Continuum Mechanics

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Abstract

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On the Continuum Theory of the Elastic Interaction of Atoms in Interstitial Solid Solutions

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In (1), a single-phase binary substitutional solid solution with an edge dislocation was consistently considered within the framework of the isotropic continuum theory of elasticity. An interstitial solid solution can also be treated as an elastic continuum with inhomogeneous properties; however, the method developed in (1) must be generalized.*

Let us consider a single-phase binary interstitial solid solution based on a body-centered cubic lattice. As is known, in a body-centered cubic lattice the atoms of the dissolved substance may occupy three different interstitial positions—along the three mutually perpendicular edges of each of the two simple cubic sublattices. In equilibrium, in the absence of external fields, all three positions are equally probable. However, in the presence of external elastic fields and elastic interaction between atoms, these positions become nonequivalent.

Let a unit volume** contain N_0 impurity atoms, with N_x, N_y, and N_z atoms located, respectively, in the interstitial positions in a cell along the directions x, y, and z ($N_x + N_y + N_z = N_0$). The total number of atoms per unit volume is N, and the number of solvent atoms is N_1 ($N_1 = N - N_0$). We introduce the concentrations of impurity atoms by interstitial positions: $c_x = N_x/N$, $c_y = N_y/N$, $c_z = N_z/N$, which in what follows we shall denote by c_ν ($\nu = x, y, z$). Obviously, $\sum c_\nu = c$, where $c = N_0/N$ is the total concentration of impurity atoms at the given point. In equilibrium, in the absence of external fields, $c_\nu = \mathrm{const} = c_0/3$, where c_0 is the average concentration of impurity atoms in the whole volume. It is natural to introduce the quantity $c^\nu = c_\nu - c_0/3$.

In an elastic crystal of arbitrary symmetry, for a nonequilibrium distribution of dissolved atoms in space and among interstitial positions, the following expansion of the free energy of a unit volume in small deformations is valid:

$$F = F_0 - \chi_{lm}\varepsilon_{lm} + \frac{1}{2}\lambda_{iklm}\varepsilon_{ik}\varepsilon_{lm}. \tag{1}$$

In this case the free energy of the entire system $\mathfrak{F}$, obviously, is equal to the functional

$$\mathfrak{F} = \int_V F(\mathbf{r})\, d\mathbf{r}. \tag{2}$$

In relation (1), F_0 is the free energy in the absence of deformations; ε_{ik} is the strain tensor; λ_{iklm} is the tensor of elastic moduli, in this case— approximation independent of the impurity concentration; $\varkappa$ is a certain tensor depending on c^ν. It is not difficult to see that (1) is a direct generalization of expression (1) from (1).

Let us expand $\varkappa_{lm}$ in a series in small c^ν: $\varkappa_{lm} = \varkappa_{lm}^{(0)} + \varkappa_{lm}^{\nu} c^\nu$ (repeated indices ν denote summation). Obviously, $\varkappa_{lm}^{0} = 0$, since at $c^\nu = 0$ the distribution of the impurity concentration is uniform, concentration stresses are absent, and expression (1) must contain only quadratic terms (for the thermoelastic case see (2)).

Further, representing $\varkappa_{lm}^{\nu}$ in the form $\varkappa_{lm}^{\nu} = \lambda_{iklm}\alpha_{ik}^{\nu}$, where α_{ik}^{ν} are certain tensors whose meaning will be clarified later, we obtain

$$F = F_0 - \lambda_{iklm}\alpha_{ik}^{\nu} c^\nu \varepsilon_{lm} + \frac{1}{2}\lambda_{iklm}\varepsilon_{ik}\varepsilon_{lm}. \tag{3}$$

For simplicity, in what follows we shall consider the isotropic case. A calculation for a cubic crystal does not lead to fundamentally new results, but is considerably more complicated.

As is known, in the isotropic case $\lambda_{iklm} = \lambda\delta_{ik}\delta_{lm} + 2G\delta_{im}\delta_{kl}$, where λ is the Lamé coefficient, $\lambda = K - \frac{2}{3}G$; K and G are the elastic moduli of hydrostatic compression and shear, respectively. If Poisson' s ratio is equal to $\frac{1}{3}$, then $\lambda = \frac{3}{4}K$, $G = \frac{3}{8}K$, and the expression is valid

$$F = F_0 - \frac{3}{4}K\left(\varepsilon_{ll}\alpha_{ll}^{\nu} + \varepsilon_{ik}\alpha_{ik}^{\nu}\right)c^\nu + \frac{3}{8}K\left(\varepsilon_{ll}^2 + \varepsilon_{ik}^2\right). \tag{4}$$

Let us calculate the stress tensor $\sigma_{ik} = \partial F/\partial\varepsilon_{ik}$. From (4)

$$\sigma_{ik} = \frac{3}{4}K\left(\varepsilon_{ll}\delta_{ik} + \varepsilon_{ik} - \alpha_{ll}^{\nu}c^\nu\delta_{ik} - \alpha_{ik}^{\nu}c^\nu\right). \tag{5}$$

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* Analogous questions, but in a somewhat different aspect, were considered in (6, 7).

** A unit volume assigned to the given point of space with coordinate $\mathbf{r}$ is meant. Therefore N_x, N_y, N_z, N_0, N, as well as c_x, c_y, c_z, c, depend on $\mathbf{r}$. The same applies to the density of free energy F.

If $\sigma_{ik} = 0$, i.e., free "concentration" expansion takes place, then, as is easily seen,

$$\varepsilon_{ik} = \varepsilon^0_{ik} = \alpha^\nu_{ik} c^\nu .$$

From this relation the meaning of the tensor α_{ik} can be clarified. Since $\varepsilon^0_{ll} = \alpha^\nu_{ll} c^\nu$, α^ν_{ll} is the volume "partial" coefficient of concentration expansion due to atoms in position ν. It is not difficult to show that for $i \neq k$ $\alpha^\nu_{ik} = 0$; the diagonal elements α^ν_{ik} can be determined from the dependence of the lattice parameters on the impurity concentration in the given interstitial position. For example, in the case of α-iron, from martensite data, if the interstitial atoms are in the z positions, it follows that $\alpha^z_{zz} = \frac{1}{a_z}\frac{\partial a_z}{\partial c^z} = 0.917$; $\alpha^z_{xx} = \alpha^z_{yy} = \frac{1}{a_x}\frac{\partial a_x}{\partial c^z} = -0.117$ (3) (a_ν are the lattice parameters in the corresponding direction). The components α^ν_{ik} for $\nu = x, y$ are obtained by a simple cyclic permutation of the diagonal elements.

The quantity F_0 appearing in the formulas is determined in the same way as in (1), on the basis of the fact that $F(\sigma_{ik} = 0) = F_{\text{chem}}$—the free energy for purely chemical interaction of atoms. Substituting in (4) $\varepsilon_{ik} = \alpha^\nu_{ik} c^\nu$, corresponding precisely to $\sigma_{ik} = 0$, we obtain:

$$F_0 = F_{\text{chem}} - \frac{3}{8} K \left(\alpha^\nu_{ll}\alpha^\eta_{ll} + \alpha^\nu_{ik}\alpha^\eta_{ik}\right) c^\nu c^\eta$$

and, finally,

$$F = F_{\text{chem}} - \frac{3}{8} K \left(\alpha^\nu_{ll}\alpha^\eta_{ll} + \alpha^\nu_{ik}\alpha^\eta_{ik}\right) c^\nu c^\eta - \frac{3}{4} K \varepsilon_{ik} \gamma^\nu_{ik} c^\nu + \frac{3}{8} K \left(\varepsilon^2_{ll} + \varepsilon^2_{ik}\right), \quad (6)$$

where $\gamma^\nu_{ik} = \alpha^\nu_{ik} + \alpha^\nu_{ll}\delta_{ik}$.

Let us note that all the preceding exposition applies not only to a body-centered cubic lattice, but to any lattice having several nonequivalent interstitial sites. In particular, if one sets

$\alpha^\nu_{ik} = \omega\delta_{ik}$, then (6) passes into expression (3) from (1)*. This limiting transition corresponds to a hydrostatic deformation of the solvent cell upon substitution or upon interstitial incorporation of an impurity atom, when there is only one interstitial position. Such a deformation apparently must occur in interstitial solid solutions based on a face-centered cubic lattice.

In the state of equilibrium the free energy of the whole system $\mathcal{F}$ must take its least value. Minimizing the functional (2) by varying independently the displacements u $\left(\varepsilon_{ik} = \frac{1}{2}(\nabla_i u_k + \nabla_k u_i)\right)$ and the numbers of particles in interstitial positions N_ν, under the condition that the total number of impurity atoms in the solution remains constant, we obtain a system of equations describing the equilibrium state:

$$\left(\frac{\partial F}{\partial N_\nu}\right)_{\varepsilon_{ik}=\text{const}} = \lambda = \text{const} \quad (\nu = x, y, z); \tag{7a}$$

$$\partial\sigma_{ik}/\partial x_k = 0. \tag{7b}$$

The first equation expresses the well-known fact of the constancy of the chemical potential $\mu^\nu = \partial F/\partial N_\nu$ of the atoms in each of the interstitial positions. The Lagrange multiplier λ can be found from the condition that the number of particles is constant, or from the value of μ^ν as $|\mathbf{r}| \to \infty$, which is usually easily calculated.

Equation (7b) is simply the equation of elasticity. The tensors ε_{ik} and σ_{ik} describe, respectively, the total deformation and the total stress. In the case where there is an external field,

$$\varepsilon_{ik} = \varepsilon_{ik}^{\text{ext}} + \varepsilon_{ik}^{c}, \tag{8}$$

where $\varepsilon_{ik}^{\text{ext}}$ is the deformation produced only by the external field; ε_{ik}^{c} is the deformation produced only by the inhomogeneous distribution of impurity atoms.

An analogous relation also holds for σ_{ik}. Here, as in (1), the validity of the superposition principle is assumed; therefore $\varepsilon_{ik}^{\text{ext}}$ and ε_{ik}^{c} each independently satisfy their own equation of elasticity (7b) with the corresponding boundary conditions. In particular, independently of the form of the external field, ε_{ik}^{c} satisfies, as follows from (5), the equation

$$\nabla_i \varepsilon_{ll}^{c} + \nabla_k \varepsilon_{ik}^{c} - \gamma_{ik}^{\nu} \nabla_k c^\nu = 0$$

or, since $\varepsilon_{ik}^{c} = \frac{1}{2}(\nabla_i u_k^c + \nabla_k u_i^c)$,

$$\frac{3}{2}\nabla_i \nabla_k u_k^c + \frac{1}{2}\nabla_k^2 u_i^c - \gamma_{ik}^{\nu} \nabla_k c^\nu = 0. \tag{9}$$

When there is only a concentration field in the system, there is no pseudovector; therefore u^c is a potential vector, and equation (9) can be represented in the form

$$\Delta u_i^c = \frac{1}{2}\gamma_{ik}^{\nu} \nabla_k c^\nu,$$

where Δ is the Laplace operator.

It is easy to show that, if as $|\mathbf{r}| \to \infty$, $|u^c| \to 0$, then

$$u_i^c = \frac{1}{8\pi} \gamma_{il}^{\nu} \nabla_l \int_V \frac{c^{\nu}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}\, d\mathbf{r}'$$

and

$$\varepsilon_{ik}' = \frac{1}{16\pi} \left(\gamma_{kl}^{\nu} \nabla_i + \gamma_{il}^{\nu} \nabla_k\right) \nabla_l \int_V \frac{c^{\nu}(\mathbf{r}')}{|\mathbf{r}' - \mathbf{r}|}\, d\mathbf{r}', \tag{10}$$

where $d\mathbf{r}' = dx'\, dy'\, dz'$, and the integration is carried out over an infinite volume.

Taking (8) into account, we represent F in the form of a sum:

$$F = F_{\text{chem}} + F_{\text{ext}} + F_c + \Phi,$$

* In paper (1), in formula (3) and below in the text, the coefficient should be 9/2, not 9/12.

where F_{ext} is the free energy of the external elastic field; F_c and Φ are the free energies of the elastic interaction of impurity atoms, respectively, with one another and with the external field. As is seen from (6),

$$F_{\text{ext}} = \frac{3}{8} K \left(\varepsilon_{ik}^{\text{ext}} - \delta_{ik} \varepsilon_{ll}^{\text{ext}}\right)^2,$$

$$F_c = -\frac{3}{8} K \left(\alpha_{ll}^{\nu} \alpha_{ll}^{\eta} + \alpha_{ik}^{\nu} \alpha_{ik}^{\eta}\right) c^{\nu} c^{\eta} - \frac{3}{4} K \gamma_{ik}^{\nu} \varepsilon_{ik}^{c} c^{\nu} + \frac{3}{8} K \left(\varepsilon_{ik}^{c} - \delta_{ik} \varepsilon_{ll}^{c}\right)^2, \tag{11}$$

$$\Phi = -\frac{3}{4} K \varepsilon_{ik}^{\text{ext}} \gamma_{ik}^{\nu} c^{\nu} + \frac{3}{4} K \left(\varepsilon_{ik}^{\text{ext}} \varepsilon_{ik}^{c} + \varepsilon_{ll}^{\text{ext}} \varepsilon_{ll}^{c}\right).$$

Then, in explicit form, equation (7a) takes the form:

$$\mu_{\text{chem}}^{\nu} - \frac{3}{4} \frac{K}{N} \left(\alpha_{ll}^{\nu} \alpha_{ll}^{\eta} + \alpha_{ik}^{\nu} \alpha_{ik}^{\eta}\right) c^{\eta} - \frac{3}{4} \frac{K}{N} \varepsilon_{ik}^{c} \gamma_{ik}^{\nu} - \frac{3}{4} \frac{K}{N} \varepsilon_{ik}^{\text{ext}} \gamma_{ik}^{\nu} = \lambda \tag{12}$$

(we have used the fact that

$$\mu^{\nu} \cong \frac{1}{N} \left(\frac{\partial F}{\partial c^{\nu}}\right)_{\varepsilon_{ik}}.$$

Here $\mu_{\text{chem}}^{\nu} = \dfrac{\partial F_{\text{chem}}}{\partial N_{\nu}}$ $(\nu = x, y, z)$.

With the aid of (10) the tensor ε^{c}_{ik} can be eliminated from (12), and then we obtain a system of equations (generally speaking, integro-differential equations) relating, in the equilibrium state, c^{ν} and $\varepsilon^{\text{ext}}_{ik}$. For each specific case $\varepsilon^{\text{ext}}_{ik}$ is determined from its own equation of elasticity. For example, in the case when the external field is created by a dislocation ($\varepsilon^{\text{ext}}_{ik} = \varepsilon^{D}_{ik}$), ε^{D}_{ik} is determined from the Volterra model (^{4}).

The free energy of the purely chemical interaction can be calculated, for example, in the regular-solution approximation. Since interstitial solutions are usually highly dilute ($c \ll 1$), the internal energy of the chemical interaction between atoms may be neglected in comparison with the elastic energy. Then $F_{\text{chem}} = -TS_{\text{chem}}$, where T is the absolute temperature, and S_{chem} is the entropy determined by known combinatorial relations.

The theory developed makes it possible to describe a number of phenomena connected with the redistribution of atoms in space and among interstitial positions. In particular, in the high-temperature approximation one can solve the problem of the formation of Cottrell and Snoek atmospheres around dislocations. Such a treatment for a solid solution of carbon in α-iron in the presence of a screw dislocation leads to values and a temperature dependence of the upper yield point, and also to a value of the radius of the Snoek atmosphere, that agree with known data (^{5}).

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