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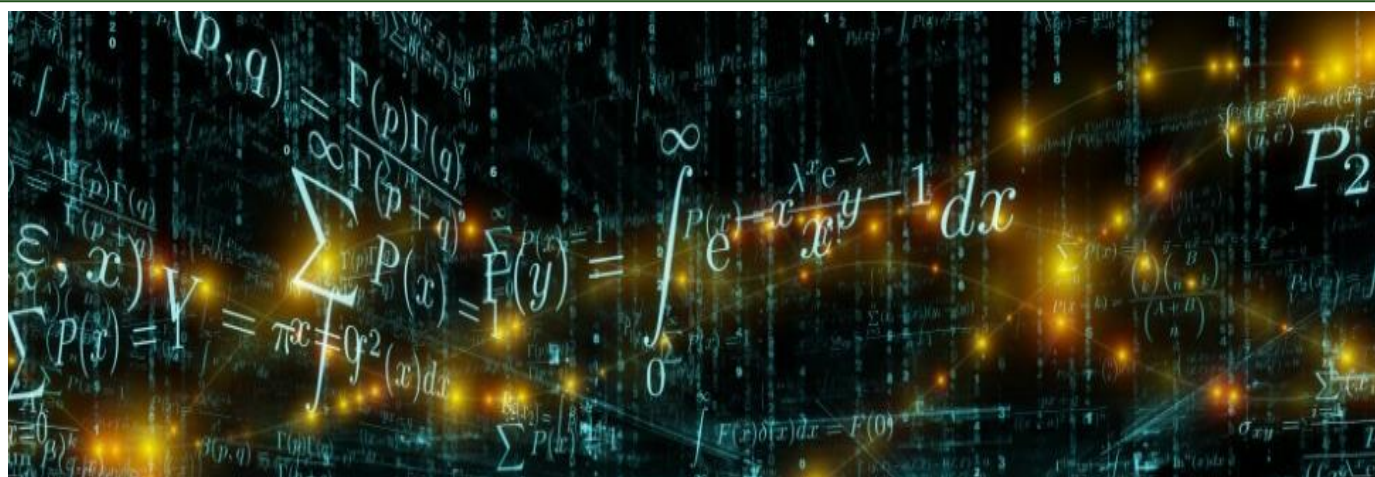
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Entropic method for calculating the maximum and effective energies of atomic structures

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The maximum and effective energies of an atomic structure equal the sum of their entropic energy components. This summation is performed for systems in equilibrium entropic state and following special rules. The spatial-energy parameter is obtained, which numerically equals the most effective energy in structural interactions. The computational and analytical method for evaluating the solubility and phase formation for complex multi-component metal systems is developed. The calculation results are quite coherent with the experimental data. The technique based on entropic principles for calculating the activation energy of self-diffusion and volumetric diffusion of atoms in solids is presented.

Keywords- entropic principles, maximum energy, effective energy, atomic structures, spatial-energy parameter, solid solutions, solubility, diffusion, activation energy.

CITATION OF THE ARTICLE



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I. INTRODUCTION

The solution of the basic problem of material science – obtaining materials with predetermined properties – can be reached only based on fundamental principles that determine the totality of physical-chemical criteria of this substance. Obviously, the quantum-mechanical conception of physics and chemistry of solids becomes such a basis. On the other hand, it can be stated that till now a sufficient amount of experimental material on physical-chemical properties of many compounds has been accumulated. Although there are several semi-empirical models for processing this information, still there is no theoretical substantiation of research trends to solve such problems in physical chemistry. Frequently such search is conducted intuitively using the “hit or miss” method. Similar problems also emerge during the practical use (for the same purposes) of the statistic Thomas-Fermi-Dirac atom model. One of the possible reasons of such discrepancy, in our opinion, is the insufficient regard for the summed parity of opposite entropic components of structural interactions.

To obtain the dependence between energy parameters of free atoms and degree of structural interactions in simple and complex systems, classical physics and quantum mechanics widely use Coulomb interactions and their varieties.

But biological and many cluster systems are electrically neutral in their structural base. And equilibrium-exchange spatial-energy interactions of non-Coulomb type have the primary meaning for them.

In this paper the method based on the application of a spatial-energy criterion (P-parameter) is developed. This criterion has been found and substantiated based on the entropic methodology of adding reciprocals of constituting energies of oppositely charged systems. P-parameter calculated for an atom following these rules gains physical sense of the most effective atom energy, i.e. the energy responsible for inter-atomic interactions.

Since P-parameter includes basic factors characterizing the atom stable state, it is possible to correlate and consequently predict many physical-chemical properties of compounds and find structural interaction energy criteria, system mutual solubility, stable phase formation, etc. with its help.

II. INITIAL DATA

The character of the change in the value of potential energy (ΔU) by its sign for different potential fields was analyzed [1](Table 1).

It was found out that the values of $-\Delta U$ and, consequently, $+\delta A$ (positive work) correspond to interactions proceeding along the potential gradient, and $+\Delta U$ and $-\delta A$ (negative work) take place during the interactions against the potential gradient.

Table 1 - Directedness of the interaction processes

No	Systems	Type of potential field	Process	U	$\frac{r_2}{r_1}$ $\left(\frac{x_2}{x_1}\right)$	U_2/U_1	Sign ΔU	Sign δA	Process directedness in potential field
1	opposite electrical charges	electrostatic	attraction	$-k \frac{q_1 q_2}{r}$	$r_2 < r_1$	$U_2 > U_1$	-	+	along the gradient
			repulsion	$-k \frac{q_1 q_2}{r}$	$r_2 > r_1$	$U_2 < U_1$	+	-	against the gradient
2	similar electrical charges	electrostatic	attraction	$k \frac{q_1 q_2}{r}$	$r_2 < r_1$	$U_2 > U_1$	+	-	against the gradient
			repulsion	$k \frac{q_1 q_2}{r}$	$r_2 > r_1$	$U_2 < U_1$	-	+	along the gradient
3	elementary masses m_1 and m_2	gravitational	attraction	$-\gamma \frac{m_1 m_2}{r}$	$r_2 < r_1$	$U_2 > U_1$	-	+	along the gradient
			repulsion	$-\gamma \frac{m_1 m_2}{r}$	$r_2 > r_1$	$U_2 < U_1$	+	-	against the gradient
4	spring deformation	field of elastic forces	compression	$k \frac{\Delta x^2}{2}$	$x_2 < x_1$	$U_2 > U_1$	+	-	against the gradient
			extension	$k \frac{\Delta x^2}{2}$	$x_2 > x_1$	$U_2 > U_1$	+	-	against the gradient
5	Photo effect	electrostatic	repulsion	$k \frac{q_1 q_2}{r}$	$r_2 > r_1$	$U_2 < U_1$	-	+	along the gradient

Therefore, after analyzing the first law of thermodynamics, we have the following:

1. All phenomena and processes in nature and world, including a human, machines, economics and ecology proceed only in two energy directions: either along the force field gradient with minimum energy input, or against the gradient with maximum energy input. The first direction corresponds to the notion of entropy and the second - to the notion of negentropy (negative entropy). In the dynamics of processes both phenomena are interrelated and complement each other.
2. In the systems in which the interaction proceeds along the potential gradient (positive work), the resultant potential energy, as well as the reduced mass are found based on the principle of adding reciprocals of corresponding values of subsystems. This is a corpuscular process, in which entropy can serve as the theoretical concept.
3. In the systems in which the interactions proceed against the potential gradient (negative work), the algebraic addition of their masses, as well as the corresponding energies of subsystems is performed. This is a wave process, in which negentropy can serve as the theoretical concept.
4. The resonance stationary state of the systems is fulfilled under the condition of equality of degrees of their corpuscular and wave interactions. In thermodynamics of open systems the entropy products in stationary state are completely compensated by the negentropy flow.

III. ATOM ENTROPIC COMPONENTS

A free atom is primarily a system of two opposite basics: the electron and atom nucleus. The nucleus positive charge generates the central force field, in which the electron cloud is located and the electrons are moving. Two acceleration components are act in kinematics of any rotary motion: centripetal - directed to the center of the field gradient. This is a corpuscular component with entropy as the theoretical concept. And there is a linear in acceleration directly tangentially from the atom, i.e. against the field gradient, with negentropy as the concept. This is the process wave part. The conditions of entropic-equilibrium state between the components determine the whole structure stabilization according to Planck's equation for atomic centers:

$$h = E/v,$$

Where E - orbital energy constant in the stationary state, the process goes along the field gradient

(entropy), v - electromagnetic wave frequency (negentropy), h - Planck's constant.

And the rear also two components of kinetic and potential energies during elastic-harmonic oscillations. Their correlation is as follows:

$$E_P/E_K = tg^2\delta,$$

where, E_K - kinetic energy, E_P - potential energy, δ - angular characteristic of oscillations.

Under the condition of equality $\delta = \varphi$, the system gets into the entropic equilibrium state (where $\varphi = 54.733^\circ$ - entropic geodesic angle). This is the angle at which a silkworm winds a silk thread onto the base.

Similar processes can be also seen in macro-processes, for example, in engineering during the production of spaceships. In this example we use the data from [2]. When producing spaceships, the extra-strong thread is wound on to the body at the geodesic angle according to the entropic correlations:

$$\sigma_\beta/\sigma_\alpha = N_\beta/N_\alpha = tg^2\varphi = 2$$

where: σ_α - axial, σ_β - circumferential stresses which are substituted by the proportional value N_α - axial "stress" and N_β - circumferential "stress".

This condition allows obtaining the equally stressed system of threads with the minimum product weight.

Between the most opposite components of the entropy the interaction type depends on the sign of their electric charge. If both components have the same electric charge, the principle of algebraic addition of their components is realized. For example, the maximum energy at elastic-oscillatory processes equals the sum of kinetic and potential energies and is always constant.

If both entropy components are electrically neutral or their values of energy parameters differ only slightly, the principle of algebraic addition is also realized. If both components have opposite electric charges, the sum of their components is found following the principle of adding their reciprocals. This also takes place in the system "electron-nucleus" and the total energy obtained this way decreases but is sufficient and the most effective in structural interactions.

Hamilton function equals the sum of kinetic and potential energies. That is - this is the total mechanical energy of the system. But Hamiltonian is realized only for systems with homogeneous function of the second degree.

For example, two particles perform free translational motion together. Both their masses and energies are summed algebraically. But if the same particles move in the field of central forces with the common energy, such particles are not homogeneous already - their masses and energies are summed following the principle of adding reciprocals. Thus, in a complex multicomponent system its total energy decreases under external technological action.

Another example: Lagrange equation for the relative motion of the isolated system of two interacting material points with masses m_1 and m_2 , which in coordinate x is as follows:

$$\mu \cdot x'' = -\frac{\partial U}{\partial x}; \frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}.$$

Here U - mutual potential energy of material points; μ - reduced mass.

At the same time, $x'' = a$ (feature of the system acceleration). For elementary portions of the interactions Δx can be taken as follows:

$$\frac{\partial U}{\partial x} \approx \frac{\Delta U}{\Delta x} \quad \text{That is: } \mu a \Delta x = -\Delta U. \text{ Then:}$$

$$\frac{1}{1/(a\Delta x)} \frac{1}{(1/m_1 + 1/m_2)} \approx -\Delta U; \quad \frac{1}{1/(m_1 a \Delta x) + 1/(m_2 a \Delta x)} \approx -\Delta U$$

Or:

$$\frac{1}{\Delta U} \approx \frac{1}{\Delta U_1} + \frac{1}{\Delta U_2}$$

Where ΔU_1 and ΔU_2 - potential energies of material points on the elementary portion of interactions, ΔU - resultant (mutual) potential energy of these interactions.

IV. SPATIAL-ENERGY PARAMETER (P-parameter)

Based on the established entropy principles, the atom maximum energy can be calculated following the principle of adding reciprocals of the initial energy components according to the following equations:

$$\frac{1}{q^2/r_i} + \frac{1}{W_i n_i} = \frac{1}{P_E} \text{ or } \frac{1}{P_0} = \frac{1}{q^2} + \frac{1}{(W n)_i}; P_E = P_0/r_i \dots\dots(1),(2),(3)$$

Where: W_i - electron orbital energy [3]; r_i - orbital radius of i orbital [4]; $q=Z^*/n^*$ [5], n_i - number of electrons of the given orbital, Z^* and n^* - nucleus effective charge and effective main quantum number, r - bond dimensional characteristics.

P_0 is called a spatial-energy parameter (SEP), and P_E - effective P-parameter (effective SEP). Effective

SEP has a physical sense of atom maximum energy and is measured in energy units, e.g. electron-volts (eV).

Values of P_0 -parameter are tabulated constants for electrons of the given atom orbital.

For dimensionality SEP can be written down as follows:

$$[P_0] = [q^2] = [E] \cdot [r] = [h] \cdot [v] = \frac{kg \cdot m^3}{s^2} = J \cdot m,$$

Where $[E]$, $[h]$ and $[v]$ - dimensions of energy, Planck's constant and velocity. Thus, such P-parameter corresponds to the processes going along the potential gradient.

The introduction of P-parameter should be considered as further development of quasi-classical notions using quantum-mechanical data on atom structure to obtain the criteria of energy conditions of phase-formation. At the same time, for the systems of similarly charged (e.g. - orbitals in the given atom) or homogeneous systems, the principle of algebraic addition of such parameters is preserved:

$$\sum P_E = \sum (P_0/r_i); \quad \sum P_E = \frac{\sum P_0}{r} \dots\dots\dots(4),(5)$$

or: $\sum P_0 = P_0' + P_0'' + P_0''' + \dots; \quad r \sum P_E = \sum P_0 \dots\dots\dots (6),(7)$

Here P-parameters are summed on all atom valence orbitals.

To calculate the values of P_E -parameter at the given distance from the nucleus either atom radius (R) or ion radius (r_i) can be used instead of r depending on the bond type.

The examples of applying such technique in material science are given further.

V. SOLUBILITY OF COMPONENTS IN METAL SYSTEM Co-W-Ni-Cr-Fe [6]

Using the value of electron bond energy as their orbital energy [3], we calculated the values of P-parameters of valence orbitals of elements in the system *Co-W-Ni-Cr-Fe* (Table 2) by the equation (1). At the same time, their effective P_E -parameters were found by the following equation:

$$P_s = \sum P_0 / R \cdot (n^* + 1), \dots\dots\dots(8)$$

Where R - atomic radius by Belov-Bokiy.

Only the significantly reduced versions of some tables are given here and further as an illustration.

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Table 2. P-parameters of atoms of alloy elements

Atoms	Valence electrons	W, eV	r _v , Å	q ² , eVÅ	ΣP _{ov} , eVÅ	R, Å	P _v /R, eV	P _v =ΣP _v /R(n ² +1), eV
C	2P ²	11.792	0.596	35.395	5.868	0.77	7.6208	2.5403
	2P ²	11.792	0.596	35.395	10.06		13.066	4.3554
	2S ²	19.201	0.620	37.240	9.021		11.715	3.9052
	2S ²	19.201	0.620	37.240	14.524		18.862	6.2874
	2P ² +2S ²				24.585		31.929	10.643
	*for Kr=12						28.587	9.5291
W	6S ²	6.1184	1.36	38.838	6.8528	1.4	4.8949	0.9413
	6S ²				11.650		8.3214	1.6003
	5d ³	12.093	0.746	161.43	23.178		16.556	3.1838
	5d ³				29.493		21.066	4.0512
	6S ² +5d ³				34.828		24.877	4.7841
	6S ² +5d ³				41.143		29.388	5.6515

The relative difference of P-parameters of elements' atoms constituting the alloy is the numerical criterion of the system solubility:

$$\alpha = \frac{P_2 - P_1}{P_2 + P_1} \cdot 200 \% , \dots\dots\dots(9)$$

Where P₁ - P_E-parameter of atoms of the first or structural component; P₂ - P_E-parameter of atoms of the second or structural component.

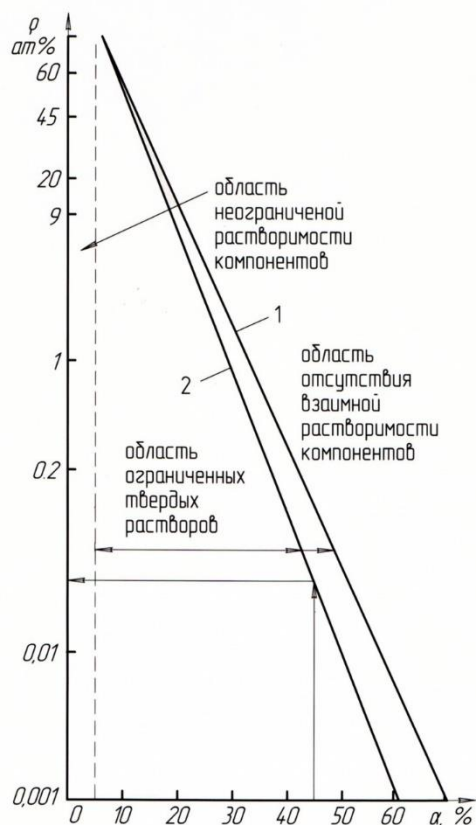


Fig. 1. Nomogram to the calculation of components' solubility ρ (in logarithmic scale) depending on coefficient α: 1 - for metal systems; 2 - for carbides

Processing of the calculation results following this technique allowed obtaining the unified nomogram of the dependence of mutual solubility of metal systems' components on coefficient α (Fig. 1, dependence 1). The logarithmic variant of such nomogram for linear dependence is given in Fig. 1. Thus, for binary metal

systems the continuous series of solid solutions is observed at α<4-6%, lack of solubility - at α>50-60%, between them - limited solubility.

Table 3. Assessment of mutual solubility of binary components in the alloy

Atom and its valence	Solubility direction	P _E , eV	P _T , eV	α, %	ρ, at%	
					calculation	experiment
1	2	3	4	5	6	7
W (5)	W → Cr	4.7841	3.9163	34.45	2.1	T ≤ 1768°K Limited solubility
Cr (6)		5.5406				
W (6)	W → Cr	5.6515	4.6263	18.1	17.5	T ≥ 2233°K
Cr (6)		5.5406				
Cr (6)	Cr → W	5.5406	6.3629	11.8	42-45	O.T.P.
W (6)		5.6515				
Cr (3)	Cr → W	2.8762	3.3030	12.13	41	T ≥ 2233°K
W (4)		3.7296				
Cr (3)	W → Cr	2.8762		5.97	100	O.T.P.
W (4)		3.7296	3.0531			
Cr (2)	W → Cr	1.7650		1.93	100	O.T.P.
W (2)		1.6003	1.7313			
Co (2)		2.1629				

Dependence of α on melting temperature of the alloy components was taken into account by the following equations:

- for the component with a higher melting temperature:

$$P_T'' = P_E'' \left(1 + 10^{-T_{mel}''/T_{mel}''} \right) / 1.1; \dots\dots\dots(10)$$

- for the component with a lower melting temperature:

$$P_T' = P_E' \left(1 - 10^{-T_{mel}'/T_{mel}''} \right) / 0.9, \dots\dots\dots(11)$$

Where P_T - reduced "temperature" value of P-parameter; T^{''} - higher melting temperature of one component; T['] - lower melting temperature of another component.

Taking into account the substitution of (10 and 11) in (9) we have:

$$\alpha_1 = \frac{P_T'' - P_E''}{P_T'' + P_E''} \cdot 200 \% , \dots\dots\dots(12)$$

$$\alpha_2 = \frac{P_T' - P_E'}{P_T' + P_E'} \cdot 200 \% \dots\dots\dots(13)$$

Using the values of calculated P-parameters (Table 2), P_T-parameters for the considered metal system Co-W-Ni-Cr-Fe reduced to the temperature of another component were found by the equations (10) and (11). At the same time, the calculations were performed in the assumption of paired interaction of atoms of elements M'-M'' for all their possible variants of combinations. Then the coefficients of structural interaction α were found by the equations (12) and (13). The calculation results are given in Table 3.

Table 4. P-parameters of systems with full solubility of components ($\rho_{max}=100\%$)

System of components (their valence)	$P'_E \rho_1, eV$	$P''_E \rho_2, eV$	$P'''_E \rho_3, eV$	$\sum P_E = P_c, eV$
$T \leq 2133^\circ K$				
Co-Ni-Fe (2-2-2)	0.721	0.727	0.716	2.164
Co-Ni-Fe (3-3-3)	0.952	0.966	0.938	2.856
$T \geq 2133^\circ K$				
W-Cr (2-2)	0.80015	0.8825	-	1.6827
W-Cr (4-3)	1.8648	1.4381	-	3.3029
W-Cr (4-3) (system with broad solubility)	2.2005	1.1792	-	3.3797

In all calculations the orbitals corresponding to the most stable oxidation degree were considered as the main valence-active ones: for iron, nickel and cobalt - (+2, +3); for chromium - (+3, +6); for tungsten - (+6, +5, +4, +2).

Table 5. Solubility of components of system (W-Cr)-(Co-Ni-Fe)

System of components and solubility direction	P'_E, eV	P''_E, eV	$P_c = \sum P_E, eV$	P_T, eV	$\alpha, \%$	$\rho, \text{at. } \%$
At the process temperatures below 1800°K ($T_{mel}/T_{mel}=1765/3680$)						
(Co-Ni-Fe) → (W-Cr)	0.80 96	4.5759	5.3806	3.4558	43.6	0.44
(W-Cr) → (Co-Ni-Fe)	0.80 96	4.5759	5.3806	4.002	33.4	2.3
At the process temperatures over 2133°K ($T_{mel}/T_{mel}=1765/3680$)						
(W-Cr) → (Co-Ni-Fe)	3.30 29	2.1634	-	2.4560	12.7	39-40
(Co-Ni-Fe) → (W-Cr)	3.30 29	2.8565	-	3.4558	4.52	100
(W-Cr) → (Co-Ni-Fe)	3.37 45	2.8565	-	2.5093	12.9	39-40
(Co-Ni-Fe) → (W-Cr)	3.37 45	2.8565	-	3.4558	2.37	100

According to the data from Table 3 it was found that the elements of the 8th group Fe, Co and Ni form continuous solid solutions with each other. For them the interaction of the most valence-active orbitals corresponds to the least external energy expenditures at lower temperatures. Elements W and Cr have limited solubility both with one another and in cobalt matrix, iron and nickel. However, the calculations demonstrate the existence of continuous solid solutions in system W-Cr for states W(4)-Cr(3) and W(2)-Cr(2) at temperatures above the chromium melting temperature. If we take into account that the molten pool temperature is 1923-2123°K and electric arc anode spot temperature reaches 2573°K [7], we can assume that all the melt elements form a solid solution with one another in the molten state. During further temperature decrease of the melt (below chromium melting temperature of 2133°K) in the process of alloy crystallization atoms of tungsten and chromium for the states W(5)-Cr(6) and W(6)-Cr(6) form limited solid solutions with one another. These results satisfactorily agree with the experimental data in [8],[9]. Therefore, taking into account the established principle of algebraic addition of P-parameters of homogeneous systems, the alloy at lower temperatures was considered as the system consisting of the components

(W-Cr) and (Co-Ni-Fe), for which P_C -parameter, P_T -parameter and α given in Tables 4 and 5 were defined.

The analysis of the data obtained demonstrated that at higher temperatures (over 2133°K) continuous solid solutions were formed ($\alpha < 4.52\%$) in the direction (W-Cr) → (Co-Ni-Fe) that confirmed the assumption put forward above. The reverse direction of the solubility process results in narrowing this region to $\alpha < 12.9\%$ and according to the nomogram (Fig. 1, dependence 1) the solubility will be $\rho = 39-40 \text{ at. } \%$. At temperatures below the chromium melting temperature their dissolution is defined by the values $\alpha_1 = 41.1\%$ and $\alpha_2 = 44.2\%$ (Table 5) and according to the nomogram (Fig. 1, dependence 1) the region of solid solutions will be significantly limited.

VI. ASSESSMENT OF ACTIVATION ENERGY OF DIFFUSION PROCESSES [10]

Since atoms of solids consist of ions and relatively free electrons moving in certain spatial regions, the interconnection between diffusion activation energy and electron interaction of atoms in the body crystalline lattice can be assumed. Based on this, diffusion activation energy (E_n) is considered as the energy of interatomic (paired) interaction of atoms A of the environment and component atom B diffusing in it. If the energy of translational motion of atom B is greater than the energy of interatomic interaction with atoms A, it diffuses outside atoms A surrounding it. If atom B has the motion energy less than the energy of its interaction with atoms A, it will be able to migrate outside these atoms. In this case, there is no exchange between atoms A and B, i.e. diffusion is impossible. Finally, if the energies of atoms are the same, there are conditions for the formation of the pair: interstitial atom - vacancy. Thus, the activation energy (in this case, diffusion energy) assessment comes down to finding the actual energy of paired or any other interaction between the diffusing atom and atoms around it.

Taking into account the entropy initial principles, we get the resultant value of the effective energy of paired interaction between atoms A and B identical to the activation energy of diffusion process as the sum of reciprocals of P-parameters:

$$\frac{1}{E_a} = 2 \left[\left(\frac{r_n}{P_o} \right)_A + \left(\frac{r_n}{P_o} \right)_B \right], \dots \dots \dots (14)$$

Where E_a - activation energy of diffusion process of atom B in the environment of atoms A; n - number of all valence electrons or the number of the valence electrons of a certain atom most distant from the nucleus.

When atom B diffuses with atoms B in the environment homogeneous in composition and similar to it, the value of E_a takes the meaning of activation

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energy of atom B self-diffusion. Based on (5) it is found as follows:

$$E_{ac} = \frac{P_o}{4r_in}, \dots\dots\dots(15)$$

The comparison of the calculation results with experimental data demonstrated their satisfactory agreement (Table 6). The error was below 5 at. %. Thus, the spatial-energy parameter is a peculiar "passport" of an atom and all the metal and alloy in general, based on which it is possible to evaluate the results of its interaction with other metals, alloys or chemical elements by means of calculations.

Table 6. Activation energy of diffusion of atoms in metal systems

Solvent			Diffusing element			E _{act} , eV	
Atoms	$\frac{P_o, eV \cdot \text{Å}}{n}$	r _n , Å	Atoms	$\frac{P_o, eV \cdot \text{Å}}{n}$	r _n , Å	Calculation by (6-7)	Reference data
γ-Fe (4S ² 3d ⁴)	29.026 3	0.67	γ-Fe (4S ²)	18.462 2	0.80	3.207	2.8-3.2
			Cr (4S ¹ 3d ²)	25.835 3	0.64	3.483	3.468
			C (2P ³)	32.458 3	2.60	1.615	1.586
			Mn (4S ²)	18.025 2	0.91	2.937	2.71-2.861
γ-Fe (4S ²)	18.462	0.80	Mn (4S ²)	18.025 2	0.91	2.665	2.419
			Ni (4S ²)	18.838 2	0.74	3.026	2.905
			Mo (5S ¹ 4d ¹)	17.475 2	0.915	2.613	2.557
			W (6S ¹ 5d ¹)	20.689 2	0.98	2.792	2.709

VII. CONCLUSIONS

1. The maximum and effective energies of atomic structure equal the sum of their entropic energy components.
2. This summation is realized for systems in equilibrium entropic state and following special rules.
3. The spatial-energy parameter numerically equal to the most effective energy in structural interactions is obtained.
4. The calculation-analytical method for evaluating solubility and phase-formation for complex multicomponent metal systems is developed. The calculation results satisfactorily agree with the experimental data.
5. The technique based on entropic principles for calculating the activation energy of self-diffusion and volumetric diffusion of atoms in solids is demonstrated.

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