ATOMIC CONFIGURATIONS OF ANTIPHASE BOUNDARIES IN Ll₂ SUPERLATTICE ALLOYS:

APB OF 1/2 <110> {110} TYPE

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An antiphase boundary of 1/2 <100> {110} type in equilibrium with atomic displacements is examined, such as occurs in an ordered alloy with Ll₂ superlattice. The effects from discrepancies in the atomic radii are evaluated along with those from differences in atomic interaction in a parallel simulation of the lattice states near planar defects in ordered Cu₃Au and Ni₃Fe. It is found that there are substantial differences in the local deformations at these boundaries by comparison with other types of planar defect: there are parallel planes involving compression and stretching together with oscillating atomic displacements perpendicular to the boundary, which die away at the eighth plane from the APB. It is found that the region of local deformation out to which the continuum theory of elasticity does not apply extends to ten planes of {110} type.

The properties of an ordered alloy are substantially dependent on the lattice states near various defects [1]. An ordered alloy may show many different planar defects: antiphase boundaries (APB) and combined packing defects (CPD) and superlattice parameter and long-range order parameter near certain APB differ from those of the ideal crystals for materials having Ll₂ and B2 superlattices. Calculations related to computer experiments have shown that there are complicated lattice states in an Ll₂ superlattice in an ordered alloy near APB of 1/2 <110> {111}, 1/2 <100> {100}, CPD, and SPD types. The evidence [4-7] indicates that there are atomic displacements localized near the defects that represent combinations of compression, stretching, and rotation, which cannot be predicted from the continuum theory of elasticity. These lattice states must be considered in constructing a work-hardening theory for such materials [8].

It is assumed [9, 10] that an APB of 1/2 <100> {110} type arises mainly as a result of thermal growth in antiphase domains. To check this and to detect the effects of such boundaries on processes associated with work hardening in ordered alloys, we have made a computer study of the atomic configurations and formation energies of APB, including the height of the potential barrier. To estimate the contributions from atomic-size discrepancies in the components and the differences in the interactions, we have made a parallel study on the model alloys of Cu₃Au and Ni₃Fe types (the atomic radii of Ni and Fe differ by less than 1%, whereas the components in Cu₃Au differ by 13%).

The formation energy for an APB of 1/2 <100> {110} type is as follows in a model based on hard spheres and the interactions between the atoms in the first three coordination spheres:

\[ \gamma = \frac{1}{a^2} \left( w_1 - 2w_2 + 2w_3 \right). \]

where \( \eta \) is the long-range order parameter, \( a \) is the lattice parameter in the ordered alloy, and \( w_i \) is the ordering energy in coordination sphere \( i \). Then the APB formation energies are 85.7 mJ/m² for Cu₃Au and 121.8 mJ/m² for Ni₃Fe. The formation energies for other APB types [4-7] show that APB of cubic orientation are preferred as regards formation energy in Cu₃Au, whereas the formation energies for all types of boundary are overestimated relative to experiment for Ni₃Fe [11]. More accurate values can be obtained for planar-defect formation energies by making calculations on defects in equilibrium as regards atomic displacements.

A variational method was applied to the equilibrium lattice state in an ordered alloy containing a single 1/2 \text{[110]} \text{[110]} APB. The interactions between the atomic pairs were approximated as sets of Morse potentials, for which the derivation method and the parameters have been given in detail in [4-7]. We examined the configuration of the completely ordered alloy at 0\degree K. The coordinate axes were as follows: the z axis was perpendicular to the defect plane, while the x and y axes lie in that plane along \text{[110]} and \text{<001>} correspondingly. The APB plane was taken as the zero one, and the subsequent \text{[110]} planes to the left and right were denoted as \pm 1, \pm 2, \pm 3, \ldots \text{ in sequence. This crystal block was chosen such that the boundary atoms showed no additional displacements during relaxation by comparison with the positions in the ideal lattice. Each atom in the block was capable of displacement in three dimensions to give the minimum in the internal energy for the entire system.}

The figures show the patterns for the atomic displacement near the equilibrium APB. Figure 1 shows the displacements on the \text{[110]} planes in a direction perpendicular to the boundary. The odd-numbered planes from the defect are mixed ones, i.e., they consist of atoms of type A and B, and the differences in the interactions cause them to split up into two monoatomic subplanes away each on relaxation. The largest splittings occurred in the first planes away from the defect: 0.0074 nm for Ni\textsubscript{3}Fe and 0.0078 nm for ordering Cu\textsubscript{3}Au. All the even planes consisted only of A atoms and did not split, being displaced as a whole on relaxation. The mean interplanar distances were reduced near the boundary; in Ni\textsubscript{3}Fe, the reduction in the distance between the zeroth and first planes was 2.5\%, but it was only 0.4\% for Cu\textsubscript{3}Au. Compression predominates near the APB in ordered Ni\textsubscript{3}Fe, which reduces the local volume around the defect somewhat; in Cu\textsubscript{3}Au, the displacements were mainly sign-varying and did not alter the volume of the crystal in the presence of the planar defect, which may be related to the size factor.

Displacements parallel to the defect plane were observed only on the even-numbered planes. The displacements were less by an order of magnitude than those along the normal to that plane. The displacements were directed in such a way as to produce alternating regions of local compression and stretching in the form of bands of width equal to the distance between the atomic rows along the y axis. The compression and expansion regions occur because the atoms of one type in adjacent odd planes approach the atoms in the related even plane, whereas the atoms of the other type recede from it. The displacements attain their maxima in the second \text{[110]} planes away from the APB and then decrease up to the eighth planes away from the defect. Figure 2 shows that the displacements parallel to the boundary are larger in Ni\textsubscript{3}Fe than in Cu\textsubscript{3}Au, which may be due to a predominant effect from the differences in the atomic interactions.

Incorporating lattice relaxation near the defect reduces the APB formation energies considerably: to 5.3 mJ/m\textsuperscript{2} for Cu\textsubscript{3}Au and to 18.3 mJ/m\textsuperscript{2} for Ni\textsubscript{3}Fe. However, although this type