NOVEL METHOD OF STRUCTURE ANALYSIS ADOPTED FOR THE LRO TERNARY Cu_2NiZn ALLOY

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Theory

The X-ray intensity from a ternary ordered alloy is given as

$$I_{\mathrm{Order}}(\mathbf{q}) = \sum_i \sum_{j(>i)} x_i x_j \left| f_i - f_j \right|^2 \alpha^{ij}(\mathbf{q}), \qquad (1)$$

$$\alpha^{ij}(\mathbf{q}) = M^{ij} + v_{\mathrm{BZ}} \sum_{\mathbf{G}} T_{\mathbf{G}}^{ij} \delta(\mathbf{q}-\mathbf{G}), \qquad (2)$$

$$T_G^{ij} = -\mathrm{Re}\left[F_G^i F_G^{j*} \right], \qquad (3)$$

where x_i and f_i are the fraction and atomic scattering factor of the ith kind of atom, respectively. M^{ij} is the uniform background due to the mixing occupation on the sublattices. $T_{\mathbf{G}}^{ij}$ means the partial intensity due to the ordering of i and j atoms at the superlattice reflection point **G**. $T_{\mathbf{G}}^{ij}$ is represented in terms of $F_{\mathbf{G}}^i$ defined as

$$F_{\mathbf{G}}^i = \frac{1}{N_{\mathrm{s}}} \sum_M (x_i^M - x_i) \exp(-2\pi i \mathbf{G} \cdot \xi_M), \qquad (4)$$

where ξ_M is the step-shift vector of the Mth sublattice. The summation is taken over N_{s} sublattices. x_i^M is the fraction of ith atom on the Mth sublattice.

$T_{\mathbf{G}}^{ij}$ can be experimentally determined in the anomalous scattering method. But this parameter cannot be easily used for analysis, because of the probability of orientational variants of ordered lattice with lower symmetry than the average lattice. Integration of eq. (2) within the Brillouin zone leads to

$$M^{ij} + D^{ij} = 1, \quad D^{ij} = \sum_{\mathbf{G}(\mathrm{BZ})} T_{\mathbf{G}}^{ij}. \qquad (5)$$

D^{ij} does not depend on the existence of the variants, and is more convenient than $T_{\mathbf{G}}^{ij}$. D^{ij} is represented as a function of x_i^M's through eqs. (3), (4) and (5), and three equations D^{ij} = $(\mathrm{constant})_{ij}$ are regarded as three planes in the $3N_{\mathrm{s}}$ dimensional space expanded with x_i^M axes. Thus, we can expect the intersections among the planes to determine a probable set of x_i^M's. Actually, there are more restrictions on the relation among a possible set of x_i^M's, i.e.

$$\sum_i x_i^M = 1, \qquad \sum_M x_i^M = N_{\mathrm{s}} \qquad (6)$$

$$0 \le x_i^M \le 1, \qquad x_i^M \le N_{\mathrm{s}} x_i. \qquad (7)$$

If the type of order could be predicted for the sample crystal, some sublattices may be identical and we have

$$x_i^M = x_i^{M'} = x_i^{M''}, \ldots, . \qquad (8)$$

Experimental

The experimental procedure on $Cu_{0.47}Ni_{0.29}Zn_{0.24}$ was reported in PF Act. Rep. #17B (1999) 206.

Results and Analysis

Our synchrotron anomalous scattering experiment for the partial intensity separation gave

$$D^{\mathrm{Cu-Ni}} = -0.36, D^{\mathrm{Ni-Zn}} = 1.21, D^{\mathrm{Zn-Cu}} = 0.95. \qquad (9)$$

We have already known that two kinds of $L1_2$ models were reported, and first tried to analyze the present result as to which model is correct. If the $L1_2$ structure is considered, 12 x_i^M's can be reduced into only 2 variables, the fractions of Ni and Zn atoms occupying the corner site of the fcc cell $x_{\mathrm{Ni}}^{\mathrm{I}}$ and $x_{\mathrm{Zn}}^{\mathrm{I}}$. Then, eqs. (9) can be drawn as 3 lines in the two dimensional coordinate system, determining $x_{\mathrm{Ni}}^{\mathrm{I}}$ and $x_{\mathrm{Zn}}^{\mathrm{I}}$ to be –0.04 and 1.0, respectively, and eventually $x_{\mathrm{Cu}}^{\mathrm{I}} = 0.04$. The occupancy probabilities were calculated to be 0.6 Cu and 0.4 Ni on the face-centered sites, being the same as the Koester's model, which is also the same as our preliminary result given in PF Act. Rep. #17 (1999) 207.