their binding energy. In this case, an increase in the quasielastic force coefficient f and, accordingly, a decrease in the RMSA h b $\sqrt{u^2}$ with an increase in the atomic number of the element in these groups are observed.

As one can see from Table 2, for a number of d-elements of groups IIIa–VIIIa, in addition to the Sc, Cu, and Zn subgroups, the quasielastic force coefficient f increases, and the RMSA $\sqrt{u^2}$ decreases with an increase in the atomic number in the groups. Figure 2 shows such a dependence for d-elements of subgroup IVa. For the rest of the d-elements of the subgroups in the V–Ni series, the same dependence is observed. The discovered regularity can be explained by the fact that, according to [5], the orbitals of d-electrons together with the orbitals of s-electrons form hybrid ds-orbitals, which define the interatomic interaction force.

For the ds-orbitals, the overlapping degree increases with the atomic number of elements (principal quantum number of valence electrons). Consequently, this leads to ian ncrease in the interatomic interaction force, which causes an increase in the quaselastic force coefficient f and a decrease in the RMSA of atomic vibrations $\sqrt{u^2}$ with an increase in the atomic number of elements of subgroup IVa. For other d-elements of subgroups in the series V → Ni, the same dependence is observed. The discovered regularity can be explained by the fact that, according to [5], in these groups, the orbitals of d-electrons together with the orbitals of s-electrons form hybrid ds-orbitals, which determine the interatomic interaction force. The overlapping degree of ds-orbitals increases with the atomic number of elements (principal quantum number of valence electrons). Consequently, this leads to an increase in the interatomic interaction force, which causes an increase in the quasielastic force coefficient f and a decrease in the RMSA $\sqrt{u^2}$ of thermal vibrations of atoms with an increase in the atomic number of the element.

In d-elements of the Sc subgroup, noble metals (copper subgroup) (Fig. 3) and the Zn subgroup, the opposite tendency is observed than in other d-elements of subgroups IIIa–VIIa. For them, a decrease in the quasielastic force coefficient f and an increase in the RMSA $\sqrt{u^2}$ with an increase in the atomic number can be observed. Among the groups of d-elements, the Sc subgroup (subgroup IIIa) is the only one which has one electron in the outer d-shell ($nd^1(n+1)s^2$), that is, the number of s-electrons n the elements of this subgroup is larger than the number of d-electrons.

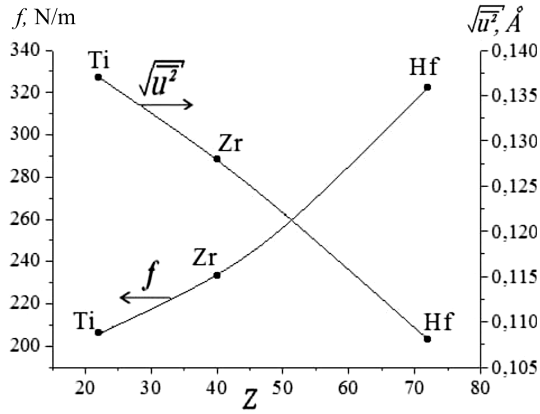

Fig. 2. Dependence of the quasielastic force coefficient and the RMS amplitude of atoms $\sqrt{u^2}$ in d-elements of group IV a (Ti–Hf) on the atomic number Z

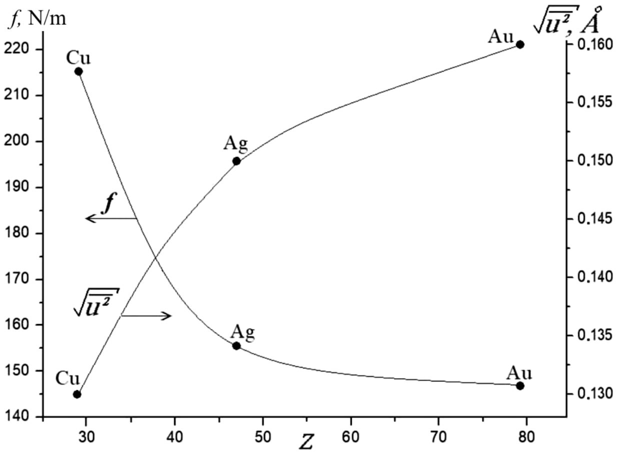

Fig. 3. Dependence of the quasielastic force coefficient f and the RMS amplitude of atoms ($\sqrt{u^2}$) in d-elements of group VIII a (Cu–Au) on the atomic number Z

Atoms of the Cu (copper) subgroup in the isolated state have an outer $d^{10}s$ electronic configuration. In these metals, s-electrons are mainly involved in the generation of binding forces during the formation of crystals [5]. In these metals, a decrease in the energy stability of s-electrons occurs, when moving from copper to gold due to an increase in the principal quantum number. When moving from Cu (copper) to gold, this leads to a decrease in the energy stability of s-electrons due to an increase in the distance of s-electrons from the nucleus and the degree of screening of the nucleus charge by internal electrons, which causes a decrease in the quasielastic force coefficient f and an increase in RMSA of thermal vibrations of atoms $\sqrt{\overline{u^2}}$ in d-elements of this group (Fig. 3). Indeed, this leads to a decrease in the modulus of normal elasticity [5], including, as it has been observed in the present study, the quasielastic force coefficient f. Obviously, this leads to an increase in the RMSA of thermal vibrations $\sqrt{\overline{u^2}}$ in the group with an increase in the atomic number of the element.

Metals of the zinc subgroup also have a d^{10}-valence subshell. In a condensed state, it is disrupted (mainly due to the excitation of the s^2-configurations) with the formation of a high concentration of unlocalized antibonding electrons [5], the antibonding degree of which increases with the atomic number of an element in the given subgroup. Naturally, this causes the weakening of interaction forces with an increase in the atomic number of an element in the given subgroup.

Note that different patterns of the dependence of interaction force characteristics and the melting temperature values [8] of the MPTCE elements in the groups on their atomic numbers correlate with one another. The nonlinear nature of the change in the interaction force characteristics of elements in groups is apparently caused by a sharp increase in the atomic mass of elements from period to period. The slightly different behaviors of the curves in the groups may be caused by the uncertainty in the Debye temperature values and the difference in the crystal structures of some elements in the same group.

4. Conclusions

1. The quasielastic force coefficient f and the root-mean-square amplitude of thermal vibrations of atoms $\sqrt{\overline{u^2}}$ are calculated via the Debye temperature in the s-, d-, and p-elements of the MPTCE. It is shown that, in s-elements of groups Ia and IIa and p-elements of groups IIIb–Vb, the quasielastic force coefficient f decreases, and the RMS amplitude of thermal vibrations of atoms $\sqrt{\overline{u^2}}$ increases with the atomic number of elements in the groups. This pattern is explained by a decrease in the binding energy of valence s- and p-electrons with an increase in their principal quantum number due to an increase in the distance from the nucleus and in the degree of screening of the nucleus charge by internal electrons.

2. It is found that, in p-elements of groups VI–VIIIb, the dependence of the quasielastic force coefficient f and the RMS amplitude of thermal vibrations of atoms $\sqrt{\overline{u^2}}$ on the atomic number in groups shows the opposite character as compared with other previous p-elements. Apparently, an increase in the number of p-electrons when moving from the left side of the groups of these elements to the right ($ns^2np^1 \to ns^2np^4$) leads to an increase in the overlapping degree of s-and p-electrons, which increases with the principal quantum number of valence electrons and leads to an increase in their binding energy values.

3. It is shown that, in the d-elements of Mendeleev's Periodic table, in addition to the Cu and Zn subgroups, the quasielastic force coefficient f increases, whereas the RMS amplitude of thermal vibrations $\sqrt{\overline{u^2}}$ decreases with an increase in the atomic number of elements in the groups. The discovered regularity can be explained by the configurational model of the electronic structure of matter. Namely, in these subgroups, the orbitals of d-electrons together with the orbitals of s-electrons form hybrid orbitals, for which the overlapping degree increases with the atomic number of elements, and, consequently, the interatomic interaction forces increase as well.

4. In noble metals (in the copper group) and in the Zn group, in contrast to the previous subgroups of d-elements, there is a decrease in the quasielastic force coefficient f and an increase in the RMS amplitude of thermal vibrations $\sqrt{\overline{u^2}}$ with an increase in the atomic number of the element. Such dependence can be explained by the fact that s-electrons are largely involved in the generation of binding forces, when crystals in the copper group are formed. The fall in the energy stability of s-electrons when moving from Cu (copper) to gold caused by an increase in the principal quantum number (due to an increase in the distance of s-electrons from the nucleus) and the degree of screening of the nuclear charge by internal electrons leads to a decrease in the interatomic

quasielastic force coefficient and to an increase in the RMS amplitude of thermal vibrations $\sqrt{\overline{u^2}}$.

5. Metals of the zinc subgroup also have a d^{10}-valence subshell. In the condensed state, it is disrupted (mainly due to the excitation of s^2-configurations) with the formation of a high concentration of unlocalized antibonding electrons. The antibonding degree of electrons increases with an increase in the atomic number of the element in the given subgroup. This leads to the weakening of the interatomic interaction force with an increase in the principal quantum number of s-electrons.

6. It is shown that the nature of the established dependences of the magnitude of quasielastic force coefficient and the RMS amplitude of thermal vibrations of atoms $\sqrt{\overline{u^2}}$ on the atomic number of elements in groups is based on the well-known and generally recognized literature data and can be well explained by the configurational model of electronic structure of matter. The nature of the dependence of the interaction force characteristics and the melting temperature of the MPTCE elements in groups on their atomic numbers correlates with each other. It can be considered that the results of this work are a good confirmation of the validity of the configurational model of the electronic structure of matter, which has been initially advanced and developed by the scientists of the Institute for Problems of Materials Science of the National Academy of Sciences of Ukraine.

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Received 18.09.21

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ЗАЛЕЖНОСТІ КОЕФІЦІЄНТА МІЖАТОМНИХ КВАЗИПРУЖНИХ СИЛ ТА СЕРЕДНЬОКВАДРАТИЧНОЇ АМПЛІТУДИ ТЕПЛОВИХ КОЛИВАНЬ АТОМІВ ВІД КОНФІГУРАЦІЇ ВАЛЕНТНИХ ЕЛЕКТРОНІВ

Розраховано коефіцієнт міжатомних квазипружних сил f та середньоквадратичну амплітуду теплових коливань $\sqrt{\overline{u^2}}$ атомів для s-, d- та p-елементів з різних груп Періодичної таблиці Менделеєва. Знайдено, що із зростанням атомного числа елемента в групі коефіцієнт квазипружних сил f та амплітуди $\sqrt{\overline{u^2}}$ теплових коливань атомів s-, d- та p-елементів змінюються по-різному в залежності від атомного числа. Ці закономірності можна пояснити в межах конфігураційної моделі електронної структури матерії.

Ключові слова: Періодична таблиця елементів Менделеєва, s-, d- та p-елементи, конфігурація орбіталей валентних електронів, коефіцієнт квазипружних сил, середньоквадратична амплітуда теплових коливань, температура Дебая, атомне число.