DOI: 10.63527/1607-8829-2025-2-25-35

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Theoretical Models of Anti-Diffusion Layers of Ternary Fe-Ni-W Systems in Thermoelectric Energy Converters

Theoretical models were developed and calculations of the chemical bond parameters of promising antidiffusion layers based on ternary systems Fe-Ni-W were performed. Calculations of the effective radii of interatomic interaction, redistribution of electron density and energy of nonequivalent chemical bonds Fe-Ni, Fe-W, Ni-W in the Fe-Ni-W system depending on the interatomic distances were presented.

Keywords: thermoelectric materials, antidiffusion layers, theoretical models, chemical bonding, quantum laws, effective radii, dissociation energy, phase diagrams, nonequivalent chemical bonds.

Introduction

Thermoelectric materials (TEM) based on the ternary systems Bi-Sb-Te of p-type and Bi-Se-Te of n-type conductivity have found wide application in the manufacture of thermoelectric coolers and generators [1].

One of the essential stages in the manufacture of thermoelectric modules is the creation of reliable connecting structures. Connection is a complex technological process that includes the creation of contact connections between the legs of the p- and n-types thermoelectric material compatible in terms of physicochemical properties with high stability, sufficient mechanical strength and resistance to thermal changes [2].

Development of the effective connections requires solving a whole range of materials science and technological issues. The first priority is the selection of materials that are intended for direct contact with semiconductor legs. The best options for connecting legs are the use of

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Citation: O.M. Manyk, M.M. Krechun, V.V. Razinkov (2025). Theoretical Models of Anti-Diffusion Layers of Ternary Fe-Ni-W Systems in Thermoelectric Energy Converters. *Journal of Thermoelectricity*, (2), 25–35. https://doi.org/10.63527/1607-8829-2025-2-25-35

metals with high thermal and electrical conductivity, for example, copper or silver. When using copper connection, it is necessary to apply anti-diffusion layers to the TEM legs, which help reduce the diffusion of copper into the thermoelectric material [3].

Considering that the need for thermoelectric cooling modules with operating temperatures above 200 °C has recently been significantly increasing, the issue of developing high-performance technologies for applying effective anti-diffusion structures to ensure reliable functioning of cooling modules at elevated temperatures is becoming particularly relevant.

The antidiffusion layer must be inert to the thermoelectric material, be characterized by high adhesion, have a low contact resistance, and have a coefficient of thermal expansion close to the coefficient of thermal expansion of the TEM.

Various methods of creating connecting structures are known, for example, the soldering method, joint hot pressing of thermoelectric legs and connecting material. However, different thermal effects on thermoelectric samples cause an increase in the diffusion of impurities from connecting materials into the TEM and deteriorate its properties. At the same time, a combination of electrochemical etching methods and electrolytic deposition of an electroneutral metal allows creating an antidiffusion barrier on the surface of the thermoelectric material with an adhesion strength that exceeds the cohesive strength of the material itself. However, at elevated operating temperatures, the functioning of such antidiffusion structures is associated with the formation of intermetallic compounds in the contact zone, which significantly reduces the service life of thermoelectric modules.

Therefore, the purpose of this paper was to develop theoretical models of anti-diffusion structures to ensure reliable operation of cooling modules at elevated temperatures by applying a comprehensive approach to the formation of a chemical bond in the contact zone.

A specifity of this approach is that a number of factors under consideration are interconnected and their influence on the properties of the materials under study is revealed indirectly through the parameters of theoretical models [4, 5, 6]. The availability of such information makes it possible to theoretically describe the connection processes and generalize the capabilities of existing models by combining thermodynamic, statistical, quantum-mechanical approaches taking into account chemical bonding.

Physicochemical properties and phase diagrams of Fe-Ni-W based antidiffusion layers

When developing theoretical models of Fe-Ni-W antidiffusion structures, it was necessary to summarize the results of studies of the physicochemical properties and quantum laws of the initial components and justify their choice.

The results of theoretical studies of the features of the chemical bond of iron (Fe) are given in [7]. Analysis of diverse information about the crystal structure, thermodynamic and quantum laws of Fe enabled establishing a theoretical model of chemical bonding, determining the constants of the microscopic theory, characteristic temperatures, which must be considered while choosing technological solutions for the synthesis of new Fe-containing materials.

The next stage of the study is aimed at establishing the dynamics of the formation of the chemical bond of the initial components during the transition to the structures of binary alloys. To describe the dependence of the temperatures of primary crystallization on the composition of binary systems, the Fe-Ni, Fe-W, Ni-W phase diagrams were used, shown in Fig. 1, where the following notations are introduced: α – solid phase based on Fe; β – solid phase based on Ni; γ – solid phase based on W; σ – solid phase based on Fe-W; Δ – solid phase based on Fe-Ni; λ – solid phase based on Ni-W; θ – solid phases based on the intermediate compound Fe-Ni-W; *L* – liquid.

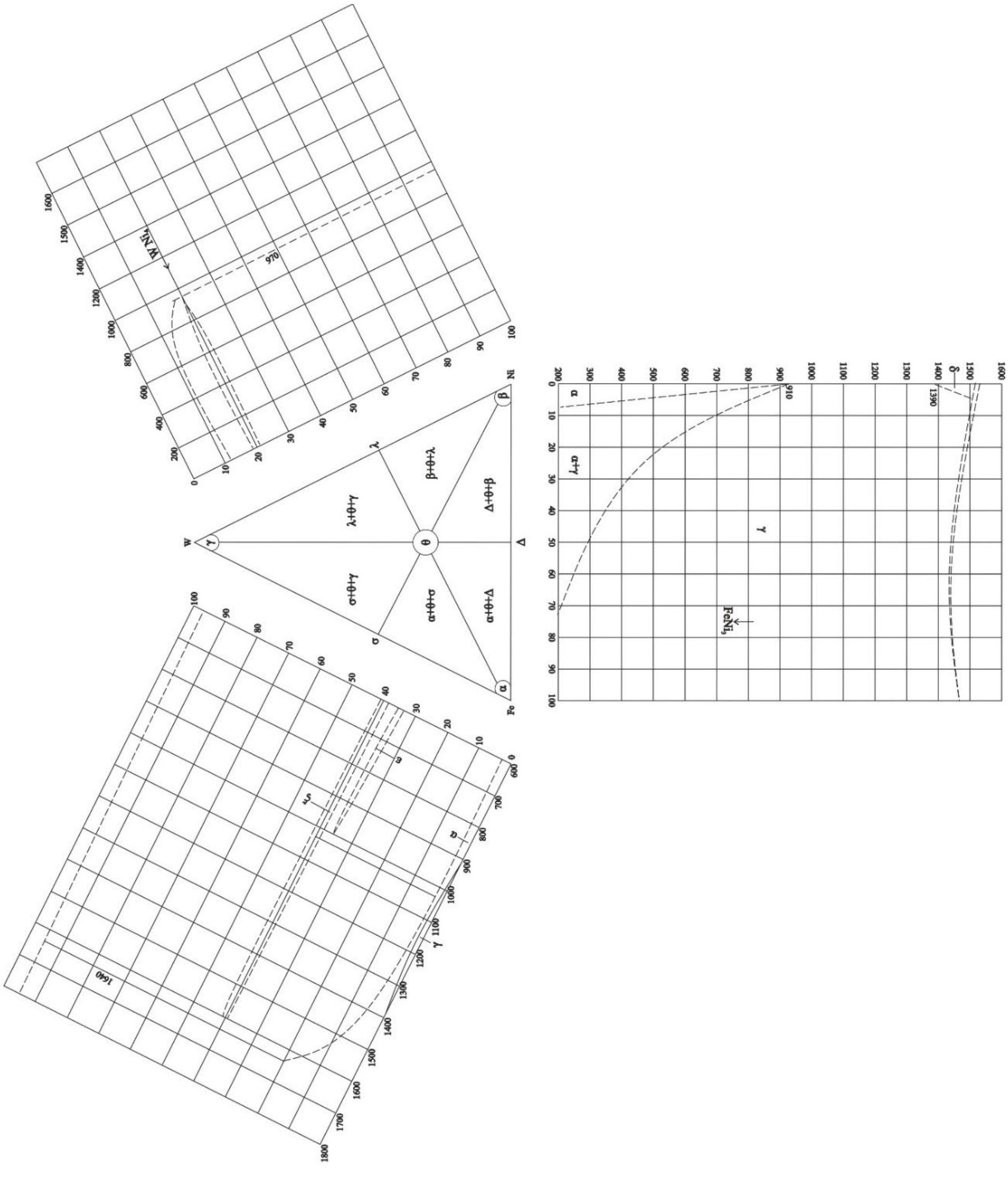

Fig. 1. Scheme of the distribution of phase regions in the Fe-Ni-W solid state.

From the analysis of the Fe-Ni phase diagrams shown in Fig. 1 [8] follows that the data on peritectic equilibria in different works differ due to the formation of metastable structures, which vary widely depending on the composition and heat treatment, as well as due to the low diffusion rate at temperatures below 500 °C. It was also established that the transformation in iron during heating and cooling is of the nature of a diffusionless martensitic transformation, which is characterized by the relationship between low-temperature polymorphic modification of the crystal lattice and high-temperature. As for the crystal structure of Fe-Ni alloys, in addition to the ordered phase $FeNi_3$ with the Cu_3Au structure, only the body-centered cubic (bcc) α-phase with the A2 type structure and the face-centered cubic (fcc) γ-phase with the A1 type structure were detected. Measurements of the lattice period showed that the introduction of Ni into Fe results in an expansion of the lattice. The period of the γ-phase reaches a maximum value at 39 at. % Ni. There is no explanation for the existence of this maximum. The periods of alloys with 50–80 % Ni in the disordered and ordered states are also given. The alloy with 75 at. % Ni has a period $a = 3.5544$ Å in the disordered state and $a = 3.5522$ Å in the ordered state.

The analysis of the Fe-W phase diagrams [9], shown in Fig. 1. demonstrates that the WFe_3, W_2Fe phases, whose existence was reported in early works, do not exist at all. It was also established that W additions reduce the temperature of the $\alpha\leftrightarrow\delta$ transformation and increase the temperature of the $\alpha\leftrightarrow\gamma$ transformation of iron. The solubility of W in solid Fe (the data available in the literature are in good agreement) is 33 wt. (13 at.) %. With a decrease in temperature, the solubility decreases. There has been much debate about how many and what compounds do exist in the Fe-W system. No correct answer has not yet been found. As for the solubility of Fe in solid W, it was initially found that at 1600 °C the solubility is 1.2 wt. %, later 1.1 wt. (3.5 at.) % and in the latest review the value is 0.8 wt. (2.6 at.) % Fe at 1640 °C. Minor changes in solubility with changes in temperature are observed. Dissolved W atoms increase the lattice period of α-iron. For compounds WFe_2 (ε-phase) is hexagonal unit cell of $MgZn_2$ type, for compounds W_2Fe_3 (ξ-phase) it is rhombohedral with $a = 9.04$ Å and $a = 30°30.5'$. Later, in addition to ξ, two more structures close to ξ were observed, which have different intensities and some shift of *X*-ray lines.

Similarly, the analysis of Ni-W phase diagrams was carried out [10]. As later works show, thermal and microscopic studies of nickel-rich alloys are of some historical interest only. In early studies, it was believed that at 940 °C an intermediate phase WNi_6 is formed from the Ni solid solution, which decomposes by a eutectoid reaction at 905 °C and 920 °C. However, it was later found that with the composition WNi_6 there is still a Ni lattice and the only intermediate phase formed by a peritectoid reaction has the formula WNi_4. The WNi_4 compound has a homogeneity interval of about 2 wt. (3 at.) % at 900 °C and it was assumed that below 850 °C its limit on the Ni side is at about 17.6 at. % W. As for the structure of WNi_4, the lattice is body-centered tetragonal (BCT) (space group 14/m) with $a = 5.730 \pm 0.001$ Å, $c = 3.553 \pm 0.001$ Å, $c/a = 0.620$ with 10 atoms per unit cell. There are conflicting data regarding the solubility of Ni in W in the solid state (4–5 wt. %), which are probably overestimated. The value of the lattice period for W saturated with Ni at 1150 °C is somewhat lower than that for pure W.

The above analysis of the results of experimental studies of the initial components for creating anti-diffusion barriers and phase diagrams of binary systems based on them allowed comparing the obtained results with the ternary TEM systems (Bi-Sb-Te) of p-type and (Bi-Se-Te) of n-type conductivity and, thus, coming to the conclusion that a number of technological problems in them are solved at different temperature intervals and are not interconnected. At the same time, the given isothermal sections enable separating the boundaries of phase equilibrium for eutectic and peritectic type diagrams and optimizing the technological modes of obtaining new materials for creating anti-diffusion barriers for TEMs in high-temperature operating ranges.

Theoretical models of the Fe-Ni-W chemical bond

Theoretical analysis of the processes of formation of antidiffusion barriers requires a revision of the foundations of the theory of interatomic interaction. Existing theoretical approaches contradict the formation of a chemical bond, which is accompanied by a restructuring of the short-range order structure of interacting atoms and a redistribution of electron density along chemical bonds.

On the other hand, taking into account statistical regularities enabled obtaining the dependence of electrons n on the outer shell of an atom on the Fermi radius r_F.

An analysis of empirical information on the properties of atoms based on the crystal chemical approach made it possible to generalize the concept of the Fermi radius for the case of electron configurations of interacting atoms depending on the length and number of bonds they form, thus introducing the concept of effective ionic radii R_U.

The most useful in searching for the bond R_U with n was the relationship $\mathrm{tg}\alpha = \frac{\Delta \lg R_U}{\Delta n}$ with the properties of atoms in the coordinates with the angle of inclination of the straight lines in the coordinates $\Delta n \lg R_U = f(n)$. Good agreement of experimental data on the properties of atoms and their ions with the values of R_U and $\mathrm{tg}\alpha$ gives the postulated dependence:

$$\lg R_{UA}^{x} = \lg R_{UA}^{0} - x\mathrm{tg}\alpha, \tag{1}$$

where $R_{U\mathrm{A}}^{0}$ is the radius of atom A in the unexcited state, and x is the valence.

Since, according to the crystal chemical approach, equation (1) describes the change in R_U of both atoms A and B when the number of electrons in the orbitals of each changes, dependence (1) takes the form of a system of equations:

$$\lg R_{UA}^{+x} = \lg R_{UA}^{0} - x\mathrm{tg}\alpha_{\mathrm{A}}, \tag{2}$$

$$\lg R_{U\mathrm{B}}^{-x} = \lg R_{U\mathrm{B}}^{0} + x\mathrm{tg}\alpha_{\mathrm{B}}, \tag{3}$$

$$d_1 = R_{UA}^{+x} + R_{U\mathrm{B}}^{-x}, \tag{4}$$

where d_1 is internuclear distance A-B.

The disadvantage of this approach is the presence of a minimum interatomic distance d_{min}, which from the standpoint of the crystal chemical approach is justified by the increase in the internuclear distance when the ionicity between the same atoms changes. However, in many cases the internuclear distances A-B in compounds and alloys are less than the value $d_{\min}$. The difficulties can be overcome only by abandoning the way of interpreting the solution of system (2)–(4) from the standpoint of the crystal chemical approach and translating system (2)–(4) into the language of quantum chemistry. It must be considered that when bonds are formed, the spherical symmetry of the electron density of atoms A and B is broken and is accompanied by a redistribution of electrons to other directions of interatomic interaction.

This condition is fulfilled if the removal (+Δ*e*) of electrons or their localization (–Δ*e*) change the values of the charges that a given pair has at $d_1 = d_{\min}$, i.e. $Z_{\text{ef}}A(B) = Z_{min}A(B) + \left(\frac{\Delta l}{2}\right)$ and are described by the system of equations:

$$d_1 = R_{UA}^{ZA} + R_{U\mathrm{B}}^{ZB}, \tag{5}$$

$$\lg R_{UA}^{ZA} = \lg R_{UA}^{0} - (Z_{\min A} + \tfrac{\Delta e}{2})\mathrm{tg}\alpha_{\mathrm{A}}, \tag{6}$$

$$\lg R_{U\mathrm{B}}^{ZB} = \lg R_{U\mathrm{B}}^{0} - \left(Z_{\min B} + \tfrac{\Delta e}{2}\right)\mathrm{tg}\alpha_{\mathrm{B}}. \tag{7}$$

Replacing *x* in the system of equations (2)–(4) by $(Z_{\min} + \frac{\Delta e}{2})$ in (5)–(7) changes the physical meaning of these equations. The function $d_1 = f(Z_{\text{ef}})$ is calculated from the standpoint of the crystal chemical approach; $(Z_A = -Z_{\mathrm{B}})$ is correct from a quantum point of view only when $d_1 = d_{\min}$, but this is enough for the system (5)–(7) to be solved for a known d_1 and the effective radii and redistribution of the electron density for all possible values of $d_1$in the compounds under consideration to be found. Thus, taking into account the quantum interpretation of the empirical material made it possible to obtain an expression for the energy of chemical bonds in the form:

$$D_{A-B}^{i} = \left(\frac{C_1\left(R_{UA}^{0} + R_{UB}^{0}\right)}{(\mathrm{tg}\,\alpha_A + \mathrm{tg}\,\alpha_B)}\right)\left(\frac{C_2 d_i}{d_i^2 - R_{UA}R_{UB}} - \frac{1}{d_i}\right), \tag{8}$$

where $R_{UA(B)}^{0}$, $\mathrm{tg}\alpha_{\mathrm{A(B)}}$ are coefficients of equations (2)–(4) for atoms A and R_{UA} and, $R_{UB}B$; are effective radii of their ions in bonds (*A*-*B*) of length d_i; i is a number of nonequivalent interatomic distances in the compounds under consideration; C_1 is a coefficient reflecting the relationship between the dimensional and energy characteristics of the interatomic interaction (measured in electron volts); C_2 is a coefficient depending on the type of crystal structure and chemical bond and chosen as dimensionless.

The given equations were used in calculations of effective charges, effective radii and dissociation energies of non-equivalent chemical bonds of ternary systems Fe-Ni-W.

The results of calculations of the coefficients of equations (2)–(4) R_U^0 and $\mathrm{tg}\alpha$ of the initial components are given in Table 1.

Table 1

Coefficients of the output component equations.

Z	Element	R_U^0(Å)	tgα
26	Fe	1.26	0.08
28	Ni	1.275	0.108
74	W	1.42	0.053

The effective charges Δq_i, effective radii $R_{U\mathrm{i}}$ and dissociation energies for nearest neighbors at different interatomic distances $d_\mathrm{i} (1 \le i \le 11)$ of structural modifications of iron are given in Table 2. The results of calculations for nickel and tungsten are given in Tables 3 and 4.

Table 2

Effective charges (Δq_i), effective radii (R_{Ui}) and dissociation energies $D(\varphi_i)$ in structural modifications of iron.

φ_i / Parameters	φ_1	φ_2	φ_3	φ_4	φ_5	φ_6	φ_7	φ_8	φ_9	φ_{10}	φ_{11}
d_i(Å)	2.5	2.6	2.7	2.8	2.9	3.0	3.1	3.2	3.3	3.4	3.5
R_{Fe} (Å)	1.25	1.3	1.35	1.4	1.45	1.5	1.55	1.6	1.65	1.7	1.75
$\Delta q_i\ (\varphi_i)$	0.00575	–0.0136	–0.030	–0.0458	–0.061	–0.0757	–0.090	–0.1038	–0.1171	–0.1301	–0.1427
$D(\varphi_i)$ (eV)	1.90907	1.8353	1.7677	1.7045	1.6458	1.5909	1.5393	1.4915	1.4463	1.4237	1.404

Table 3

Effective charges (Δq_i), effective radii (R_{Ui}) and dissociation energies $D(\varphi_i)$ in structural modifications of nickel.

φ_i / Parameters	φ_1	φ_2	φ_3	φ_4	φ_5	φ_6	φ_7	φ_8	φ_9	φ_{10}	φ_{11}
d_i(Å)	2.5	2.6	2.7	2.8	2.9	3.0	3.1	3.2	3.3	3.4	3.5
R_{Ni} (Å)	1.25	1.3	1.35	1.4	1.45	1.5	1.55	1.6	1.65	1.7	1.75
$\Delta q_i\ (\varphi_i)$	0.0796	–0.0781	–0.2298	–0.3761	–0.5172	–0.6535	–0.7854	–0.913	–1.0368	–1.1568	–1.2734
$D(\varphi_i)$ (eV)	1.574	1.5736	1.4575	1.4055	1.361	1.312	1.27	1.23	1.193	1.1574	1.1245

Table 4

Effective charges (Δq_i), effective radii (R_{Ui}) and dissociation energies $D(\varphi_i)$ in structural modifications of tungsten.

φ_i Parameters	φ_1	φ_2	φ_3	φ_4	φ_5	φ_6	φ_7	φ_8	φ_9	φ_{10}	φ_{11}
d_i(Å)	2.5	2.6	2.7	2.8	2.9	3.0	3.1	3.2	3.3	3.4	3.5
R_W (Å)	1.25	1.3	1.35	1.4	1.45	1.5	1.55	1.6	1.65	1.7	1.75
$\Delta q_i\ (\varphi_i)$	1.0449	0.7235	0.4142	0.1461	–0.1713	–0.4491	–0.7178	–0.578	–1.123	–1.4747	–1.7122
$D(\varphi_i)$ (eV)	3.5723	3.435	3.3077	3.1903	3.08	2.977	2.907	2.7909	2.706	2.6266	2.552

As for the above parameters for the compounds Fe-Ni, Fe-W, Ni-W, they are given in Tables 5, 6, 7.

Table 5

Effective charges (Δq_i), effective radii (R_{Ui}) and dissociation energies $D(\varphi_i)$ depending on interatomic distances d_i Fe-Ni.

φ_i Parameters	φ_1	φ_2	φ_3	φ_4	φ_5	φ_6	φ_7	φ_8	φ_9	φ_{10}	φ_{11}
d_i(Å)	2.5	2.6	2.7	2.8	2.9	3.0	3.1	3.2	3.3	3.4	3.5
R_{UFe} (Å)	1.24	1.28	1.34	1.39	1.44	1.49	1.54	1.59	1.64	1.69	1.74
R_{UNi} (Å)	1.26	1.32	1.36	1.41	1.46	1.51	1.56	1.61	1.66	1.71	1.76
$\Delta q_i\ (\varphi_i)$	0.0595	–0.1134	–0.2824	–0.4453	–0.6024	–0.7542	–0.901	–1.043	–1.181	–1.349	–1.445
$D(\varphi_i)$ (eV)	1.9354	1.8904	1.7887	1.728	1.6683	1.6128	1.5775	1.512	1.466	1.423	1.3826

Table 6

Effective charges (Δq_i), effective radii (R_{Ui}) and dissociation energies $D(\varphi_i)$ depending on interatomic distances d_i Fe-W.

φ_i Parameters	φ_1	φ_2	φ_3	φ_4	φ_5	φ_6	φ_7	φ_8	φ_9	φ_{10}	φ_{11}
d_i(Å)	2.5	2.6	2.7	2.8	2.9	3.0	3.1	3.2	3.3	3.4	3.5
R_{UFe} (Å)	1.175	1.222	1.27	1.32	1.36	1.41	1.44	1.50	1.55	1.6	1.645
R_{UW} (Å)	1.325	1.378	1.43	1.48	1.54	1.59	1.66	1.70	1.75	1.8	1.855
Δq_i (φ_i)	0.4736	0.2064	−0.0506	−0.2984	−0.5374	−0.7683	−0.9916	−1.2079	−1.4176	−1.6208	−1.8183
$D(\varphi_i)$ (eV)	2.6738	2.5712	2.4877	2.3884	2.3161	2.2283	2.1715	2.0881	2.019	1.9664	1.909

Table 7

Effective charges (Δq_i), effective radii (R_{Ui}) and dissociation energiesD (φ_i) depending on interatomic distances d_i Ni-W.

φ_i Parameters	φ_1	φ_2	φ_3	φ_4	φ_5	φ_6	φ_7	φ_8	φ_9	φ_{10}	φ_{11}
d_i(Å)	2.5	2.6	2.7	2.8	2.9	3.0	3.1	3.2	3.3	3.4	3.5
R_{UNi} (Å)	1.18	1.23	1.26	1.325	1.372	1.42	1.47	1.51	1.561	1.6	1.65
R_{UW} (Å)	1.32	1.37	1.44	1.475	1.528	1.58	1.63	1.69	1.739	1.8	1.85
Δq_i (φ_i)	0.4587	0.2192	−0.0113	−0.2334	−0.4478	−0.6548	−0.8551	−1.049	−1.237	−1.4193	−1.596
$D(\varphi_i)$ (eV)	3.5435	3.4083	3.2753	3.165	3.0514	2.9542	2.8857	2.7666	2.683	2.6068	2.5331

In the given Tables, the values of the coefficients C_1 and C_2 in the calculations in the first approximation are chosen to be equal to unity.

Conclusions

As follows from the results obtained in the paper, shown in Figure 1 and in Tables (1)–(7), the use of a comprehensive approach ensured systematizing and summarizing the available empirical and theoretical material on the physicochemical properties of the initial components, information on the phase diagrams of the binary systems Fe-Ni, Fe-W and Ni-W, and also, considering statistical and quantum-chemical regularities, building theoretical models to describe the ordering processes in alloys of Fe-Ni-W based ternary systems

Such an approach made it possible to describe the processes of formation of interatomic interaction at different technological levels from the standpoint of chemical bonding. In order to track various possible options for the formation, destruction and dynamics of formation of different types of chemical bonds in the system under study, calculations of chemical bond parameters were carried out in the paper depending on the interatomic distances: $2.5\ \text{Å} \le d_i \le 3.5\ \text{Å}$.

This enabled establishing the limits of the appearance of the donor effect (change in the sign of the electron density depending on certain distances). Thus, for Fe, Ni, W, as well as for binary compounds based on them, this occurred within the limits of: Fe $(2.5\ \text{Å} \le d_i \le 2.6\ \text{Å})$; Ni $(2.5\ \text{Å} \le d_i \le 2.6\ \text{Å})$; W $(2.8\ \text{Å} \le d_i \le 2.9\ \text{Å})$; Fe-Ni $(2.5\ \text{Å} \le d_i \le 2.6\ \text{Å})$; Fe-W $(2.6\ \text{Å} \le d_i \le 2.7\ \text{Å})$; Ni-W $(2.5\ \text{Å} \le d_i \le 2.7\ \text{Å})$.

The results thus obtained confirm the experimentally established fact that the initial elements Fe, Ni, W can have different oxidation states, and in compounds the oxidation state can take values from – 3 to + 5.

The calculations of the chemical bond parameters allowed confirming the fine structure of the chemical bond, determinig the hysteresis patterns of both individual elements (for example, in iron) and in intermetallics of intermediate compounds of the initial elements.

The results in question can be used to create antidiffusion barrier layers from Fe, Ni, W and binary compounds based on them to suppress interdiffusion in compounds with traditional contact compounds based on Cu, Pb, Sn.

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Submitted: 21.05.2025

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Теоретичні моделі антидифузійних шарів потрійних систем Fe-Ni-W в термоелектричних перетворювачах енергії

Розроблено теоретичні моделі та проведені розрахунки параметрів хімічного зв'язку перспективних антидифузійних шарів на основі потрійних систем Fe-Ni-W. Представлено розрахунки ефективних радіусів міжатомної взаємодії, перерозподілу електронної густини та енергії нееквівалентних хімічних зв'язків Fe-Ni, Fe-W, Ni-W в системі Fe-Ni-W в залежності від міжатомних відстаней.

Ключові слова: термоелектричні матеріали, антидифузійні шари, теоретичні моделі, хімічний зв'язок, квантові закономірності ефективні радіуси, енергія дисоціації, діаграми стану, нееквівалентні хімічні зв'язки.

Надійшла до редакції 21.05.2025