

ON THE DETERMINATION OF INTERATOMIC CORRELATION PARAMETERS IN ALLOYS WITH h. c. p. STRUCTURE

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An additional term is obtained in the expression for the intensity of diffuse X-ray scattering for alloys with close radii of the neighboring coordination spheres. A technique is suggested for determining interatomic correlation parameters corresponding to these spheres.

A large number of investigations [1] are devoted to studying interatomic correlations in solid solutions using the diffuse X-ray scattering (DXRS) method. These investigations were primarily carried out for f. c. c. and b. c. c. alloys. A considerably smaller number of works are devoted to the study of alloys with h. c. p. structure [2-10]. The h. c. p. alloys are characterized by close values of the radii of some coordination spheres, owing to which the traditional analysis cannot be applied [1]. In a number of studies the coordination spheres with close radii were combined, and the effective values of interatomic correlation parameters were determined for them. When the signs of the combined parameters are different, their effective values may turn out to be nearly zero although the parameters themselves may have substantial magnitudes.

The present paper is devoted to the development of a method of calculating the interatomic correlation parameters for alloys with close radii of neighboring coordination spheres.

In accordance with [11] and neglecting the static displacements, the intensity of the DXRS by a single crystal alloy can be written in the form

$$I = N \sum_{\gamma\gamma'=1,2} (\Delta f)^2 \left[C(1-C)\delta_{\gamma\gamma'} + \sum_{\rho_{\gamma\gamma'}} \varepsilon(\rho_{\gamma\gamma'}) \exp\{i\mathbf{Q}\rho_{\gamma\gamma'}\} \right], \quad (1)$$

where $(\Delta f)^2$ is the square of the difference of the component atomic factors, $\gamma = 1, 2$ is the index of the site in the cell, C is concentration, $\varepsilon(\rho_{\gamma\gamma'})$ is the correlation parameter, \mathbf{Q} is the scattering vector, and $\delta_{\gamma\gamma'}$ is the Kronecker delta.

When studying polycrystal alloys it is necessary to average expression (1) over all orientations of the scattering vector:

$$I_p = \frac{1}{4\pi q^2} \int_S I(q) dS, \quad (2)$$

where $q = 4\pi \sin \theta / \lambda$ and λ is the X-ray radiation wavelength. The integration in (2) extends over a sphere S of radius q in the reciprocal lattice space. Taking into account that the relation $\varepsilon(-\rho) = \varepsilon(\rho)$, the integration results in

$$I_p = 2N(\Delta f)^2 \left[C(1-C) + \sum_{\rho_{11}^i} C_{11}^i \varepsilon(\rho_{11}^i) \frac{\sin q\rho_{11}^i}{q\rho_{11}^i} + \sum_{\rho_{12}^i} C_{12}^i \varepsilon(\rho_{12}^i) \frac{\sin q\rho_{12}^i}{q\rho_{12}^i} \right], \quad (3)$$

where C_{11}^i and C_{12}^i are the coordination numbers, $\varepsilon(\rho_{11}^i)$ is the correlation parameter for the i th coordination sphere of atoms located at the sites of the first sublattice, $\varepsilon(\rho_{12}^i)$ is the same parameter for atoms one of which is at a site in the first sublattice and the other are at the sites of the second sublattice, ρ_{11}^i is the radius of the i th coordination sphere in the first sublattice, and ρ_{12}^i is the radius of the i th coordination sphere joining the sites of the first sublattice to those in the second sublattice.

Let the radii ρ_{11}^1 and ρ_{12}^0 be close to each other. The resulting contribution to the intensity corresponding to them can be written as

$$\frac{\Delta I}{2N(\Delta f)^2} = C_{11}^1 \varepsilon(\rho_{11}^1) \frac{\sin q\rho_{11}^1}{q\rho_{11}^1} + C_{12}^0 \varepsilon(\rho_{12}^0) \frac{\sin q\rho_{12}^0}{q\rho_{12}^0}. \quad (4)$$

Passing from the values of $\varepsilon(\rho_{12}^0)$, $\varepsilon(\rho_{11}^1)$ and ρ_{11}^1 , ρ_{12}^0 to their average values and differences we rewrite (4) as

$$\frac{\Delta I}{2N(\Delta f)^2} = C_{11}^1 \left(\bar{\varepsilon} + \frac{\Delta\varepsilon}{2} \right) \frac{\sin q(\bar{\rho} + \Delta\rho/2)}{q(\bar{\rho} + \Delta\rho/2)} + C_{12}^0 \left(\bar{\varepsilon} - \frac{\Delta\varepsilon}{2} \right) \frac{\sin q(\bar{\rho} - \Delta\rho/2)}{q(\bar{\rho} - \Delta\rho/2)}, \quad (5)$$

where

$$\bar{\varepsilon} = [C_{11}^1 \varepsilon(\rho_{11}^1) + C_{12}^0 \varepsilon(\rho_{12}^0)]/2, \quad (6)$$

$$\Delta\varepsilon = C_{11}^1 \varepsilon(\rho_{11}^1) - C_{12}^0 \varepsilon(\rho_{12}^0), \quad (7)$$

$$\bar{\rho} = (\rho_{11}^1 + \rho_{12}^0)/2, \quad (8)$$

$$\Delta\rho = \rho_{11}^1 - \rho_{12}^0. \quad (9)$$

Expression (5) can be transformed to obtain

$$\frac{\Delta I}{2N(\Delta f)^2} = \bar{\varepsilon}_{\text{eff}} \cos q \frac{\Delta\rho}{2} \frac{\sin q\bar{\rho}}{q\bar{\rho}} + \Delta\varepsilon_{\text{eff}} \sin q \frac{\Delta\rho}{2} \frac{\cos q\bar{\rho}}{q\bar{\rho}}, \quad (10)$$

where

$$\bar{\varepsilon}_{\text{eff}} = \frac{1}{\bar{\rho}} C_{11}^1 \varepsilon(\rho_{11}^1) \rho_{12}^0 + C_{12}^0 \varepsilon(\rho_{12}^0) \rho_{11}^1, \quad (11)$$

$$\Delta\varepsilon_{\text{eff}} = \frac{1}{\bar{\rho}} C_{11}^1 \varepsilon(\rho_{11}^1) \rho_{12}^0 - C_{12}^0 \varepsilon(\rho_{12}^0) \rho_{11}^1. \quad (12)$$

When deriving (10) we neglected the term $(\Delta\rho/2)^2/\bar{\rho}^2$. Therefore the condition for the applicability of expression (10) is the inequality

$$\frac{(\Delta\rho/2)^2}{\bar{\rho}^2} \ll 1. \quad (13)$$

It is obvious that condition (13) is fulfilled at least for $\Delta\rho < 0.5 \text{ \AA}$ (for cadmium we have $\Delta\rho \sim 0.3$). On the other hand, if $\Delta\rho \sim 0.01$ (manganese), then (10) goes into the earlier applied expression, however with a different method of averaging the sphere radii and correlation parameters.

The method of averaging these quantities suggested in this paper seems to be more consistent.

The numerical estimates show that in the case of different signs of the parameters $\varepsilon(\rho_{11}^1)$ and $\varepsilon(\rho_{12}^0)$ the magnitude of the second term in (10) may substantially exceed the contribution of the first term. Therefore, when carrying out investigations of interatomic correlations in alloys with close neighboring radii of coordination spheres it is necessary to take into account the term proportional to $\cos q\bar{\rho}/q\bar{\rho}$.

Expression (10) implies that the angular dependence is qualitatively different for the two terms. Therefore, in the determination of interatomic correlation parameters, for instance, by the least squares method, it is suggested that not the parameters $\varepsilon(\rho_{11}^1)$ and $\varepsilon(\rho_{12}^0)$ themselves but the values of $\bar{\varepsilon}_{\text{eff}}$ and $\Delta\varepsilon_{\text{eff}}$ should be determined, after which the desired parameters are found with the aid of (11) and (12).

Earlier only the effective values of the parameters were determined, the methods of averaging the parameters and the corresponding radii having the form

$$\varepsilon_{ij} = \frac{C_i \varepsilon_i \sin(qr_i)/qr_i + C_j \varepsilon_j \sin(qr_j)/qr_j}{(C_i + C_j) \sin(q\bar{r}_{ij})/q\bar{r}_{ij}}, \quad (14)$$

$$\bar{r}_{ij} = (C_i r_i + C_j r_j)/(C_i + C_j). \quad (15)$$

These averaging methods seem to be insufficiently accurate. Their application may lead to additional errors in the determination of the interatomic correlation parameters.

Hence, in the present paper, within the framework of the DXRS method, an expression is obtained for the additional term in the formula for the DXRS intensity of disordered alloys characterized by substantial closeness of radii of some coordination spheres, and a method is suggested for separate determination of the corresponding interatomic correlation parameters. For the case of close coordination spheres definitions of effective interatomic correlation parameters are introduced that differ from those used traditionally.

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