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Influence of Element Concentration on Kinetic and Dynamic Properties of High-Entropy Solid Solutions

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Previously obtained calculation data on the dependence of dynamic characteristics (lattice parameter (a) and Debye temperature Θ_D) and experimental data on kinetic characteristics (resistivity ρ and mean free path of electrons λ) on the concentration of elements in high-entropy alloys (HEAs) were generalized. In the first case, calculations were carried out for bulk solid solutions with an FCC lattice based on Cu, Co, Ni, Fe, Cr, Al, or Ti atoms; in the second case, on the basis of experimental data.

A correlation was established between Θ_D and a, and between ρ and λ^{-1} in four- and five-component solid solutions, in which Al and Ti atoms are absent. The reason for the unsatisfactory correlation in the presence of Al and Ti atoms is explained by the relatively large value of the parameter δ – the difference in atomic radii (5.2–7.1%) in solid solutions containing Al and Ti atoms. The individual parameter δ_i has an even larger value: 10.3% (Al) or 12.0–15.4% (Ti). Relatively large values of δ and δ_i can cause deformation of the solid-solution lattice, which manifests itself in the absence of correlation between Θ_D and a, as well as between ρ and λ^{-1}.

Keywords: High-entropy alloys, Solid solutions, Lattice parameter, Debye temperature, Resistivity, Mean free path, Thin films, Correlation, Atomic radius difference parameter.

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Introduction

At the moment, in the study of the properties of high-entropy alloys (HEAs), one of the varieties of which is solid solutions (s.s.), significant experimental material has been accumulated regarding the physical, mechanical and magnetic properties of multicomponent metal coatings in the form of HEAs or their nitrides. In our work, we analyze the effect of the concentration of paramagnetic and magnetic components on the electrophysical properties of films [1–3] and the dynamic characteristics (lattice parameter and Debye temperature) of bulk solid solutions [4–6].

The cited works addressed issues related to the formation of the phase composition without secondary phases; electrophysical studies (resistivity, temperature coefficient of resistance, gauge factor) and magnetoresistive properties (normal and anisotropic magnetoresistance) as a function of the concentration of doping atoms. This opens up potential opportunities for producing sensitive elements for functional electronics devices with predictable characteristics, as well as promising applications of HEAs in aerospace, energy, and instrumentation industries.

The aim of our study is to generalize previously obtained [1–6] experimental data for individual components (resistivity ρ and mean free path of electrons (MFPE) – λ) and calculated results for bulk metals (Debye temperature – Θ_D and lattice parameter – a) from the point of view of the influence of the concentration (atomic fraction) of individual HEA components on the mentioned properties and characteristics.

In the equiatomic approximation, data were analyzed for HEAs in which: four-component solid solutions were formed based on Cu, Co, Ni, and Fe; five-component ones were based on these four elements with the addition of Cr or Al; six-component alloys, in which the sixth component was either HCP-Ti atoms or virtual FCC-Ti atoms. In the latter case, the parameters a_{FCC} and atomic radius r of Ti were calculated using the relationships $a_{FCC} = \sqrt{2} \cdot a_{HCP}$

and $4r = \sqrt{2}\, a_{FCC}$.

I. Working Relationships, Methodology of Calculations

The calculation of the lattice parameter, Debye temperature, resistivity, and mean free path for high-entropy solid solutions was carried out on the basis of relationships presented in our previous works [3–6], which, in accordance with the principle of additivity, are written as follows:

$$a = \frac{1-x}{n-1}\sum_{i=1}^{n-1} a_i \; + \; x\, a_n \; ;$$

$$\theta_D = \frac{1-x}{n-1}\sum_{i=1}^{n-1} \theta_{Di} \; + \; x\, \theta_{Dn}; \qquad (1)$$

$$\rho = \frac{1-x}{n-1}\sum_{i=1}^{n-1} \rho_i \; + \; x\, \rho_n + \rho_r$$

and

$$\lambda^{-1} = \frac{1-x}{n-1}\sum_{i=1}^{n-1} \lambda_{\mathrm{i}}^{-1} \; + \; x\, \lambda_n^{-1}$$

where the multiplier $\frac{1-x}{n-1}$ denotes the equiatomic composition of the phase-forming system of elements; n – the number of components; i– the index of the doping element; x – atomic fraction; ρ_r – residual resistivity, which satisfies the condition $\rho_r \ll \rho$.

We proceed from the assumption that the principle of additivity can be applied when calculating the magnitudes of properties or characteristics of high-entropy solid solutions if, for each component, the property or characteristic is not collective in nature but an individual one. These may include atomic sizes, mass, magnetic moment; Debye temperature; relative change of resistivity upon annealing or deformation.

It should be noted that resistivity ρ itself is not a strictly individual characteristic. However, since

$$\rho = \frac{\mathrm{A}}{N\lambda}, \qquad (2)$$

where A is a certain constant; N is the concentration of conduction electrons, then the value λ^{-1} can be considered conditionally as an intrinsic characteristic, although it is more correct to consider the value $(N\lambda)^{-1}$as such.

In Section II, we will attempt to establish correlations between the ρ i (λ^{-1}), which will serve as confirmation or refutation of the considerations given above.

It is very important to emphasize the following. The concentration dependences of ρ and λ were calculated for HEA thin films, while those of a and Θ_D were calculated for bulk alloys. For this purpose, we used our extensive experimental data on the properties of single-component films with a thickness of 50–70 nm (see [1,3,5] and references therein). As for the values of λ in single-component films, they were obtained after processing experimental dimensional and temperature dependences of ρ within the theoretical models of Tellier, Tosse, and Pishar (see details in [7]).

In the case of concentration dependences of a and Θ_D, we used tabulated data [8,9]. It should be noted that experimental data for films could also be used in this case, since the difference $\Delta a = a_f - a_0$ (index "0" denotes bulk single-component samples) is negligible, about 0.001–0.003 nm. At the same time, the value of ρ_f in films is larger ρ_0 by an order of magnitude, while for λ and λ_0 this difference is even more significant. With regard to Θ_D, it can only be stated that it differs noticeably between films and bulk single-component metals, but such data for single-component films, which could be used, are absent in the literature.

II. Results of Calculations and Their Discussion

2.1. Lattice Parameter and Debye Temperature

Using relations (1), calculations were carried out for the dependence of the lattice parameter (Table 1) and the Debye temperature (Table 2) on the concentration x of the doping n-th element, where each HEA component was alternately considered as a dopant. The right columns of these tables present extrapolated data for dependencies $a(x)$ and $\Theta_D(x)$ given in [6], which are not related to HEAs but correspond to the stability region of multicomponent alloys (MCAs).

Several features of the concentration dependences of a can be noted. In the case of a four-component HEA, the maximum lattice parameter a = 0.350 nm and the minimum a = 0.334 nm (highlighted in Table 1) are realized at x = 0.10 when the dopant is Fe or Cu.

For a five-component HEA, the minimum and maximum values of a occur at x = 0.30 and x = 0.10, respectively. For a six-component HEA, the smallest value a = 0.320 nm is observed at x = 0.10 (dopant Cu), and the largest a = 0.326 nm at x = 0.10 (dopant Fe or Cr).

Thus, by changing the number of components and the concentration of the dopant, HEAs can be obtained whose lattice parameters vary within $\Delta a \approx 0.04$ nm. In our opinion, such changes in the lattice parameter affect the gauge factor of HEA films, as we described in [1].

In Table 2, the results of calculations of Θ_D as a function of the atomic fraction x of the dopant element are presented. It is noteworthy that Θ_D varies within the following ranges: $\Delta\Theta_D$ = 25 K (n = 4), 50 K (n = 5), and 24 K (n = 6). This opens the possibility of influencing the temperature dependence of the heat capacity of HEAs.

A comparison of Tables 1 and 2 shows that there exists a correlation between Θ_D and a, the essence of which is the following.

Since

$$\theta_D = \frac{\hbar\, \omega_{max}}{k} \sim \frac{1}{\lambda_{min}}$$

(where $\hbar$ – Dirac's constant; k is Boltzmann's constant; $\lambda_{min} = 2a_{min}$ is the minimal phonon wavelength), the maximum lattice parameter corresponds to the minimum value of Θ_D, and vice versa (the corresponding values are marked in Tables 1 and 2). It should be noted that in the case of five- and six-component alloys, when Al (n = 5) and Ti (n = 6) are added to the classical group of elements Cu, Co, Ni, and Fe, only a conditional correlation can be observed. This suggests that Al and HCP-Ti or virtual

FCC-Ti atoms do not fully satisfy the third criterion for HEA formation — the difference in atomic radius δ should not exceed 6.6% [10] or 8.5% [11] (other values in the range δ = (6.7 -7.3) % [12,13], are also found in the literature, depending on element concentrations).

In the equiatomic approximation, we calculated δ according to the relation:

$$\delta = \sqrt{\sum_{i=1}^{n} c_i (1 - {}^{r_i}/_{\bar{r}})^2} \ , \qquad (3)$$

Table 1.

Influence of concentration (atomic fraction) *x* doping elements (DE) on the lattice parameter (nm) of four-, five-, and six-component alloys

x \ DE	Cu	Co	Ni	Fe	Cr \ Al	Ti^{FCC} \ Ti^{HCP}	Cu	Co	Ni	Fe	Cr \ Al	Ti^{FCC} \ Ti^{HCP}
Calculations of the HEA lattice parameter, nm							Extrapolation of the MCA lattice parameter, nm					
0.00	0.328	0.330	0.331	0.353	-	-	-	-	-	-	-	-
0.10	**0.334**	0.336	0.336	**0.350**	-	-	-	-	-	-	-	-
0.15	0.338	0.337	0.337	0.346	-	-	-	-	-	-	-	-
0.20	0.339	0.338	0.338	0.342	-	-	-	-	-	-	-	-
0.30	0.340	0.340	0.340	0.335	-	-	-	-	-	-	-	-
0.40	-	-	-	-	-	-	0.344	0.342	0.341	0.327	-	-
0.50	-	-	-	-	-	-	0.347	0.344	0.349	0.321	-	-
0.60	-	-	-	-	-	-	0.349	0.345	0.344	0.313	-	-
0.00	0.349	0.351	0.352	0.368	0.339 / -	-	-	-	-	-	-	-
0.10	0.351	0.352	0.352	**0.360**	**0.345** / -	-	-	-	-	-	-	-
0.15	0.351	0.352	0.352	0.356	0.349 / -	-	-	-	-	-	-	-
0.20	0.352	0.352	0.352	0.352	0.352 / -	-	-	-	-	-	-	-
0.30	0.353	0.352	0.352	**0.344**	**0.359** / -	-	-	-	-	-	-	-
0.40	-	-	-	-	-	-	0.353	0.352	0.350	0.332	0.364 / -	-
0.50	-	-	-	-	-	-	0.355	0.353	0.352	0.328	0.368 / -	-
0.60	-	-	-	-	-	-	0.357	0.353	0.352	0.319	0.377 / -	-
0.00	0.340	0.341	0.342	0.355	- / 0.354	0.329 / -	-	-	-	-	-	-
0.10	0.342	0.343	0.344	**0.348**	- / 0.345	**0.338** / -	-	-	-	-	-	-
0.15	0.343	0.343	0.344	0.345	- / 0.344	0.342 / -	-	-	-	-	-	-
0.20	0.344	0.344	0.343	0.341	- / 0.342	0.345 / -	-	-	-	-	-	-
0.50	-	-	-	-	-	-	0.351	0.346	0.346	0.320	- / 0.321	0.372 / -
0.60	-	-	-	-	-	-	0.354	0.348	0.347	0.313	- / 0.314	0.382 / -
0.00	0.315	0.317	0.317	0.330	- / 0.330	- / 0.329	-	-	-	-	-	-
0.10	**0.320**	0.321	0.321	**0.326**	- / **0.326**	- / 0.325	-	-	-	-	-	-
0.15	0.322	0.322	0.323	0.324	- / 0.324	- / 0.324	-	-	-	-	-	-
0.20	0.325	0.324	0.324	0.322	- / 0.322	- / 0.322	-	-	-	-	-	-
0.50	-	-	-	-	-	-	0.338	0.336	0.334	0.307	- / 0.308	- / 0.310
0.60	-	-	-	-	-	-	0.342	0.339	0.337	0.303	- / 0.305	- / 0.308

where $\bar{r}$ is the average atomic radius.

The results are: δ = 1.05 % (HEA – CuCoNiFe); 5.2% (CuCoNiFeAl); 5.4% (CuCoNiFeCr HCP-Ti) and 7.1% (CuCoNiFeCr FCC-Ti).

These data confirm that Al and Ti atoms do not fully meet the requirements of the third HEA formation criterion. Additionally, we propose considering the parameter δ_i – the individual difference of atomic radius of components:

$$\delta_i = \frac{\bar{r}-r_i}{\bar{r}}. \qquad (3')$$

For the HEAs analyzed, the following values were obtained δ_i for four-component HEA: -1.6% (Cu), 0.8% (Co,Ni) and -0.8% (Fe); five-component HEA: 1.2% (Cu), 3.5% (Co,Ni), 2.0% (Fe) and -10.3% (Al); six-component HEA: -4.1% (Cu), -1.6% (Co,Ni), -3.3% (Fe), -5.7% (Cr) and 15,4% (atomic FCC-Ti); six-component

Table 2.

Influence of concentration *x* of doping elements on the Debye temperature (K) of four-, five-, and six-component alloys

DE / *x*	Cu	Co	Ni	Fe	Al / Cr	Ti^{HCP}	Cu	Co	Ni	Fe	Al / Cr	Ti^{HCP}
Calculations of the HEA Debye temperature, K							Extrapolation of the MCA Debye temperature,K					
0.00	435	419	393	392	-	-	-	-	-	-	-	-
0.10	**429**	420	404	**404**	-	-	-	-	-	-	-	-
0.15	424	418	407	407	-	-	-	-	-	-	-	-
0.20	419	416	411	410	-	-	-	-	-	-	-	-
0.30	409	412	412	417	-	-	-	-	-	-	-	-
0.40	-	-	-	-	-	-	398	408	421	422	-	-
0.50	-	-	-	-	-	-	387	405	430	431	-	-
0.60	-	-	-	-	-	-	378	401	439	440	-	-
0.00	495	484	464	463	414 / -	-	-	-	-	-	-	-
0.10	479	474	464	463	**439** / -	-	-	-	-	-	-	-
0.15	472	469	464	464	451 / -	-	-	-	-	-	-	-
0.20	464	464	464	463	464 / -	-	-	-	-	-	-	-
0.30	449	454	464	464	**489** / -	-	-	-	-	-	-	-
0.40	-	-	-	-	-	-	430	448	464	464	508 / -	-
0.50	-	-	-	-	-	-	417	438	465	465	530 / -	-
0.60	-	-	-	-	-	-	400	425	465	466	565 / -	-
0.00	472	463	447	446	- / 414	457	-	-	-	-	-	-
0.10	**459**	455	448	448	- / **435**	453	-	-	-	-	-	-
0.15	452	451	450	449	- / 447	451	-	-	-	-	-	-
0.20	445	447	450	450	- / 457	448	-	-	-	-	-	-
0.40	-	-	-	-	-	-	418	430	454	454	- / 501	435
0.50	-	-	-	-	-	-	403	422	456	457	- / 520	430
0.60	-	-	-	-	-	-	380	413	460	461	- / 542	417

HEA: 7.7% (Cu), 3.8% (Co,Ni), 2.3% (Fe), 0.8% (Cr) and -12.0% (atomic HCP-Ti).

This confirms the conclusion that Al and Ti components do not fully satisfy the third HEA formation criterion. Large δ_i values can be the cause of significant lattice microstresses and deformation of the phonon spectrum.

2.2. Resistivity and Mean Free Path

Figure 1 and Tables 3 and 4 present the dependences of resistivity $\rho(x)$ and mean free path $\lambda(x)$, calculated according to relation (1) for ρ and λ^{-1}. As noted in Section I, the values of ρ and λ at $x = 0$ for individual components correspond to experimental data for single-component films, while all other calculated data refer to HEAs. Although we compare only ρ and λ (since no data on the carrier concentration N are available), it can be stated that the largest (or smallest) values of ρ correspond to the smallest (or largest) values of λ, i.e., a correlation between $\rho \sim \lambda^{-1}$ exists.

Furthermore, a comparative analysis of the data in Tables 3 and 4 indicates a tendency for resistivity to increase when the mean free path decreases, and vice versa. Additionally, it should be noted that resistivity

Table 3.

Dependence of resistivity (Ohm·m) on the concentration of the doping element in four- and five-component HEAs based on Cr, Ni, Co, Fe, and Cu atoms.

DE / x	Cr	Ni	Co	Fe	Cu	Remark
0.00	5.50	5.15	4.00	3.35	-	The factor 10^{-7} Ohm·m around the value of the resistivity is omitted.
0.05	**5.40**	5.15	4.15	**3.65**	-	
0.10	5.20	4.95	4.25	3.80	-	
0.15	4.95	4.80	4.25	4.00	-	
0.20	4.62	4.60	4.30	4.25	-	
0.23	4.40	4.40	4.40	4.40	-	
0.00	4.85	4.65	3.75	3.00	4.55	
0.05	**4.60**	4.40	3.75	**3.40**	4.35	
0.10	4.45	4.35	3.95	3.70	4.30	
0.15	4.35	4.30	4.07	3.95	4.25	
0.20	4.23	4.23	4.23	4.25	4.23	

Table 4.

Dependence of the mean free path (nm) on the concentration of the doping element in four- and five-component HEAs based on Cr, Ni, Co, Fe, and Cu atoms.

DE / x	Cr	Ni	Co	Fe	Cu	Cr	Ni	Co	Fe	Cu
0.00	37.1	41.8	42.0	40.3	-	35.1	39.5	40.0	39.0	38.0
0.05	**37.5**	**42.4**	41.8	40.4		**35.8**	38.2	39.3	**38.5**	37.4
0.10	37.8	41.3	40.8	40.0	-	36.9	38.8	39.3	38.5	38.1
0.15	39.0	41.2	40.5	40.3	-	38.0	38.9	39.6	39.0	39.4
0.20	40.1	41.3	41.2	40.8	-	38.6	39.8	38.5	38.6	38.4
0.21	-	-	-		-	38.7	38.8	38.8	38.7	38.7
0.25	41.1	41.0	41.0	41.0	-	-	-	-	-	-

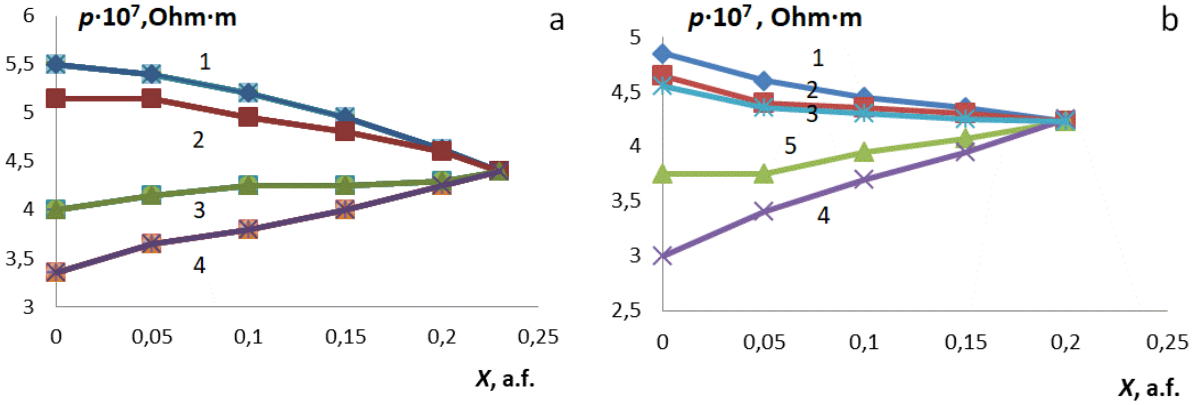

Fig. 1. Dependence $\rho(x)$ for four-component HEA
(a): $(FeCoNi)_{1-x} - Cr_x$ (1); $(FeCoCr)_{1-x} - Ni_x$ (2); $(FeNiCr)_{1-x} - Co_x$ (3) та $(CoNiCr)_{1-x} - Fe_x$ (4) and for five-component HEA
(b): $(FeCoNiCu)_{1-x} - Cr_x$ (1); $(FeCoCrCu)_{1-x} - Ni_x$ (2); $(FeCoNiCr)_{1-x} - Cu_x$ (3); $(FeNiCrCu)_{1-x} - Co_x$ (4) and $(CoNiCrCu)_{1-x} - Fe_x$ (5).

growth is observed when Co and Fe act as dopant elements, which correlates with the magnitude of the average atomic magnetic moment (μ) of the HEA.

Although in the case of Ni atoms both $\rho(x)$ and $\lambda(x)$ dependencies do not exhibit a clearly pronounced trend (they appear "smeared"), it can still be stated that they show partial correlation.

Our corresponding calculations indicate that the value of μ (in units of Bohr magneton) changes with increasing x from 0 to 0.20 in the following intervals: 1.135 – 0.908 (dopant elements Cu і Cr); 0.984 -0.912 (Co) та 0.580 – 0.908 (Fe). The change of resistivity $\rho(x)$ in accordance with the change of $\bar{\mu}$ is associated not only with electron–phonon interaction but also with spin–orbit interaction.

Conclusions

Generalized previously obtained calculation results (for lattice parameter and Debye temperature) and experimental data (resistivity and mean free path of electrons) for four- to six-component high-entropy alloys in the form of FCC solid solutions allow us to draw the following conclusions:

A correlation exists between Debye temperature Θ_D and lattice parameter a, which is determined by the individuality of these dynamic characteristics, for which the principle of additivity holds.

This correlation is realized more clearly in HEAs based on Cu, Co, Ni, Fe, and Cr, and to a lesser extent in alloys where the fifth or sixth component is Al or Ti.

The weaker correlation Θ_D і a is explained by relatively large values of the parameter δ (atomic radius difference) for the HEA as a whole: 5.2-7.1% with doping elements Al and Ti atoms; and individual parameter δ_i values of: 10.3 % (doping elements Al) end (12.0-15.4)% (Ti).

Relatively large δ and δ_i values can cause deformation of the lattice and the phonon spectrum, which in turn results in the absence of correlation between Θ_D and a.

Al and Ti atoms, as HEA components, may also influence the correlation between resistivity and mean free path of electrons (MFPE), since phonon spectrum deformation leads to reduction MFPE and corresponding increase values $\rho(x)$.

In addition to electron–phonon interaction $\rho(x)$ is strongly dependent on the spin–orbit interaction of conduction electrons, which is particularly effective in the presence of magnetic components.

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Вплив концентрації елементів на кінетичні та динамічні властивості високоентропійних твердих розчинів

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Здійснено узагальнення раніше отриманих розрахункових даних стосовно залежності динамічних (параметр решітки (a) та температура Дебая Θ_D) та експериментальних даних стосовно кінетичних характеристик (питомий опір (ρ) та середня довжина вільного пробігу електронів (λ)) від концентрації елементів у високоентропійних сплавах. У першому випадку розрахунок проводився на прикладі масивних т.р. із ГЦК решіткою на основі атомів Cu,Co,Ni,Fe,Cr, Al або Ti, а у другому випадку – на основі експериментальних даних для плівкових високоентропійних т.р. на основі тих же елементів за виключенням Al і Ti. У обох випадках розрахунки здійснювалися у еквіатомному наближенні для чотири-шести компонентних т.р. Була встановлена кореляція між Θ_D і a та ρ і λ^{-1} у чотири- п'яти компонентних т.р., в яких відсутні атоми Al і Ti. Причину незадовільної кореляції при наявності атомів Al і Ti ми пояснюємо відносно великим значенням параметра δ – різниця атомних радіусів (5,2 – 7,1%) у т.р. із атомам Al і Ti. Індивідуальний параметр δ_i має ще більше значення: 10,3% (Al) або 12,0-15,4% (Ti). Відносно великі значення δ та δ_i можуть обумовити деформацію решітки т.р., що проявиться у відсутності кореляції Θ_D і a та ρ і λ^{-1}.

Ключові слова: Високоентропійні сплави, Тверді розчини, Параметр решітки, Температура Дебая, Питомий опір, Середня довжина вільного пробігу, Плівка, Кореляція, Параметр різниці атомних радіусів.