STUDY OF POINT DEFECTS FOR B2 STRUCTURES WITH A
ω-TYPE MARTENSITIC PHASE

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The molecular dynamics method has been used to study the effects of the inheritance from point defects in B2 structures having an ω-like martensitic transformation with different final reaction products. For order defects, antistructural atoms, and their simplest complexes it has been shown that in several cases the number of atoms in the defects increases sharply for martensite during the transition to austenite. Here the fraction of chemical energy accumulated by the defects grows. A certain type of defect in the B2 structure in martensite corresponds to the appearance of high-energy linear disordered chains in directions of the [111]B2 type. This can play a substantial role in the determine the path of the reverse martensitic transformation.

Interest in questions of the inheritance by martensitic phases of defects from the high-temperature phase arises because they strongly affect the thermodynamic properties of the phases and the kinetics of the transition [1, 2]. There is a broad class of materials, for example ordered intermetallic alloys with the B2 structure, NiTi, NiAl, FeMn, FeNi, CuMn, AuCd, InTi, etc. in which the elementary event of plasticity occurs due to a reversible martensitic transition and a number of other processes. In these alloys in particular one can observe complete or partial reversibility of the inelastic deformation imparted to them [1]. The recovery is initiated by forces of mechanical and chemical origin (forces on the side of stacking faults and antiphase boundaries, point defects).

While the mechanical stress always tends toward recovery of the deformation the thermodynamic force proportional to the difference in the thermodynamic potentials of the phases can be in one or the other direction depending on the temperature. Then the overall direction of the reaction or direction of development of the deformation will be determined by the sum of mechanical and chemical forces. It is important to note that the chemical forces often predominate over the mechanical ones; therefore the microstress just like the stress arising from an external load, exerts only a small perturbing effect on the development of the transition. The introduction of defects can change the relation between the "chemical" and mechanical forces and strengthen the effect of mechanical stress on the transition.

A phase transition in a material containing defects causes the reaction products to accumulate high-energy defects as a result of their inheritance. During an "exactly reversed" reaction there is full restoration of the initial low-energy structure. The other conceptual idea of the path of the reverse transition is one where the high-energy defects inherited from the forward reaction acquire still higher energies. Consequently an energy arises in the lattice which tends to produce a reverse martensitic transition with certain transition paths since only during such reactions is there complete restoration of the initial low-energy defect structure.

This conclusion turns out to be valid not only for dislocations but also for point defects or complexes of them where the change in short-range order turns out to be important [1].

Moreover the point defects can turn out to influence the path of the reverse martensitic transition and can also change the sequence of forward martensitic transitions. Thus while in nickel titanium containing 50.2 at. % Ni a B2(β) → B19' phase transition is observed, in annealed alloys with excess nickel (for example Ti49Ni51) the martensitic transition occurs in the sequence B2 → R → B19' [3]. This fact is related to the strong effect of the regions of local nickel enrichment and more rapid growth of the fraction of nonordered atoms in the disordered system in comparison with a concentrationally disordered one [3]. An increase in the number of localized regions with order defects and a change of the distribution of the defect spectrum during annealing affects the sequence of transitions.

No theory explaining the regularities in the inheritance of defects has been given to the present time. The question of the inheritance during martensitic transformations of dislocational defects has been treated in [1].

Interest in the study of point defects during martensitic transformations arises because in alloys with the ordered B2 (CsCl) structure the degree of long-range order $\eta$ as a rule is less than unity even for the stoichiometric state. For example $\eta$ does not exceed 0.84 in TiNi [3]. These alloys contain a substantial quantity of point defects connected with local disorder. A deviation from stoichiometry also lowers the degree of long-range order. The excess atoms which occupy sites in the foreign sublattice form substitutional defects. When they are inherited by martensite not only are these changes in the short-range surroundings about a defect in the reaction product, but as shown in [4] new point ordering defects and their complexes can be generated. The simplest complex of substitutional defects and ordering defects can decay into several defects [4].

The martensitic transformation can change the local surroundings about a point defect. As a result, if before the transformation the contribution from point defects to the thermodynamic potential was $G_0$, then after the transformation it changes by $\Delta G$ on account of the difference in the energies of the defects and their numbers [4] in the initial phase and the reaction products. The change $\Delta G$ leads to the appearance of additional chemical forces which should arise during the martensitic transformation. With a "soft" lattice (low shear modulus) the defects are stimulated to form defect superlattices on account of the lowering of the energy by relaxation. The formation of such superlattices can stimulate the martensitic transformation.

Here we consider the fine structure of the point defects and their simplest complexes during $\omega$-like martensitic transformation of an ordered B2 lattice.

We used the molecular dynamics method [5, 6] with computational cells of variable size and shape and periodic boundary conditions to study the problem of inheritance of point defects. With a soft lattice the distortion about a defect reached the boundary of the computational cell and the defect cannot be regarded as isolated. In this case the use of periodic boundary conditions is equivalent to considering an infinite superlattice of defects with primitive translation vectors equal to edges of the computational cell. Modeling of the martensitic transformation process in a crystal has certain limitations connected with the periodic boundary conditions due to the simultaneous nature of the processes in all primitive cells of the defect superlattice.

The computations were done with empirical pairwise potentials fitted to the elastic constants, interaction energy, and equilibrium lattice parameters for pure Ti and Ni [4] and the superstructure B2 of TiNi. Consideration of multiparticle interactions was done by introducing in the energy of formation of the intermetallic compound TiNi of a volume-dependent term which was represented as a Fourier series.

Figure 1 shows the point defects in the B2 structure introduced by the martensitic transition [4] in the hexagonal closest-packed structure. This phase is obtained from the B2 lattice by the collapse of three (111)-type planes which contain atoms of the same sort. Formation of this martensitic phase occurs through an intermediate martensitic of rhombohedral symmetry. The intermediate martensite is also a layered ordered structure whose (111) planes contain atoms of a different type with concentrations $C_A = 1/3$ and 2/3 in the alternating planes.

We studied the following types of defect: order defects (Fig. 1a) produced by interchange of the Ti and Ni atoms in the first coordination sphere; antistructure Ti atoms and order defects which form linear chains along the [111] direction (Fig. 1b); defects forming isosceles triangles with base a lying in (110) planes whose vertices are excess Ti atoms and order defects (Fig. 1c).

An arbitrary scheme for the displacements of the B2 lattice planes during the transition into the martensitic phase is shown in Fig. 2. We show from above the packing of the (111)$_2$ planes in the computational cell. The planes occupied by Ti are denoted by dark circles and those occupied by Ni by open circles. The positions of the sites which contain defects and