



Condensed Matter and Interphases

Kondensirovannyye Sredy i Mezhfaznye Granitsy
<https://journals.vsu.ru/kcmf/>

Original articles

Research article

<https://doi.org/10.17308/kcmf.2023.25/11265>

Heat capacities and thermal expansion coefficients of iron triad metals

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Abstract

One of the complex problems relating to the thermodynamics of a substance is creating an adequate description of its thermal properties. For example, the Einstein and Debye models (as well as in various modifications of these models) the heat capacity is calculated only when mechanical vibrations of the lattice are taken into account. This leads to the impossibility of describing the increase in heat capacity with increasing temperature for most substances, including iron triad metals. In addition, there is not a single theoretical construction capable of calculating the temperature dependences of the heat capacity and thermal expansion coefficient during polymorphic transformations and structural, magnetic and other phase transitions in the system. They appear on the charts in the form of final jumps, peaks and holes. As a result, there is a need to develop a new approach to the calculation of thermal characteristics. It should take into account the occurrence of local equilibrium in small areas in initially non-equilibrium metal samples for research. The nonequilibrium of a sample can be caused by the presence of impurity atoms, defects, volatile components in it, residual stresses, the occurrence of irreversible processes, etc. For the analytical description of arrays of measured values, experimenters use different exponential expressions in different temperature intervals, sometimes with negative powers. Such theoretical and experimental approaches cannot be considered satisfactory. Therefore, for the creation of the new model, it is necessary to choose such values that would be sensitive to changes in the state of the system. Within the framework of the proposed model of a two-phase locally equilibrium region, such quantities are the absolute temperature of the system, the order parameter in the form of the difference in volume fractions of coexisting ideal phases, the phase composition of the ordering phase, and its derivative with respect to temperature. The developed model allows to calculate the temperature dependences of the heat capacities and coefficients of thermal linear expansion of the iron triad metals (Fe, Co, Ni) with a change in the aggregation state (crystal - liquid), the presence of structural, magnetic and other phase transitions.

It has been shown that the used expressions adequately describe the experimental data in a wide temperature range, and also allow to extend the plotted curves to experimentally unexplored regions. A possible structural transition in cobalt at a temperature of about 1600 K, the existence of which requires additional experiments, was established. The obtained expressions are distinguished by their simplicity and universality of applicability; they can be used to create an automatic calculation of the thermophysical properties of not only iron triad metals, but also other solid substances.

Keywords: Thermodynamic model, Order parameter, Structural rearrangement, Polymorphic transformations, Transition metal

For citation: Terekhov S. V. Heat capacities and thermal expansion coefficients of iron triad metals. *Condensed Matter and Interphases*. 2023;25(1): 406–414. <https://doi.org/10.17308/kcmf.2023.25/11265>

Для цитирования: Терехов С. В. Теплоемкости и коэффициенты теплового расширения металлов триады железа. *Конденсированные среды и межфазные границы*. 2023;25(3): 406–414. <https://doi.org/10.17308/kcmf.2023.25/11265>

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1. Introduction

Iron triad elements are transition metals: iron Fe, cobalt Co, and nickel Ni. At room temperature, the elements form structures: Fe – BCC, Co – HCP, Ni – FCC. They are used in the production of structural steels, metallic glasses, ferromagnetic materials (for Fe, the Curie temperature $T_c = 1041$ K, for Co - 1390 K, for Ni – 631 K), etc.

Products made from them may be subject to seasonal temperature variations or a change in operating mode, therefore it is important to know the temperature dependence of the thermophysical properties of the components. The internal reaction of the alloy to a change in the temperature of the external medium can be accompanied by rearrangements of the electronic, atomic, phonon, vacancy, and other subsystems of quasiparticles with the possible nucleation of new phases in them. Important thermal characteristics of pure metals, sensitive to changes in the internal state of the system, are the heat capacity and the coefficient of thermal linear expansion. The course of the phase transition is reflected in their temperature dependences in the form:

- final jump (structural transition) of the baseline (see explanation in the text after formula (12));

- narrow in width, sharp and large peak (magnetic transition);

- symmetric or asymmetric peaks/pits with a rounded top, depending on the sign of the transition enthalpy or other physical quantity (polymorphic and aggregate transitions). The asymmetry of these graphical features is probably associated with a succession of phase transitions in the atomic system and subsystems of quasiparticles.

The evolution of the internal structure can occur by local nucleation of new phases (first-order phase transitions) or by creating conditions for the simultaneous appearance of a new phase in the entire volume (second-order phase transitions) both in the system itself and in its subsystems. Thus, internal phenomena and processes affect the measuring equipment.

The scatter of experimental values, for example, the heat capacities of Fe, Co, and Ni [1–8] depends on the temperature range in

which they were obtained, the chosen research method, the equipment used, the atmosphere in it, the chemical indifference of the crucible, sample pretreatment, and internal processes in it. Such kinetic phenomena include [9]: structure rearrangement, redistribution of atoms over positions in the unit cell, thermal expansion, transition of volatile impurities into the atmosphere of the calorimeter, etc. In this case, the thermal effects of a change in the internal state of the sample are summed up by the measuring equipment, which causes a discrepancy between the experimental data of different authors.

In the absence of phase transitions, experimental data on the temperature dependence, in particular, on the heat capacity of a substance, are often smoothed out by approximating functions [10–12], which contain a divergence at absolute zero temperature. The applied theoretical developments do not use one continuous function (or the sum of continuous functions) to describe the heat capacity graph of the system, especially in the presence of phase transitions [10, 13]. Therefore, there is a need to search for a new theoretical approach to describing the behaviour of the heat capacity of a solid in the temperature range from 0 K to the melting point.

The aim of this study was the description of the temperature dependences of the heat capacities and coefficients of thermal linear expansion of Fe, Co, Ni during the implementation of phase transitions of various nature in the studied temperature range using the ratios of the two-phase local equilibrium region model [14]. The model showed a fairly good agreement with the experimental data [14–19].

2. Heat capacities of iron, cobalt and nickel in the presence of structural, magnetic and aggregate phase transitions

2.1. Model of ideal phases (model of a two-phase locally equilibrium region)

Let us consider a locally equilibrium region of a condensed medium with a volume V , in which two ideal phases coexist, containing N_1 and N_2 elements with volumes ω_1 and ω_2 respectively [14]. In other words, phase 1 has the volume of $V_1 = \omega_1 N_1$, phase 2 has the volume of $V_2 = \omega_2 N_2$,

and the volume V of the region (with total number of elements $N = N_1 + N_2$) is equal to:

$$V_1 + V_2 = V. \quad (1)$$

It should be noted that one element of the local region accounts for the volume $\omega = V/N$, which depends on the concentration $c_i = N_i/N$ ($i = 1, 2$) of elements in phases. For simplicity of reasoning, we will further assume that the elements of the phases have the same or very close volumes, i.e., the condition $\omega_1 = \omega_2 = \omega$.

Dividing the equality (1) by the volume V , we obtain the ratio for the volume fractions of the phases:

$$x_1 + x_2 = 1, \quad (2)$$

where $x_i = V_i/V = N_i/N = c_i$ is the volume fraction of the phase $i = 1, 2$.

Let us introduce the order parameter η according to the formula:

$$\eta = x_1 - x_2. \quad (3)$$

From (2) and (3) it follows that:

$$x_1 = (1 + \eta) / 2, \quad x_2 = (1 - \eta) / 2. \quad (4)$$

Formulas (4) show that the order parameter η takes values from the interval from -1 to $+1$, since volume fractions x_i vary from 0 to 1.

Gibbs energy G of one mole of a substance (or per unit of dimensionless volume of the system) is equal to:

$$g = G / N = G\omega / V = \mu_1 x_1 + \mu_2 x_2, \quad (5)$$

where μ_{i0} are the chemical potentials of phase elements at temperature T , set by known formulas for an ideal system:

$$\mu_i = \mu_{i0} + k_B T \ln x_i, \quad (6)$$

Here μ_{i0} are the standard values of chemical potentials for each of the phases, which include a summand in the form $k_B T \ln N$, connected by the equation for the state of the medium with pressure and temperature, k_B is the Boltzmann constant. The extremum of the Gibbs energy (5) along the argument η , which corresponds to the local equilibrium value of the order parameter, is observed at:

$$(dg / d\eta) \Big|_{\eta=\eta_0} = 0 \Rightarrow \eta_0 = -\text{th}(\varphi / T), \quad (7)$$

where the argument is $\varphi = \Delta\mu_0 / 2k_B$, the function is $\Delta\mu_0 = \mu_{10} - \mu_{20}$. Therefore, the equilibrium

fraction, for example, of the crystalline phase in an amorphous alloy during its isochronous crystallization is described by the function:

$$x_1 = [1 - \text{th}(\varphi / T)] / 2. \quad (8)$$

If we expand the function φ in a Taylor series near the extreme point of thermal effect of the phase transition T_x with only the linear terms of the series preserved, than:

$$\begin{aligned} \varphi / T &= (\partial\varphi / \partial T)(T - T_x) / T = \\ &= a_0(q)[(T_x / T) - 1], \end{aligned} \quad (9)$$

where parameter is $a_0(q) = -\partial\varphi / \partial T$, q is the rate of sample heating. Model parameter $T_x(q)$, at which the maximum of the first derivative $u_x(q) = (dx_1 / dT) \Big|_{T=T_x}$ on the volume fraction of phase 1 and the extremum of the phase transition heat is observed, related to temperature by the ratio:

$$a_0(q) = 2T_x(q)u_x(q). \quad (10)$$

2.2. Heat capacity baseline (local heat capacity)

The local (partial) derivative of a function characterizes its changes in the vicinity of a single point. Thus, the entropy of the system at a fixed phase composition $x = x_1$ is defined by the formula [20]:

$$\begin{aligned} \sigma_x &= -(\partial g / \partial T)_x = -\partial\mu_{20} / \partial T - x\partial(\Delta\mu_0) / \partial T - \\ &- k_B [x \ln x + (1 - x) \ln(1 - x)] = \sigma_1 + \sigma_2 x + \sigma_3, \end{aligned} \quad (11)$$

where entropy: mother phase $\sigma_1 = -\partial\mu_{20} / \partial T$, phase differences $\sigma_2 = -\partial(\Delta\mu_0) / \partial T$, and their mixing $\sigma_3 = -k_B [x \ln x + (1 - x) \ln(1 - x)]$. Then the local heat capacity of the system:

$$\begin{aligned} C_b &= T(\partial\sigma_x / \partial T)_x = T(\partial\sigma_1 / \partial T)_x + \\ &+ T(\partial\sigma_2 / \partial T)_x x = k_1 T + k_2 x, \end{aligned} \quad (12)$$

where coefficients $k_1 = T(\partial\sigma_1 / \partial T)_x$ and $k_2 = T(\partial\sigma_2 / \partial T)_x$ we considered to be constant. In this case, formula (12) describes within the experimental error *heat capacity baseline* of the substances (*temperature dependence of local heat capacity* calculated at a constant phase composition) [17, 19]. The first summand in (12) depends linearly on temperature and describes the contribution of the electron subsystem to the heat capacity of the substance, while the internal evolution of the substance is represented by the second term.

2.3. Substantial heat capacity (heat capacity of the test sample)

Unlike the partial derivative of a function, its total derivative describes the behaviour of the function at any point in the system and during the transition from one point to another. We will use this fact for the study of the heat capacity of the investigated sample (substantial heat capacity of locally-equilibrium region), i.e., substantive entropy:

$$\begin{aligned} \sigma &= -(dg / dT) = \\ &= -[(\partial g / \partial T)_x - (\partial g / \partial x)_T \partial(dx / dT)] = \quad (13) \\ &= \sigma_x + \varepsilon_T u, \end{aligned}$$

where is the density energy of phase coexistence:

$$\varepsilon_T = -(\partial g / \partial x)_T = -\Delta\mu_0 - k_B T \ln[x / (1 - x)], \quad (14)$$

$u = dx / dT$ is “rate” of change in the phase composition x upon thermal transition to a new state. Thus, the local equilibrium entropy (11) coincides with its substantial definition (13) when the equation $\varepsilon_T = 0$ is satisfied, which generates formula (8).

Substantial heat capacity:

$$\begin{aligned} C &= T \frac{d\sigma_x}{dT} = \\ &= T \left[\left(\frac{\partial \sigma}{\partial T} \right)_{x,u} + \left(\frac{\partial \sigma}{\partial x} \right)_{T,u} \left(\frac{dx}{dT} \right) + \left(\frac{\partial \sigma}{\partial u} \right)_{T,x} \left(\frac{dx}{dT} \right) \right] = \quad (15) \\ &= C_b + C_k + C_d. \end{aligned}$$

The kinetics of the formation of a new phase affects the function (15), as was indicated in [9]. The “kinetic” component of heat capacity:

$$C_k = \{2\xi_T - Tu / [x(1 - x)]\} Tu = k_3 Tu, \quad (16)$$

here $\xi_T = (\partial \varepsilon_T / \partial T)_{x,u}$, $k_3 = 2\xi_T - Tu / [x(1 - x)]$. At a constant coefficient k_3 formula (16) describes the peaks ($k_3 > 0$) and pits ($k_3 < 0$) of polymorphic transformations, aggregate and magnetic transitions. “Dynamic” heat capacity component:

$$C_d = T \varepsilon_T w \quad (17)$$

where $w = du / dT$ for establishing local equilibrium ($\varepsilon_T = 0$) equals zero. Thus, the theoretical relation for calculating the temperature dependence of the heat capacity of a condensed medium upon reaching a local equilibrium state takes the form:

$$C = C_b + C_k. \quad (18)$$

2.4. Heat capacity of iron triad elements (Fe, Co, Ni)

Since when the temperature changes, the formation of a singularity β on the graph and the rearrangement of the subsystem i (fluctuation, vacancy, phonon, magnetic, etc.) substance can occur, the heat capacity C_b and C_k in formula (18) are calculated as:

$$C_b = k_1 T + \sum_{\beta,i} k_{2\beta i} x_{1\beta i}, \quad (19)$$

$$C_k = T \sum_{\beta,i} k_{3\beta i} u_{1\beta i}. \quad (20)$$

For the transition metals iron Fe, cobalt Co, and nickel Ni, the model parameters are shown in Table 1, and the calculation result is shown in Fig. 1. Fig. 1 demonstrates an adequate description of the experimental data using a single continuous function consisting of the sum of continuous values. As can be seen in Fig. 1, the above formulas describe quite well the temperature dependences

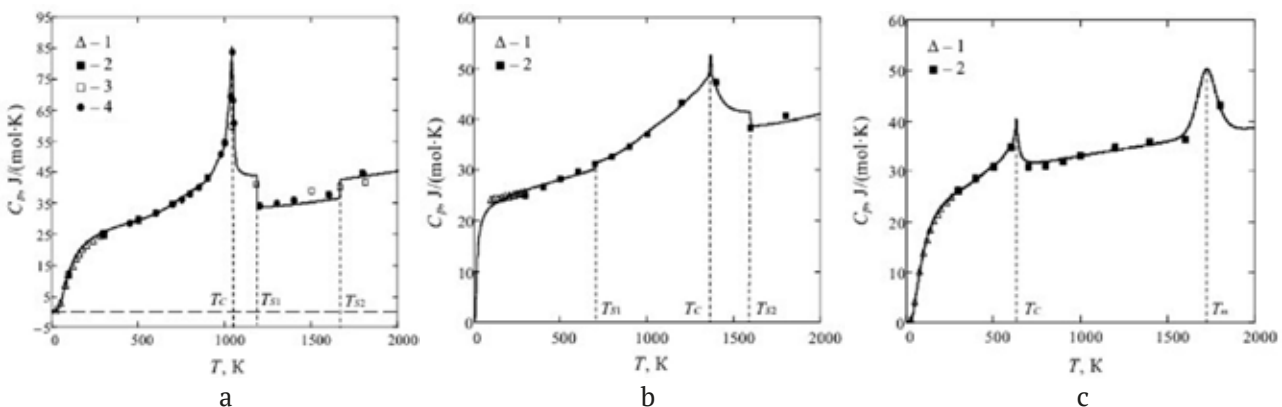


Fig. 1. Heat capacities of iron Fe (a), cobalt Co (b), and nickel Ni (c): 1 – data [1], 2 – [2], 3 – [3], 4 – [4]; solid line – theory

Table 1. Parameters of the theoretical model for calculating the heat capacities of metals

Parameters \ Metals		Fe ($T_m = 1811$ K [32])	Co ($T_m = 1767$ K [32])	Ni ($T_m = 1728$ K [2,32])
a_{01}		0.79	0.6	0.56
T_{x01} , K		140	27	156
$k_1 \cdot 10^4$		87	92	50
k_{201}		32.9	31	38.7
a_{02}	$\beta \rightarrow \gamma$ (Fe)	$T_{s1} = 1183$ K [2]	$T_{s1} = \sim 700$ K	–
	$\alpha \rightarrow \beta$ (Co)	2000	2000	–
T_{x02} , K		1188 ($T_{cubic} = 1189$ K [2])	698	–
k_{202}		–10.1	1.2	–
a_{03}	$\gamma \rightarrow \delta$ (Fe)	$T_{s2} = 1665$ K	$T_{s2} = ?$	–
	$\alpha \rightarrow ?$ (Co)	2000	2000	–
T_{x03} , K		1667 ($T_{s2} = 1667$ K [2])	1600	–
k_{203}		6.0	–2.8	–
Phase transitions in subsystems				
a_{111}		3.1	4.0	1.9
T_{x11} , K		955 ($T_c = 910$ K [32]) $\alpha_{amph} \leftrightarrow \beta$)	1190	492
k_{211}		5.0	–	–
k_{311}		3.4	2.3	2.8
a_{121}		15	10	4.0
T_{x21} , K		997	1314	543
k_{321}		1.1	0.9	1.0
a_{131}		58	29	12
T_{x31} , K		1022	1350	603
k_{231}		–	0.1	–
k_{331}		0.4	0.06	0.5
a_{141}		92	28	40
T_{x41} , K		1041	1368	632 ($T_c = 631$ K [32])
k_{341}		0.6	0.28	0.23
a_{151}		520	220	200
T_{x51} , K		1043 ($T_c = 1043$ K [2])	1369 ($T_c = 1390$ K [32])	633
k_{351}		0.027	0.04	0.023

of the heat capacities of the above metals for the structural (transition temperature T_s), magnetic (T_c) and aggregate (T_m) transitions. From Table 1 and Fig. 1b it can be seen that in cobalt at a temperature $T = \sim 1600$ K, a polymorphic transformation of the β phase may occur with

a change in the structure of the metal occurs, which is reflected in its temperature dependence as the jump. Apparently, at this temperature, the premelting process starts, which destroys the β -structure of the metal, since the temperature of the aggregate transition of cobalt $T_m = 1767$ K.

It should also be noted that the obtained results coincide with the data provided for Fe in [5, 21 p. 30], cobalt Co – [5, 8] and nickel Ni – [5, 7, 22, 23].

3. Thermal expansion coefficients of iron triad elements

Isobaric coefficient of thermal (linear – $\alpha_L = (\partial L / \partial T)_p / L$ or volumetric – $\alpha_V = (\partial V / \partial T)_p / V$) expansion depends on the aggregate state of the object, its chemical and phase compositions, structure and other internal phenomena and processes. At the microlevel, an increase in temperature is accompanied by an increase in the mobility of atoms, the appearance of new degrees of freedom, rearrangement of the phonon subsystem, and evolution of other subsystems of quasiparticles [24]. At the macro level, these phenomena lead to: the appearance of singular points (kinks) on the temperature dependences of the measured quantities; the appearance of diffuse phase transitions [25, 26]; the growth of cracks in solids due to emerging elastic and thermal stresses, as well as other irreversible processes.

Relationship of isobaric coefficient α_V with specific heat capacity c_V was first obtained by Grüneisen (see, for example, [27, p. 13; 28, p. 26]):

$$\alpha_V / c_V = \gamma\beta / V_m \approx \text{const}, \tag{21}$$

where γ is the Grüneisen parameter from the interval [1.5; 2.5], $\beta = (\partial V / \partial P)_T / V$ is coefficient of isothermal compressibility of metal, V_m is molecular volume, which is practically independent of temperature. Formula (21) indicates the similarity of the temperature curves for α_V and specific heat capacity c_V .

On the other hand, in accordance with the mixing rule (see, for example, [29]), the thermal expansion coefficient of a two-phase locally equilibrium region is:

$$\alpha = \alpha_1 x + \alpha_2 (1 - x) = \alpha_2 + x\Delta\alpha, \tag{22}$$

here α_i ($i = 1, 2$) is coefficient α_V (or α_L) of phase i , $\Delta\alpha = \alpha_1 - \alpha_2$ is phase thermal difference coefficient. In study [30] the behaviour of metallic glass using the above formulas both during cooling of the melt and during heating of the amorphous alloy was simulated. It was demonstrated that the presence of kinks on straight lines is associated with the occurrence of a diffuse phase transition.

Equations (21) and (22) allow us to calculate the coefficient $\alpha_L \cdot 10^6$ according to the formula:

$$\alpha_L \cdot 10^6 = q_1 T + q_2 x + \sum_{\beta, i} q_{3\beta i} T u_{\beta i}. \tag{23}$$

The parameters of the theoretical model are shown in Table 2, and temperature dependences of the coefficients of linear thermal expansion

Table 2. Parameters of the theoretical model for calculating the linear thermal expansion coefficients

Parameters \ Metals	Fe	Co	Ni
a_0	0.756	0.96	0.735
T_{x0}	154	114	134
$q_1 \cdot 10^4$	80	32	57
q_2	14	15.8	16
Phase transitions in subsystems			
a_{011}	5.28	–	23.4
T_{x11}	1063 ($T_{\gamma \rightarrow \delta} = 1038 \text{ K}$ [27])	–	639 ($T_c = 633 \text{ K}$ [27])
q_{311}	–1.68	–	1.06
a_{021}	9.3	–	12.2
T_{x21}	1810 ($T_m = 1811 \text{ K}$ [32])	–	670
q_{321}	–0.76	–	–0.5
a_{031}	–	–	3.4
T_{x31}	–	–	1728
q_{331}	–	–	2.0

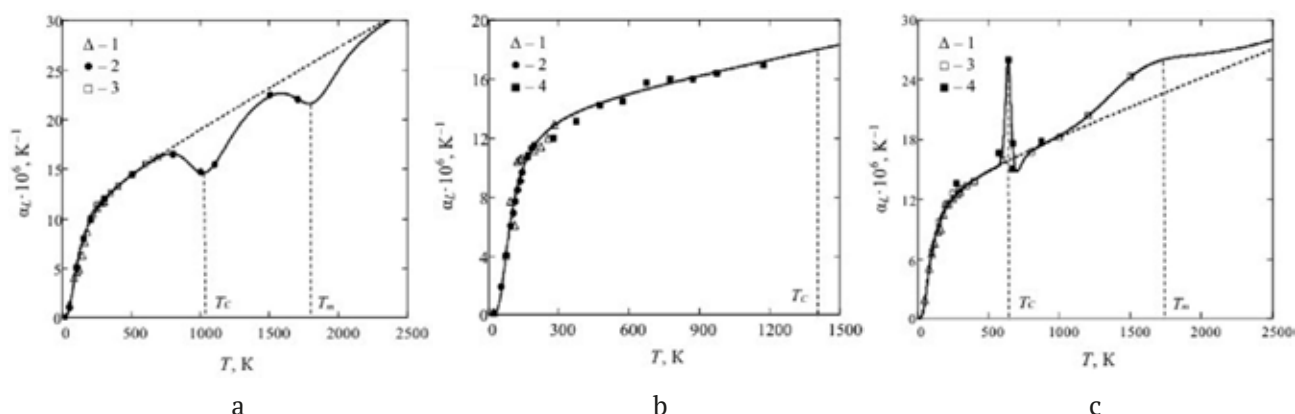


Fig. 2. Linear thermal expansion coefficients of iron Fe (a), cobalt Co (b), and nickel Ni (c): 1 – data [1], 2 – [27], 3 – [31], 4 – [32]; dotted line – base line, solid line – theory

of the iron triad elements are shown in Fig. 2. It should be noted that for iron the temperature T_{x11} is close to its Curie temperature T_C , and the temperature T_{x21} almost the same as the melting point T_m . Therefore, the proposed approach allows to analytically calculate not only the base lines of heat capacities and thermal expansion coefficients of iron triad elements, but also take into account the implementation of phase transformations in their subsystems.

Thus, the nonmonotonic and complex behaviour of the linear thermal expansion coefficient (Fig. 2b and c), for example, for nickel (Fig. 2c) did not receive an explanation during the experimental study [27, p. 203]. This study, taking into account “kinetic” additives allows to explain the non-monotonic nature of the temperature dependence curves by the occurrence of phase transitions. For iron (Fig. 2a) the presence of rounded extrema, probably, is associated with a series of polymorphic transformations, which are set with increasing temperature by rearrangements of atoms in the unit cells of the metal. For nickel, the sharp peak and the following minimum of the thermal expansion coefficient are determined by the successive implementation of the magnetic phase transition and polymorphic transformation in the temperature range from 500 to 800 K. A further increase in temperature causes a new transition: the system begins to rearrange into a new (liquid) aggregate state.

4. Discussion

The calculations carried out within the framework of the model of coexistence of two ideal phases in the local equilibrium region

showed a fairly good agreement between the theoretical results and different experimental data arrays on the heat capacities and thermal expansion coefficients of iron triad elements. According to most experimental data, the relative calculation error does not exceed 5–7%, and for transition temperatures it does not exceed 3%. The use of total temperature derivatives of specific entropies and the second Grüneisen rule allow to describe the temperature graphs of the indicated values in the implementation of structural, magnetic, and aggregate transitions.

Unlike the CALPHAD method, which uses functionally different dependences with divergence at 0 K, the presented approach uses the sum of continuous functions. The presence of features on the graphs (jumps, peaks/pits with sharp and rounded peaks) is due to the influence of the “kinetic” additive associated with rearrangements of quasiparticle subsystems. Their implementation should be taken into account when developing materials with specific thermophysical properties and during the use of finished products.

5. Conclusions

The simplicity of the ratios obtained in the proposed model and the reliability of the calculated data allow us to hope for its use in the algorithms for designing new materials. In addition, the applicability of the theoretical construction to solids of different physical and chemical nature, demonstrated in other studies of the author, indicates the universal nature of the assumptions of the model.

Conflict of interests

The author declares that they has no known competing financial interests or personal relationships that could have influenced the work reported in this paper.

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* Translated by author of the article.

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Received 10.01.2023; approved after reviewing 25.03.2023; accepted for publication 15.04.2023; published online 25.09.2023.

Translated by Valentina Mittova