

wave for two cases: water droplets, $N \sim 10^{13} \text{ cm}^{-3}$, $D = 30 \text{ \AA}$, using the value of the complex dielectric constant for a radiation frequency $\nu = 1000 \text{ cm}^{-1}$, and also metallic spheres of copper having the same dimension and the same density, at the same frequency. The photon free path in a two-phase medium is $\lambda \sim 1/N\sigma$, and in the former case $\lambda \sim 0.1 \text{ km}$ while in the latter it is 30 times larger (σ is the total-attenuation cross section).

The authors are grateful to Yu.B. Konev, I.I. Sobel'man, and D.T. Shalunov for useful discussions.

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ELECTROSTATIC ENERGY OF A DISORDERED ALLOY

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Submitted 15 January 1971

ZhETF Pis. Red. 13, No. 4, 318 - 321 (20 February 1971)

The electronic theory of alloys, based on the method of pseudopotentials, is presently being successfully developed (cf., e.g., [1, 2]). As follows from the theory, an important contribution to the total energy of the alloy is made by the electrostatic energy of the ion lattice in the field of the uniformly-distributed negative charge. The expression for the electrostatic energy E_{es} of a completely disordered binary alloy was obtained in [1] by generalizing the corresponding expression for the E_{bs} of the band structure of the alloy. It turned out that both E_{es} and E_{bs} consist of two parts each, the energy of the "average" ion lattice (which contains the sum over the reciprocal-lattice points) and the so-called difference energy, which is proportional to $(Z_A - Z_B)^2$ (Z_A and Z_B are the charges of the ions of type A and B), and expressed in the form of a sum over all the reciprocal-space points allowed by the cyclic boundary condition, with the exception of the reciprocal-lattice vectors.

As is well known, the electrostatic energy of a system of charges in a homogeneous compensating field is conveniently determined with the aid of the Ewald transformation. Ewald's method employs a parameter η , which characterizes the dimensions of the Gaussian charge-distribution "caps" over the lattice points. The value of η is chosen such as to ensure optimally rapid convergence of the series. The final result should in this case be independent of η . However, the expression given in [1] for E_{es} does not satisfy this requirement, since the first term (the electrostatic energy of the "average" crystal) does not depend on η , whereas the second is a function of η .

We shall show in this paper how to effect the Ewald transformation for an alloy with an arbitrary ion placement. It turns out here that in a disordered alloy, in the absence of short-range order (the case considered in [1]), the expression for E_{es} has no difference term at all. If, on the other hand, there is a correlation in the placement of the ions (short-range order), then the

terms proportional to $(Z_A - Z_B)^2$ differ from zero, and the corresponding expression is independent of η , as it should be.

Let us consider a crystal lattice at whose sites are located, in arbitrary fashion, positive pointlike ions with charges Z_A and Z_B . The numbers of ions A and B in the cyclic volume $\Omega = N\Omega_0$ are $N_A = cN$ and $N_B = (1 - c)N$ (Ω_0 is the average atomic volume, N is the total number of the ions, $N = N_A + N_B$, and c is the concentration of the ions A). The lattice is immersed in a uniformly distributed negative charge of density \bar{Z}/Ω , where $\bar{Z} = Z_A c + Z_B(1 - c)$. In the general case, the charge density produced at the point r by the distribution of the pointlike ions in the lattice sites can be written in the form

$$\rho(r) = \sum_{\mathbf{R}} \{Z_A C_{\mathbf{R}} + Z_B(1 - C_{\mathbf{R}})\} \delta(r - \mathbf{R}), \quad (1)$$

where the summation is over all the lattice sites and $C_{\mathbf{R}}$ is a random quantity equal to unity if the site \mathbf{R} is occupied by the ion A and to zero if the site \mathbf{R} is occupied by the ion B. Obviously $C_{\mathbf{R}}^2 = C_{\mathbf{R}}$.

Let us determine the potential produced by the distribution (1) together with the uniform negative charge¹⁾. We calculate first the potential ϕ_1 of the negative charge and of the aggregate of Gaussian distributions of positive charge $\Delta\rho_1$:

$$\Delta\rho_1 = \sum_{\mathbf{R}} \{Z_A C_{\mathbf{R}} + Z_B(1 - C_{\mathbf{R}})\} (\eta/\pi)^{3/2} e^{-\eta(r - \mathbf{R})^2}. \quad (2)$$

Expanding $\Delta\rho_1$ in a Fourier series in the volume Ω and solving then the Poisson equation, we obtain

$$\phi_1(r) = \frac{4\pi}{\Omega} \sum_{\mathbf{q}} \frac{1}{q^2} e^{-q^2/4\eta} e^{i\mathbf{q}r} \sum_{\mathbf{R}} \{Z_A C_{\mathbf{R}} + Z_B(1 - C_{\mathbf{R}})\} e^{-i\mathbf{q}\mathbf{R}}, \quad (3)$$

where the vector \mathbf{q} runs through all the values of the quasicontinuum with the exception of $q = 0$, and the summation over \mathbf{R} extends over all lattice sites.

Let us determine now the potential ϕ_2 produced by the distribution of the positive pointlike charges (1) and by the distribution of the Gaussian "caps" of negative charge $\Delta\rho_2 = -\Delta\rho_1$. Direct integration of the Poisson equation yields

$$\phi_2(r) = \sum_{\mathbf{R}} \{Z_A C_{\mathbf{R}} + Z_B(1 - C_{\mathbf{R}})\} \frac{1 - \text{erf}[\sqrt{\eta}|r - \mathbf{R}|]}{|r - \mathbf{R}|}. \quad (4)$$

The total potential ϕ should not depend on η . It is easy to verify that this requirement is fulfilled if the integration constant of the Poisson equation is taken to be

$$= -\frac{\pi}{\eta\Omega} \sum_{\mathbf{R}} \{Z_A C_{\mathbf{R}} + Z_B(1 - C_{\mathbf{R}})\} = -\frac{\pi N \bar{Z}}{\eta\Omega}.$$

Then

¹⁾We follow the Ewald-method variant given in [3].

$$\phi(\mathbf{r}) = \phi_1(\mathbf{r}) + \phi_2(\mathbf{r}) - \frac{\pi}{\eta\Omega_0} \bar{Z}, \quad (5)$$

The total energy of the distribution of the charge (1) in the field (5) is obviously

$$\frac{1}{2} \int_{\Omega} d^3r \rho(\mathbf{r}) \phi(\mathbf{r}),$$

and all terms pertaining to the same lattice site should be excluded from the product $\rho\phi$. Thus, the electric energy per ion is

$$\begin{aligned} E_{es} = & \frac{1}{2} \left\{ \frac{4\pi}{\Omega_0} \sum_q' \frac{1}{q^2} e^{-q^2/4\eta} |Z_B S_q + (Z_A - Z_B) C_q|^2 + \right. \\ & + \frac{1}{N} \sum_{\mathbf{R}} \sum_{\substack{\mathbf{R}' \\ \mathbf{R} \neq \mathbf{R}'}} [Z_B + (Z_A - Z_B) C_{\mathbf{R}}] [Z_B + (Z_A - Z_B) C_{\mathbf{R}'}] \frac{1 - \text{erf}[\sqrt{\eta} |\mathbf{R} - \mathbf{R}'|]}{|\mathbf{R} - \mathbf{R}'|} \\ & \left. - \frac{\pi}{\eta\Omega_0} (\bar{Z})^2 - 2\sqrt{\frac{\eta}{\pi}} (\bar{Z}^2) \right\}. \end{aligned} \quad (6)$$

Here

$$S_q = \frac{1}{N} \sum_{\mathbf{R}} e^{iq\mathbf{R}}; \quad C_q = \frac{1}{N} \sum_{\mathbf{R}} C_{\mathbf{R}} e^{iq\mathbf{R}}$$

and we use the notation $(\bar{Z}^2) = Z_A^2 c + Z_B^2 (1 - c)$. The last term in the curly brackets cancels exactly the contribution of the terms with $\mathbf{R} = \mathbf{R}'$ retained in the first sum over q .

Expression (6) is valid for an arbitrary distribution of the ions A and B over the lattice sites. We now assume that the distribution is random and average. If there is no short-range order then (cf., e.g., [4])

$$\overline{C_{\mathbf{R}} C_{\mathbf{R}'}} = \begin{cases} c^2 & \text{for } \mathbf{R} \neq \mathbf{R}' \\ c & \text{for } \mathbf{R} = \mathbf{R}' \end{cases}; \quad \overline{C_q} = c S_q; \quad \overline{C_q C_{q'}} = \begin{cases} c^2 |S_q|^2 & \text{for } q = h \\ \frac{c(1-c)}{N} & \text{for } q \neq h \end{cases}$$

(h is any reciprocal-lattice vector). Then

$$E_{es} = \bar{E}_{es} + \frac{1}{2} \left\{ c(1-c)(Z_A - Z_B)^2 \frac{4\pi}{\Omega} \sum_q'' \frac{1}{q^2} e^{-q^2/4\eta} - 2\sqrt{\frac{\eta}{\pi}} [(\bar{Z}^2) - (\bar{Z})^2] \right\}. \quad (7)$$

The double primes denote summation over all points of the quasicontinuum with the exception of the reciprocal-lattice points. \bar{E}_{es} in (7) is the electrostatic energy of the "average" lattice, i.e., of the lattice of the positive ions of charge \bar{Z} in the homogeneous field of a charge of density \bar{Z}/Ω :

$$\bar{E}_{es} = \frac{(\bar{Z})^2}{2} \left\{ \frac{4\pi}{\Omega_0} \sum_q' \frac{1}{q^2} e^{-q^2/4\eta} |S_q|^2 + \sum_{\mathbf{R}} \frac{1 - \text{erf}[\sqrt{\eta} |\mathbf{R}|]}{|\mathbf{R}|} - \frac{\pi}{\eta\Omega_0} - 2\sqrt{\frac{\eta}{\pi}} \right\}. \quad (8)$$

We note that the expression for E_{es} in [1] contains only the first two terms of (7). We shall now show that the sum of the last two terms in (7) is equal to zero. Indeed, the contribution made to the sum over the quasicon- tinuum by the reciprocal-lattice sites is negligibly small ($\sim 1/N$) and therefore we can replace this sum by the integral over all of reciprocal space. The latter can be readily evaluated, and as a result we find that the last two terms in (7) cancel each other exactly. Finally we get

$$E_{es} = \bar{E}_{es}. \quad (9)$$

We recall, however, that relation (9) was obtained under the assumption that there is no short-range order at all in the alloy. Allowance for the short-range order leads immediately to the appearance of an additional contri- bution to the electrostatic energy

$$\Delta E_{es} = \frac{1}{2} (Z_A - Z_B)^2 \left\{ \sum_{\mathbf{R}} \epsilon(\mathbf{R}) \frac{1 - \text{erf}[\sqrt{\eta}|\mathbf{R}|]}{|\mathbf{R}|} + \frac{4\pi}{\Omega} \sum_{\mathbf{q}} \frac{1}{q^2} e^{-q^2/4\eta} \right\}. \quad (10)$$

Here $\epsilon(\mathbf{R})$ are the correlation parameters defined by the relation [4]

$$\overline{C_{\mathbf{R}} C_{\mathbf{R}'}} = c^2 + \epsilon(\mathbf{R} - \mathbf{R}'), \quad \epsilon(\mathbf{q}) = \frac{1}{N} \sum_{\mathbf{R} \neq 0} \epsilon(\mathbf{R}) e^{i\mathbf{q}\mathbf{R}}.$$

It is easy to verify that ΔE_{es} does not depend on η ($\partial \Delta E_{es} / \partial \eta = 0$), as should be the case in accordance with the requirements of the Ewald transformation.

In conclusion we note that the results are valid for both a Bravais lat- tice and for a lattice with a basis.

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PLANAR MODEL OF A BRANCHED DOMAIN STRUCTURE OF A CUBIC FERROMAGNET

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Submitted 19 January 1971

ZhETF Pis. Red. 13, No. 4, 222 - 224 (20 February 1971)

It is well known that in cubic ferromagnets cut in the form of plates perpendicular to the easy axis, a domain structure with closed triangles is possible [1]. There is no anisotropy energy in this case, so that the total energy is made up of the energy of the surface tension on the phase boundaries and the magnetostriction energy, which is concentrated near the surface of the sample at distances on the order of the domain widths. The magnetostriction energy is very small in most cases (e.g., in iron). The total energy is there- fore also small, and as a result this structure hardly ever becomes branched. According to an estimate by Lifshitz [1], branching in an iron plate cut per- pendicular to the easy axis should begin only when the plate thickness is