Formation of off-phase domains in $L1_2$ type ordering

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Domain structures consisting of multiple off-phase variants are generally formed in ordering process in binary alloy systems. Multiple order parameters should be defined in order to describe the ordered states including such domain structures. The present authors previously developed a Time-dependent Ginzburg-Landau (TDGL) formulation for ordering process of $L1_2$ type in binary alloys [1]. The $L1_2$ type order is formed in $A_{3-\varepsilon}B_{1+\varepsilon}$ alloys on the basis of a face-centered-cubic (fcc) lattice, in which the major A atoms are preferentially located on the face-centered lattice sites, while the minor B atoms are on the corner sites. In this type of order, there exist four distinct crystallographic variants, anyone of which is displaced from the other three by one of the three primitive translations of the fundamental fcc lattice. In the $L1_2$ phase the fcc lattice is divided into four simple cubic sublattices. The atomic occupation probabilities on the sublattices are represented by three independent order parameters ξ, η and ζ, and a composition parameter ε. The order parameters can be measured independently to each other through crystal structure factors. If the state of order of atomic arrangement is represented by a point in the three dimensional Euclidean space spanned by the three order parameters, the four equivalent variants are defined by the four tips of a regular tetrahedron centered on the origin for the disordered state. A mean-field free energy is defined in a form of Landau type expansion with the order parameters and the composition parameter. Interfacial energies due to local variations of degrees of order and concentration are given in a gradient square approximation with the cubic symmetry. Kinetic equations for time-evolution of the order parameters and the concentration are derived from the Ginzburg-Landau type potential consisting of the mean-field free energy density and the interfacial energy terms. Formation of off-phase variants was simulated by treating the kinetic equations numerically in a three-dimensional cell scheme.

Figure 1 shows an example of simulation results of off-phase domain structures formed in the $L1_2$-type ordering. Here off-phase boundaries of ordered variants appear in dark contrast. One may recognize that the $L1_2$ type ordering results in formation of rectangular type of variant structures. It is known that there exist two kinds of off-phase boundaries in the $L1_2$ variants. When the displacement vector for the phase shift between variants lies on the boundary plane, the off-phase boundary is called conservative type, otherwise non-conservative. The interface energy density of the former type is usually lower than that of the latter type. Therefore the off-phase boundaries sometimes show preferential orientations to {100} in the cubic lattice system. Figure 2 gives a TEM (Transmission Electron Microscopy) image of Cu_3Au binary alloys with $L1_2$ order. The characteristic rectangular type of off-phase domains is observed in the real alloy system. Thus, the present formulation of kinetic equations can be applied to simulate time-evolution of ordered domain structures with the characteristic anisotropy of cubic symmetry in $L1_2$ type ordering.

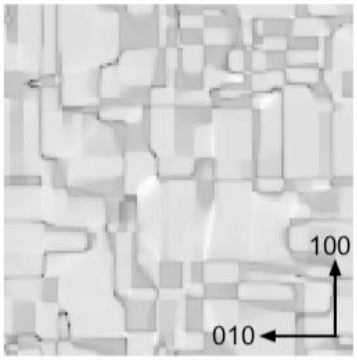

Fig. 1: An off-phase domain structure of $L1_2$ type ordering obtained by three-dimensional simulation.

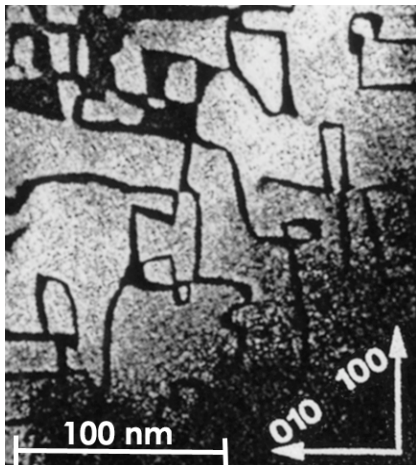

Fig. 2: 110 dark field image in the [001] orientation [2].Off-phase boundaries with dark contrast are shown along [100] and [010] direction.

References

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[2] L. Potez and A. Loiseau: Interface Sci. 2, 91 (1994).