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On the Possibility of Applying the Principle of Physical Quantities Additivity of Multicomponent Metallic Materials

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In the phenomenological approach, the problem of the possibility of applying the additivity principle to the calculation of physical quantities or characteristics of multicomponent solid metal solutions, including high-entropy ones, is analyzed. These values and characteristics include the lattice parameter and the Debye temperature, since they can be considered indirectly through the radius and mass of an atom as their own, rather than collective, characteristics of individual components, such as, for example, the magnetic moment of an atom, magnetization, heat capacity. It is proposed to consider the relative change in resistance when measuring the thermal coefficient of resistance or the strain coefficient as conditionally individual characteristics of individual components. At the same time, applying the principle of additivity to collective quantities or characteristics (melting temperature, Fermi energy, mean free path of electrons) can give very approximate values.

Keywords: Multicomponent materials, High-entropy alloys, Solid Solution, Individual values and characteristics, Collective values and characteristics, Principle (rule) of additivity.

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1. INTRODUCTION

In previous works [1-3], we made an attempt to predict some physical quantities of multicomponent materials in the form of solid solutions (s.s), including and high-entropy (HEA). The methodological basis of such a forecast is the concept (principle) of additivity of physical quantities. The essence of the concept can be illustrated by the following ratios:

$$\overline{\varepsilon_d} = \sum_{i=1}^{n} c_i \cdot \varepsilon_{di}, \quad (1)$$

where $\overline{\varepsilon_d}$ is the average value of the energy level of d-orbital; c_i – the atomic fraction of component i in the alloy; ε_{di} – the d- orbital energy level of element i [4];

$$\overline{T_m} = \sum_{i=1}^{n} c_i \cdot T_{mi}, \quad (2)$$

where $\overline{T_m}$ is the average melting temperature of the alloy; T_{mi} is melting point i components [5,6].

In works [1-3] is presented a large array of calculation data for resistivity – ρ; thermal resistance coefficient (TCR) – β_T; longitudinal strain coefficient – γ_l; lattice parameter s.s. – a; Debye temperature – Θ_D; melting point s.s. – T_m and others. Some of them (a, ρ, TCR and γ_l) quantitatively agree with our experimental data for film HEA.

Since agreement can be expected in the case of the lattice parameter and TCR, we set ourselves the task of analyzing the question of in which cases the principle of additivity can claim accuracy and the principle possibility of its application in the calculation of physical quantities of multicomponent alloys.

2. INDIVIDUAL OR COLLECTIVE CHARACTERISTICS OF ATOMS AND ELECTRONS

By individual characteristics, we mean those that do not change (or change to an insignificant extent, as in the case of $\overline{\varepsilon_d}$ [4], when an isolated electron or atom falls into the s.s. crystal lattice with its internal potential.

Such characteristics include the atoms size (then the parameter a will act as its own characteristic); the mass of an atom (the Debye frequency as a function of the mass of an atom can be considered its own characteristic); magnetic moment of an electron (μ). In this case, the additivity principle of physical quantities can be written in the form of ratios [7]:

$$\Theta_D^{s.s.} = \sum_{l=1}^{n} c_i \Theta_{Di}, \; a_{s.s.} = \sum_{l=1}^{n} c_i \, a_i$$

$$\overline{\mu_{s.s.}} = \sum_{i=1}^{n} c_i \; \mu_i \quad (3)$$

$$\text{and} \quad \overrightarrow{M_{s.s.}} = \sum_{i=1}^{n} c_i \, \overrightarrow{\mu_i};$$

where $\overrightarrow{M}$ is magnetization vector.

Note that the relations given in (1) and (2), as well as in (3), were "constructed" by analogy with Vegard's rule for a two-component s.s.:

$$a = c_1 \cdot a_1 + c_2 \cdot a_2.$$

Regarding the possibility of applying the principle of additivity to other physical quantities (ρ, β_T, γ_l, T_m, Fermi energy – ε_F, mean free path of electrons – λ_0), some doubts arise and require additional analysis.

In the case of resistivity ρ, which is a collective characteristic of s.s., the principle of additivity can most likely be applied when the Fermi surfaces of individual components differ little from the Fermi surface of s.s. Note that this is a very partial case that does not apply to the general case of multicomponent s.s.

Since the resistivity can be represented as

$$\rho = \frac{A}{\lambda_0 \, n} \quad \text{and} \quad \lambda_0 = \frac{A}{\rho \, n},$$

where n is concentration of free electrons; A is some constant, then λ_0 also cannot act as a characteristic of electrons, i.e ρ and λ_0 is non-additive property and characteristic. The situation is somewhat different in the case β_T and γ_l, since they are expressed through derivatives with respect to temperature or longitudinal deformation:

$$\beta_T = \frac{d\ ln\rho}{dT} \text{ and } \gamma_l = \frac{d\ lnR}{d\ lnl} = \frac{d\ ln\rho}{d\ lnl} + 1 + 2\mu_f, \quad (4)$$

where R is the sample resistance; $d\ lnl = \frac{dl}{l} = d\varepsilon_l$ is longitudinal deformation; μ_f is Poisson's ratio. Multiplier $d\ ln\rho = \left(\frac{d\rho}{\rho_{(T)}}\right)$ and $\left(\frac{d\rho}{\rho_{(\varepsilon_l)}}\right)$ in ratios for β_T and γ_l can be considered to some extent as the own characteristics of individual components. At the same time, T_m and ε_F act as collective (non-additive) characteristics, since melting s.s. occurs when bonds between atoms are broken i and k component, which will be less affected by energy bonds between atoms of the same type. The Fermi energy can also be only a collective characteristic, the value of which will be completely determined by the internal potential of the s.s.

3. CONCLUSIONS

Qualitative analysis makes it possible to draw conclusions regarding a fairly accurate or approximate prediction of the properties of multicomponent metallic s.s. The prediction can claim to be sufficiently accurate if we are talking about the intrinsic characteristics of the atoms, which almost do not differ in free or s.s. atoms. This, first of all, is about the size of atoms, their mass, magnetic moment. We come to the conclusion that the relative change in resistivity in thermal or deformation processes can be considered a conditionally characteristic characteristic, although the resistivity itself is a collective characteristic of s.s. and

$$\rho_{s.s.} = \sum_{i=1}^{n} c_i\ \rho_i\ , \quad (5)$$

most likely not legitimate. In our opinion, the self-diffusion coefficient of atoms in the case can be attributed to the conditionally proper characteristic of atoms HEA.

With regard to the forecast for T_m, λ_0 and ε_F, then it will have a very approximate character, since all three quantities have a collective character, as in the case of equation (5).

Finally, we note the following. Ratio (1) includes the characteristic of atoms ε_d, although, in our opinion, $\overline{\varepsilon_d}$ cannot be a collective characteristic and cannot be a physical quantity or characteristic s.s., because, to a large extent, it has no physical content (such as, for example, the average temperature of patients in a hospital).

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Про можливість застосування принципу адитивності фізичних величин багатокомпонентних металевих матеріалів

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У феноменологічному наближенні проаналізоване питання про можливість застосування принципу адитивності для розрахунків фізичних величин або характеристик багатокомпонентних твердих металевих розчинів, в тому числі і високоентропійних. До цих величин і характеристик можна віднести параметр гратки і температуру Дебая, оскільки вони опосередковано через радіус і масу атома можуть розглядатися як власні, а не колективні характеристики окремих компонентів як і, наприклад, магнітний момент атома, намагніченість, теплоємність. Запропоновано розглядати відносну зміну опору при вимірюванні термічного коефіцієнту опору або коефіцієнту тензочутливості як умовно індивідуальні характеристики окремих компонентів. У той же час застосування принципу адитивності до колективних величин чи характеристик (температура плавлення, енергія Фермі, середня довжина вільного пробігу електронів) може давати дуже наближені значення.

Ключові слова: Багатокомпонентні матеріали, Високоентропійні сплави, Тверді розчини, Власні величини і характеристики, Колективні величини і характеристики, Принцип (правило) адитивності.