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Effective Characteristics of Solute Atoms in a Multicomponent Alloy

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Modified model of 'inclusion in the matrix' is proposed to determine the solute-atoms' characteristics in a multicomponent alloy at different temperatures. The model allows calculating the effective diameter of dissolved atom and the effective shear modulus attributed to it for each component. This becomes possible with the correct interpretation of the input parameters for modelling, in particular, with the correct determination of the correction factors for atomic sizes, shear moduli, and Poisson's ratios for alloy components in a certain temperature range. It depends on the type of crystal lattices of the pure components and the alloy. The same atom in crystal lattices

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with a different co-ordination numbers will exhibit a different size, and the lattice of a pure component may differ from that of an alloy. Statements about different shear moduli and Poisson's ratios, which can be attributed to atoms in pure components and dissolved atoms in an alloy, if their crystal lattices are different, are also valid. The effective diameters and shear moduli for the dissolved atoms make it possible to determine the temperature dependence of atomic-sizes' misfits and elastic-moduli misfits. This is enough to calculate the temperature dependence of the lattice distortion of the alloy. Using the example of CrCoNiFeMn alloy, it is shown that the distortion determined using the proposed model increases with temperature.

Key words: lattice distortion, solid solution, solute atom, inclusion, matrix, multicomponent alloy.

Запропоновано модифікований модель «включення в матриці» для визначення характеристик розчинених атомів у багатокомпонентному стопі за різних температур. Модель уможливлює розрахувати ефективний діяметер розчиненого атома й ефективний модуль зсуву, що йому приписується, для кожного компонента. Це стає можливим за умови правильної інтерпретації вхідних параметрів для моделювання, зокрема, за умови правильного визначення поправочних коефіцієнтів для розмірів атомів, модулів зсуву та Пуассонових коефіцієнтів для компонентів стопу в певному діяпазоні температур. Це залежить від типу кристалічних ґратниць чистих компонентів і стопу. Один і той самий атом у кристалічних ґратницях з різними координаційними числами матиме різний розмір, а ґратниці чистого компонента можуть відрізнятися від кристалічних ґратниць стопу. Також справедливі твердження про різні модулі зсуву та Пуассонові коефіцієнти, які можна віднести до атомів у чистих компонентах і розчинених атомів у стопі, якщо їхні кристалічні ґратниці різні. Ефективні діяметри та модулі зсуву розчинених атомів уможливлюють визначити температурну залежність невідповідностей розмірів атомів і невідповідностей модулів пружности. Цього достатньо для розрахунку температурної залежности дисторсії кристалічних ґратниць стопу. На прикладі стопу CrCoNiFeMn показано, що дисторсія, визначена за допомогою запропонованого моделю, зростає з температурою.

Ключові слова: дисторсія ґратниць, твердий розчин, розчинений атом, включення, матриця, багатокомпонентний стоп.

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1. INTRODUCTION

Multicomponent alloys are a promising class of materials from the point of view of engineering applications and, in many cases, represent substitutional solid solutions [1, 2]. The solid solution strengthening, *i.e.*, an increase in the yield strength of the corresponding material, is the result of the fact that there is resistance to the movement of dislocations in the glide plane due to the shear stresses created by solute at-

oms. The solute atom differs from the atoms surrounding it. This difference leads to local distortion of the crystal lattice, and this, in turn, creates stresses. Local distortion changes with temperature, and understanding the features of these changes is important for determining the temperature dependence of the yield strength of a material.

Various aspects of solid solution strengthening have been considered theoretically and experimentally in many works [3–21]. Lattice distortion and yield strength in multicomponent alloys can be determined in various ways [22–26]. Characteristics of the distribution of shear stresses in the glide plane in a solid solution can be calculated both by direct summation of contributions from many solute atoms [27, 28] and by using a special statistical method [29]. The main four parameters of such a distribution are the standard deviation and correlation length of the short-wave component of the stochastic shear-stress field in the glide plane and the standard deviation and correlation length of the long-wave component of the field. The distribution of shear stresses is a major factor in modelling dislocation motion in the glide plane by the method of discrete dislocation dynamics [30, 31]. This simulation, in particular, shows the reality of the sequential action on the dislocation motion of the short- and long-wave components of the shear-stress field, and clarifies the sinusoidal shape of the bulges on the dislocation line, which are formed and disappear under the action of an external load as well as by means of which the dislocation itself moves.

Since multicomponent alloys are often used at high temperatures, the temperature dependence of their yield point is also important. In many cases, such dependence exhibits an almost constant yield-point value within the certain temperature range known as the ‘plateau’. In Ref. [32], the idea was first proposed that the mechanism of ‘plateau’ formation may be associated with an increase in crystal-lattice distortion with increasing temperature. This distortion results from the displacement of atoms in the process of thermal vibrations, which changes the equilibrium position of the atoms and, in particular, leads to thermal expansion of the material with increasing temperature. In other words, these displacements, namely, the root-mean-square displacements of atoms from ideal positions in the crystal lattice, lead to an increase in the distortion of the crystal lattice with increasing temperature.

A solute atom in a solid solution may exhibit characteristics, such as size, which are different from those it exhibits in the pure metal. The atom’s environment affects its effective characteristics.

The goal of this work is to develop a model to determine the effective characteristics of solute atoms in a multicomponent alloy at various temperatures and to derive the temperature dependence of the average distortion of the multicomponent-alloy crystal lattice.

2. CALCULATION ALGORITHMS

As a simple model of a solute atom, we take a sphere ('inclusion') inserted into a spherical cavity in an infinite block ('matrix') of elastic material [33]. Such a model is schematically depicted in Fig. 1. To determine the effective elastic characteristics of an inclusion inserted into the cavity, we modify the model by applying a pressure p on the outer surface of the matrix. An elastic ball with radius r_0 is inserted into a spherical cavity with radius r_m in the centre of another elastic ball with radius R. In this case, the following conditions $u_r, u_r', r_0 - r_m << r_0, r_{ii}, r_m << R$ are satisfied, which actually ensure the 'infinity' of the matrix. In addition, K' is the bulk modulus of the inclusion in the free state, μ' is the shear modulus of the inclusion in the free state, ν' is the Poisson's ratio of the inclusion in the free state; K is the bulk modulus of the matrix, μ is the shear modulus of the matrix, ν is the Poisson's ratio of the matrix. After inserting the ball into the cavity, all the elastic displacements obey spherical symmetry relative to the centre of the inclusion, *i.e.*, only radial displacements are nonzero. This spherical symmetry is not violated by the pressure p applied in the modified model on the outer surface of the matrix. The points of the ball surface have radial elastic displacements $u_r'(r_0)$, and the points of the cavity surface have radial elastic displacements $u_r(r_0)$. After inserting the ball into the cavity, the surfaces of the ball and the cavity coincide and create a single spherical surface with radius r_{ii}. According

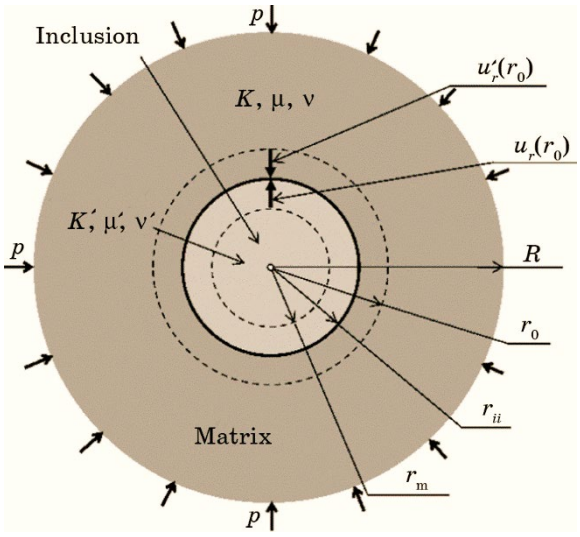

Fig. 1. The dashed lines show the surfaces of the sphere (larger circle) and the cavity (smaller circle) in the free state before the sphere is inserted. The solid line shows these surfaces after the sphere is inserted into the cavity.

to the analysis given in Ref. [33], the radial displacements of the points of the inclusion and the matrix will be

$$u_r'(r) = C'r\ ,\ \ u_r(r) = Cr^{-2} + C_{\rm I}r\ , \tag{1}$$

respectively, where C, C' and $C_{\rm I}$ are the constants, r is the radial coordinate. Then, the radial components of elastic stresses associated with these displacements will be

$$\sigma_{rr}'(r) = 3K'C'\ ,\ \ \sigma_{rr}(r) = -4\mu Cr^{-3} + 3KC_{\rm I} \tag{2}$$

for the points of the inclusion and the matrix, respectively.

For the model shown in Fig. 1, the following conditions must be met:

$$\begin{cases} \sigma_{rr}(R) = -p, \\ \sigma_{rr}'(r_0) = \sigma_{rr}(r_0), \\ 4\pi r_0^2[u_r(r_0) - u_r'(r_0)] = \delta\Omega, \end{cases} \tag{3}$$

where the difference in the volumes of the inclusion sphere and the spherical cavity is as follows:

$$\delta\Omega = 4\pi r_0^2(r_0 - r_{\rm m})\ . \tag{4}$$

Taking into account (1), (2) and (4), conditions (3) can be rewritten as a set of equations for the constants C, C' and $C_{\rm I}$:

$$\begin{cases} -4\mu CR^{-3} + 3KC_I = -p, \\ 3K'C' = -4\mu Cr_0^{-3} + 3KC_{\rm I}, \\ C + C_{\rm I}r_0^3 - C'r_0^3 = \delta\Omega\ /\ (4\pi). \end{cases} \tag{5}$$

After solving set (5), we find that:

$$C = \frac{3K'r_0^2(r_0 - r_{\rm m})}{4\mu + 3K'} - \frac{3(K - K')}{4\mu + 3K'}\frac{p}{3K}r_0^3\ , \tag{6a}$$

$$C' = \frac{4\mu(r_{\rm m} - r_0)}{r_0(4\mu + 3K')} - \frac{4\mu + 3K}{4\mu + 3K'}\frac{p}{3K}\ , \tag{6b}$$

$$C_{\rm I} = -\,p/(3K)\ . \tag{6c}$$

It should be noted that each of the constants C and C' has the term, which does not depend on p (*i.e.*, the value of a constant at $p = 0$), and the term, which is directly proportional to p. The constant $C_{\rm I}$ is directly proportional to p and equals 0 at $p = 0$. Usually, the 'inclusion in the matrix' model was considered only at $p = 0$, but taking into account

non-zero values of p allows us to obtain effective elastic characteristics of the inclusion, when it is inserted into a cavity within the matrix. These effective characteristics may differ from the elastic properties of a 'free' inclusion, when it is not within the matrix. If the expressions for the constants are substituted into Eq. (1), we obtain the following expressions for the displacements in the case $r = r_0$:

$$u_r'(r_0) = \frac{4\mu(r_m - r_0)}{4\mu + 3K'} - \frac{4\mu + 3K}{4\mu + 3K'} r_0 \frac{p}{3K}, \tag{7a}$$

$$u_r(r_0) = \frac{3K'(r_0 - r_m)}{4\mu + 3K'} - \frac{4\mu + 3K}{4\mu + 3K'} r_0 \frac{p}{3K}. \tag{7b}$$

Here, there are also terms, which correspond to $p = 0$ and are directly proportional to p. Using Eq. (7), it is easy to obtain an expression for the radius of the inclusion, when it is inserted into a cavity within the matrix:

$$r_{ii} = r_0 + u_r'(r_0) = r_m + u_r(r_0) = \frac{3K'r_0 + 4\mu r_m}{4\mu + 3K'} - \frac{4\mu + 3K}{4\mu + 3K'} r_0 \frac{p}{3K}. \tag{8}$$

The dilation or relative change in volume of an inclusion inserted into a cavity within the matrix, when pressure p is applied, will be

$$\Delta = 3\frac{r_{ii} - r_{ii}\big|_{p=0}}{r_{ii}\big|_{p=0}} = -\frac{p}{K_{ii}}, \tag{9}$$

where

$$r_{ii}\big|_{p=0} = \frac{3K'r_0 + 4\mu r_m}{4\mu + 3K'}, \tag{10}$$

and K_{ii} is the effective bulk modulus of the inclusion, when it is inserted into a cavity within the matrix:

$$K_{ii} = \frac{3K'r_0 + 4\mu r_m}{4\mu + 3K}\frac{K}{r_0} = \frac{r_{ii}\big|_{p=0}}{r_0}\frac{4\mu + 3K'}{4\mu + 3K}K. \tag{11}$$

Note that $\dfrac{r_{ii}\big|_{p=0}}{r_0} \cong 1$ due to the fact that $u_r, u_r' << r_0, r_{ii}, r_m$, and thus,

$$K_{ii} \cong \frac{4\mu}{4\mu + 3K}K + \frac{3K}{4\mu + 3K}K' = f_K K + f_{K'}K', \tag{12}$$

where $f_K + f_{K'} = 1$, and $0 \le f_K, f_{K'} \le 1$. These conditions lead to the fact that the value of the effective modulus K_{ii} always lies between the val-

ues K and K'.

The relationships between the bulk moduli and the shear moduli will be as follow:

$$K' = 2(1 + \nu')\mu' / [3(1 - 2\nu')], \quad K = 2(1 + \nu)\mu / [3(1 - 2\nu)], \tag{13a}$$

$$K_{ii} = 2(1 + \nu_{ii})G_{ii} / [3(1 - 2\nu_{ii})], \tag{13b}$$

where ν_{ii} is the effective Poisson's ratio of the inclusion, when it is inserted into a cavity within the matrix, G_{ii} is the effective shear modulus of such an inclusion. If we use Eqs. (12) and (13), we can derive the equation

$$G_{ii} = f_{\mu}\mu + f_{\mu'}\mu', \tag{14}$$

where

$$f_{\mu} = \frac{2(1 - 2\nu_{ii})(1 + \nu)}{3(1 + \nu_{ii})(1 - \nu)}, \quad f_{\mu'} = \frac{(1 - 2\nu_{ii})(1 + \nu)(1 + \nu')}{3(1 + \nu_{ii})(1 - \nu)(1 - 2\nu')}. \tag{15}$$

The unknown parameter ν_{ii} can be determined from the condition

$$f_{\mu} + f_{\mu'} = \frac{1 + \nu}{1 - \nu}\frac{1 - \nu'}{1 - 2\nu'}\frac{1 - 2\nu_{ii}}{1 + \nu_{ii}} = 1. \tag{16}$$

In this case, we have

$$\nu_{ii} = \frac{\nu' + 2\nu - 3\nu'\nu}{3 - 4\nu' + \nu} \tag{17}$$

and

$$f_{\mu} = \frac{2(1 - 2\nu')}{3(1 - \nu')}, \quad f_{\mu'} = \frac{1 + \nu'}{3(1 - \nu')}. \tag{18}$$

Note that f_{μ} and $f_{\mu'}$ depend only on the Poisson's ratio of the inclusion in the free state.

Equations (14), (16), (18) lead to the fact that the value of the effective shear modulus G_{ii} always lies between the values μ and μ'.

Now, it is necessary to interpret the parameters of the 'inclusion in the matrix' model from the point of view of the solute atom. Firstly, $r_0 = k_i s_i/2$, where s_i is the distance between the nearest atoms (atomic diameter) in the pure component i, and k_i is the correction factor for the interatomic distance, which is due to the fact that the same atom in different crystal lattices with different co-ordination numbers will exhibit different sizes (interatomic distances), and the lattice of the pure component i may differ from the lattices of the alloy. For example, we

know about the Goldschmidt's correction, which allows us to convert the size of an atom in the lattice of a metallic material with a certain co-ordination number into the size that this atom would have in a close-packed lattice with a co-ordination number of 12. In particular, if an atom in a b.c.c. lattice with a co-ordination number of 8 has a certain size (the distance between the nearest atoms), then, this atom in an f.c.c. lattice with a co-ordination number of 12 will exhibit a size approximately 1.03 times larger. Secondly, $r_m = s_{lat}/2$, where s_{lat} is the average distance between the nearest atoms in the alloy (the average material—the virtual matrix-solvent). Thirdly, $r_{ii}|_{p=0} = s_{ii}/2$, where s_{ii} is the effective diameter of the atom of component i, which is dissolved in the matrix-solvent. In addition, $\mu' = g_i G_i$, $\mu = G$, $\nu' = n_i \nu_i$, where G_i is the shear modulus of the pure component i, g_i is the correction factor for the shear modulus, which is related to the fact that the same atom in different crystal lattices can be assigned a different shear modulus similarly to different size, G is the shear modulus of the alloy (virtual matrix-solvent), ν_i is the Poisson's ratio of the component i, n_i is the correction factor for the Poisson's ratio, which is related to the fact that the same atom in different crystal lattices can be assigned the different Poisson's ratios similarly to different sizes and shear moduli. Let us add that ν is also the Poisson's ratio of the alloy (virtual matrix-solvent).

It should be explained here that an individual solute atom certainly does not have a real shear modulus and Poisson's ratio, and the attribution of these characteristics to such an atom is purely conditional. For clarity, one can imagine that such elastic properties are possessed by some virtual material, which has a crystal lattice such as an alloy has and consists entirely of atoms identical to the solute; nevertheless, this will be only an approximation. In fact, the shear modulus and Poisson's ratio attributed to a solute atom characterize indirectly its potential for interatomic interaction. The use of elastic characteristics attributed to a solute atom is successfully used in modelling solid solutions [33, 34].

It should also be added that averaging the corrected atomic sizes of the components should give us the average distance between the nearest atoms in the alloy (the average atomic diameter in the alloy). For the shear moduli and Poisson's ratios, the only assumption that will be valid is that the shear modulus and Poisson's ratio of the alloy should lie between their respective estimates by Voigt's and Reuss's formulae, which are made using the corrected values of the shear moduli and Poisson's ratios of the components. Thus, the following conditions should be satisfied:

$$s_{lat} = \sum_i k_i s_i X_i \,, \quad G_R \le G \le G_V \,, \quad \nu_R \le \nu \le \nu_V \,, \tag{19}$$

where X_i is the atomic fraction of component i (note that the sum of the atomic fractions of all components is equal to unity), $G_{\mathrm{V}} = \sum_i g_i G_i X_i$ is the estimate of shear modulus of the alloy by Voigt, $G_{\mathrm{R}} = 1/\sum_i [X_i/(g_i G_i)]$ is the estimate of shear modulus of the alloy by Reuss, $\nu_{\mathrm{V}} = \sum_i n_i \nu_i X_i$ is the estimate of Poisson's ratio of the alloy by Voigt, $\nu_{\mathrm{R}} = 1/\sum_i [X_i/(n_i \nu_i)]$ is the estimate of Poisson's ratio of the alloy by Reuss.

Note that G_{ii} and ν_{ii} can be interpreted as the effective shear modulus and Poisson's ratio of the atom of component i, which is dissolved in the matrix-solvent, *i.e.*, is surrounded by atoms of other components.

Determination of correction factors k_i, g_i and n_i is a separate task for each alloy. Here, we show, as an example, a possible algorithm for determining these factors for the Cantor's alloy CrCoNiFeMn. Let us set $i = 1$ for Cr, $i = 2$ for Co, $i = 3$ for Ni, $i = 4$ for Fe, $i = 5$ for Mn. Firstly, this alloy has an f.c.c. lattice, which is close-packed with a co-ordination number of 12. Secondly, the pure components Co and Ni have an h.c.p. lattice and an f.c.c. one, respectively, which are also close-packed with a co-ordination number of 12; thus, we can assume that the size, shear modulus and Poisson's ratio for the atoms of these components will be the same in the lattices of the pure components and in the lattice of the alloy, *i.e.*, the correction factors k_i, g_i and n_i for these components will be equal to unity at all temperatures ($k_2 = k_3 = 1$, $g_2 = g_3 = 1$, $n_2 = n_3 = 1$). Thirdly, the pure Cr and Fe components have b.c.c. lattices with a co-ordination number of 8. Thus, we can assume that k_i for these components are the same and close to 1.03 according to the Goldschmidt's correction ($k_1 = k_4 = k$). Fourthly, the pure Mn component has a special cubic lattice, in which there is no single co-ordination number; nevertheless, we assume that the correction factor $k_5 = \zeta_s k$ for its atomic size will be close to the corresponding correction factors of Cr and Fe, where ζ_s is a number close to unity. When k_5 and k are sufficiently close to each other over a wide temperature range, the temperature dependence of ζ_s can be neglected. Similarly, we can assume that $g_1 = g_4 = g$, $n_1 = n_4 = n$ and $g_5 = \zeta_g g$, $n_5 = \zeta_n n$, where ζ_g is a number close to unity, the dependence of which on temperature can be neglected, ζ_n is the same for all temperatures, since the temperature dependence of Poisson's ratio can be neglected. If we set ζ_s, then, we can find k and k_5 from the balance Eq. (19) for a given temperature with known temperature dependences of s_{lat}, s_1, s_2, s_3, s_4, and s_5. The task of finding g, g_5, n, and n_5 is more complicated. In addition to selecting ζ_g and ζ_n, we must set and solve for each temperature the auxiliary equations $(G_{\mathrm{V}} - G) / (G_{\mathrm{V}} - G_{\mathrm{R}}) = \xi_G$, $(\nu_{\mathrm{V}} - \nu) / (\nu_{\mathrm{V}} - \nu_{\mathrm{R}}) = \xi_\nu$, where ξ_G and ξ_ν determine the exact positions of G and ν between the corresponding estimates according to the Voigt's and Reuss's formulae. The parame-

ters ξ_G and ξ_ν can take values between 0 and 1. The auxiliary equations replace essentially inequalities (19). It should be noted that the bulk modulus and Young's modulus of the alloy at each temperature must also lie between their corresponding estimates according to the Voigt's and Reuss's formulae, which are made using the bulk moduli and Young's moduli of the components, which are found through the corrected shear moduli and Poisson's ratios of the components.

Thus, taking into account formulae (10), (14), and the abovementioned interpretation of the model parameters, both the effective diameter and the effective shear modulus of the solute atom of component i required to calculate the average distortion of the alloy will be

$$s_{ii} = f_{\text{lat}} s_{\text{lat}} + f_s k_i s_i , \tag{20}$$

where

$$f_{\text{lat}} = \frac{2(1 - 2n_i\nu_i)G}{2(1 - 2n_i\nu_i)G + (1 + n_i\nu_i)g_i G_i} , \; f_s = \frac{(1 + n_i\nu_i)g_i G_i}{2(1 - 2n_i\nu_i)G + (1 + n_i\nu_i)g_i G_i} \tag{21}$$

and

$$G_{ii} = f_G G + f_{G'} g_i G_i , \tag{22}$$

where

$$f_G = \frac{2(1 - 2n_i\nu_i)}{3(1 - n_i\nu_i)} , \; f_{G'} = \frac{1 + n_i\nu_i}{3(1 - n_i\nu_i)} . \tag{23}$$

Average distortion of the alloy crystal lattice is defined [27] as

$$\chi = \left(\sum_{i=1}^{N} (\eta_i'^2 + \alpha_0^2 \delta_i^2) X_i \right)^{2/3} , \tag{24}$$

where α_0 is a constant, which is equal to 16 for edge dislocations [22, 27, 35], $\delta_i = (1/s_{\text{lat}})(ds_{\text{lat}}/dX_i)$ is the size mismatch of the solute atoms of component i compared to the atoms of the virtual matrix-solvent, and $\eta_i' = \eta_i / (1 + 0.5|\eta_i|)$, $\eta_i = (1/G)(dG/dX_i)$ is the elastic modulus mismatch of the solute atoms of component i compared to the atoms of the matrix-solvent [27]. In accordance with Ref. [22], the parameters δ_i and η_i can be calculated as

$$\delta_i = 2\frac{s_{ii} - s_{\text{lat}}}{s_{ii} + s_{\text{lat}}} , \; \eta_i = 2\frac{G_{ii} - G}{G_{ii} + G} . \tag{25}$$

To find the temperature dependence of the average distortion $\chi(T)$ of the crystal lattices of the alloy, it is necessary to determine $\delta_i(T)$ and

$\eta_i(T)$ for different temperatures, *i.e.*, to determine $s_{ii}(T)$ and $G_{ii}(T)$; for this purpose, it is necessary to use the dependences $s_i(T)$, $s_{lat}(T)$, $G_i(T)$, $G(T)$, and Poisson's ratios ν_i (the parameters ν_i can be approximately considered independent of temperature).

Next, it is useful to calculate and analyse the temperature dependences of the relative shear modulus $G(T)/G(0)$, the relative average distortion $\chi(T)/\chi(0)$, and the factor $\kappa(T) = \chi(T)G(T)/(\chi(0)G(0))$.

3. RESULTS AND DISCUSSION

To verify the modified 'inclusion in the matrix' model for determining the effective characteristics of solute atoms in a multicomponent alloy, the CrCoNiFeMn alloy was chosen. The temperature dependences of $s_i(T)$, $s_{lat}(T)$, $G_i(T)$ and $G(T)$ for its individual components and the alloy itself are described in Ref. [36]. The CrCoNiFeMn alloy is a substitutional solid solution with an f.c.c. lattice. At $T = 0$ K, this alloy has an average distance between the nearest atoms $s_{lat} = 0.253$ nm, a shear modulus $G = 84$ GPa, a Poisson's ratio $\nu = 0.25$, a bulk compressive modulus $K = 140$ GPa, and a Young's modulus $E = 210$ GPa. The atomic sizes, shear moduli, and Poisson's ratios of the pure components at $T = 0$ K are given in Table 1.

To calculate the effective diameter s_{ii} of the solute atom of component i and its effective shear modulus G_{ii} according to formulae (20) and (22) at various temperatures, it is necessary to determine the cor-

TABLE 1. Atomic sizes, shear moduli and Poisson's ratios of the pure components, correction factors and corrected values of sizes, shear moduli and Poisson's ratios for solute atoms in the CrCoNiFeMn alloy.

i	Cr	Co	Ni	Fe	Mn
	1	2	3	4	5
X_i	0.2	0.2	0.2	0.2	0.2
s_i at $T = 0$ K, nm	0.252	0.249	0.249	0.248	0.25
G_i at $T = 0$ K, GPa	110	84	88	87	86
ν_i	0.21	0.34	0.32	0.29	0.22
k_i at $T = 0$ K	1.021	1	1	1.021	1.037
g_i at $T = 0$ K	0.879	1	1	0.879	0.87
n_i	0.642	1	1	0.642	1.284
$k_i s_i$ at $T = 0$ K, nm	0.257	0.249	0.249	0.253	0.259
$g_i G_i$ at $T = 0$ K, GPa	97	84	88	76	75
$n_i \nu_i$	0.14	0.34	0.32	0.19	0.29

rection factors k_i, g_i and n_i for each temperature. We will do this according to the algorithm described above for the CrCoNiFeMn alloy.

Since Co and Ni as pure components have close-packed lattices with a co-ordination number of 12, we assume that the sizes, shear moduli and Poisson's ratios for the atoms of these components will be the same in the lattices of the pure components and in the lattices of the alloy, *i.e.*, at all temperatures, $k_2 = k_3 = 1$, $g_2 = g_3 = 1$, and $n_2 = n_3 = 1$. For the temperature-dependent diameter of the solute atom of Mn, we assume that $\zeta_s = 1.016$ in the entire temperature range considered. That is, we assume that the correction factor for the size of the solute atoms of Mn is slightly larger than the factor for the sizes of the solute atoms of Cr and Fe. Then, $k_1 = k_4 = k$ and k_5 can be calculated in the entire temperature range considered taking into account the balance equation for the dimensions (19), s_i and s_{lat}, for each temperature (Fig. 2). It is seen that these coefficients depend weakly on temperature and are very close to 1.03, *i.e.*, to the Goldschmidt's correction factor (with transition from co-ordination number of 8 to co-ordination number of 12). This is an indirect proof of the correctness of such an approach.

Let us also assume that $\zeta_g = 0.99$ in the entire temperature range considered, *i.e.*, the correction factor for the shear modulus of solute atoms of Mn is slightly smaller than the factor for the shear moduli of solute atoms of Cr and Fe. This is plausible, since it is logical to associate a slightly smaller shear modulus with a slightly larger diameter of solute atom of Mn. For the auxiliary equation corresponding to the shear modulus, we will assume $\xi_G = 0.5$ that is the best value for esti-

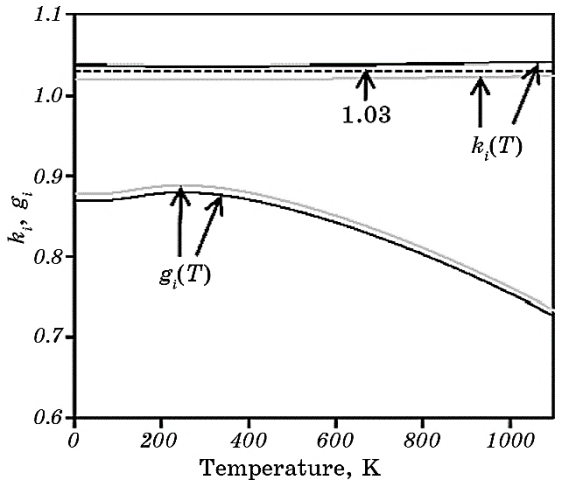

Fig. 2. Dependences of correction coefficients k_i and g_i on temperature for Cr, Fe and Mn atoms. Gray lines are for Cr and Fe atoms; black lines are for Mn atoms.

mating the shear modulus.

Then, $g_1 = g_4 = g$ and g_5 can be calculated in the entire temperature range considered using the auxiliary equation, G_i, and G for each temperature (Fig. 2). These coefficients depend on temperature more strongly than the coefficients for the atomic sizes and are less than unity that corresponds to a decrease in the effective shear modulus of the solute atom relative to the modulus of the pure component. An increase of the atomic size contributes to a corresponding decrease of the shear modulus. The task of determining $n_1 = n_4 = n$ and n_5 is more difficult. The parameters ζ_n and ξ_ν must be determined, so that the bulk modulus and Young's modulus of the alloy lay between their corresponding estimates according to the Voigt's and Reuss's formulae at each temperature. These estimates should be made using the bulk moduli K_i^{corr} and Young's moduli E_i^{corr} of the components, which are found through the corrected shear moduli and Poisson's ratios of the components: $K_i^{\text{corr}} = 2(1 + n_i\nu_i)g_iG_i/[3(1 - 2n_i\nu_i)]$, $E_i^{\text{corr}} = 2(1 + n_i\nu_i)g_iG_i$.

In addition, it should be taken into account that the average distortion of the alloy, according to formula (24), at $T = 0$ K should be $\chi = 0.094$ as calculated in Ref. [36]. Taking into account these conditions, we have $\zeta_n = 2$ and $\zeta_\nu = 0.095$. Then, the auxiliary equation for Poisson's ratio allows us to calculate the correction factors $n_1 = n_4 = n$ and n_5 (Table 1).

When all the correction factors are determined, we can calculate the effective diameter s_{ii} of the solute atom of component i and its effective shear modulus G_{ii} according to formulae (20) and (22) at various temperatures (Fig. 3). The temperature dependences $s_{ii}(T)$ and $G_{ii}(T)$ look qualitatively like the corresponding dependences $s_{\text{lat}}(T)$ and $G(T)$ for

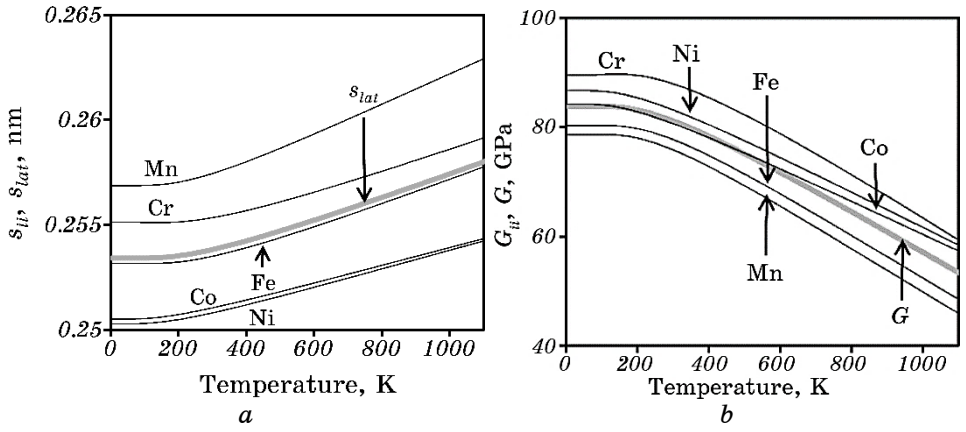

Fig. 3. Dependences of the distances between the nearest atoms $s_{ii}(T)$ and s_{lat} (*a*) and the shear moduli G_{ii} and G (*b*) on temperature for the CrCoNiFeMn alloy.

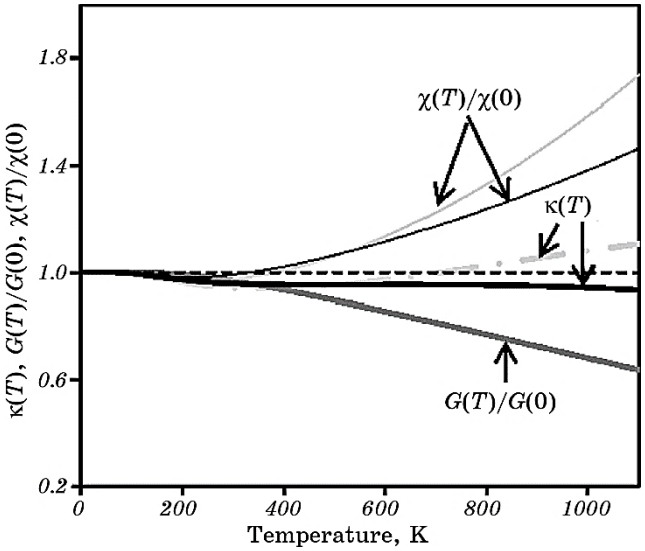

Fig. 4. Dependences of the relative shear modulus $G(T)/G(0)$ of the alloy, its relative average distortion $\chi(T)/\chi(0)$, and the factor $\kappa(T)$ on temperature for the CrCoNiFeMn alloy. Black lines are calculated in this work; grey lines are calculated in work [36].

the alloy, but lie above and below the latter. Thus, we can calculate the atomic-size mismatch and elastic-modulus mismatch of the solute atoms of component i compared to the atoms of the virtual matrix-solvent using formulae (25) throughout the entire considered temperature range.

Next, according to formula (24), the average distortion χ of the crystal lattice is calculated for various temperatures; then, the relative average distortion $\chi(T)/\chi(0)$ and the factor $\kappa(T) = \chi(T)G(T)/(\chi(0)G(0))$ are calculated. The temperature dependences of these parameters together with the dependence of the relative shear modulus are shown in Fig. 4. It can be seen that the relative average distortion, which is calculated using the effective characteristics of solute atoms determined using the modified model proposed here, increases with temperature.

In general, complementing the calculations made in Ref. [36], the modified model allows us to calculate the effective characteristics of solute atoms in a multicomponent alloy at various temperatures.

4. CONCLUSION

A modified 'inclusion in the matrix' model is proposed to determine the effective characteristics of solute atoms in a multicomponent alloy at various temperatures. The model allows calculating the effective

diameter of a solute atom and the effective shear modulus assigned to it for each component. This becomes possible with the correct interpretation of the input parameters for modelling, in particular, with the correct determination of the correction factors for atomic sizes, shear moduli, and Poisson's ratios for alloy components in a certain temperature range depending on the type of crystal lattices of pure components and the alloy. The effective diameters and shear moduli of solute atoms make it possible to determine the temperature dependences of the mismatches of atomic sizes and elastic moduli, *i.e.*, to calculate the temperature dependence of the average distortion of the crystal lattice of the alloy.

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