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A rationale for transformation twins in ordered alloys

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A mechanism based on the growth of the ordered phase in the disordered matrix is advanced to explain the presence of numerous transformation twins in the ordered structure. The merits of this mechanism are considered on the basis of available experimental results on ordered alloys.

1. Introduction

Twins, like banded microstructures, are often observed in ordered alloys where the ordering transformation involves a change in the crystal system. As early as 1916, Kurnakov and his co-workers [1] reported observing such a microstructure in ordered equiatomic CuAu. Later investigations have confirmed this observation not only in CuAu [2, 3, 4] but in many other systems [5-8] as well. By electron diffraction, Pashley and Presland [3] identified the bands in CuAuI as twins and determined the composition plane to be {101}. Hirabayashi and Weissman [4] have confirmed this observation and attributed the twinning to misfit stresses created during ordering. Tanner and Ashby [9] have shown that twinning can cancel some of the components of the transformation strain ϵ_{ij}^{t}, though not the transformation strain arising from a volume change. In this paper we propose a growth mechanism for the formation of transformation twins during ordering and show how this mechanism can neatly explain all the experimental observations.

2. A proposed growth mechanism

Consider the following hypothetical ordering system. Phase A is disordered and phase B is an ordered phase of lower symmetry. The transformation strains ϵ_{ij}^{t*} are small and there is no volume change, i.e., $\epsilon_{ii}^{t} \approx 0$. The number of atoms in the unit cell remains constant. Let us also assume that the coherent interface between A and B is a symmetry plane of phase A. This assumption is justified for CuAu, where experimental results are available [11] showing {101} as the coherent plane for the growth of the ordered matrix.

Since the components of the transformation strain are small, the atom movements (considering atoms sites only) required to propagate the ordered phase are also small. If during growth, atom movement takes place in the $+x$

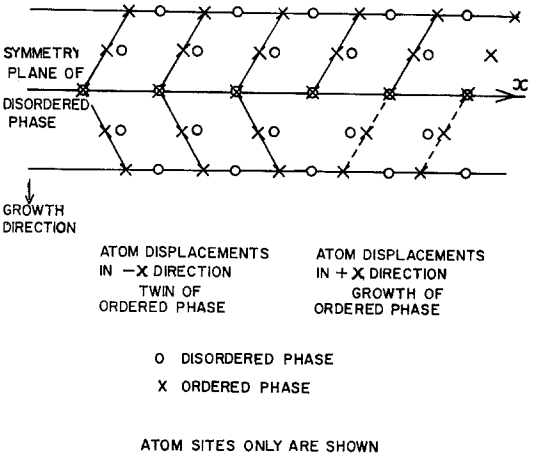

Figure 1 A schematic diagram illustrating the growth of ordered phase or a twin from the disordered matrix.

*The transformation strain ϵ_{ij}^{t} relates the unstrained parent phase to the unstrained ordered phase. Eshelby [10] has shown how to calculate displacements, stresses and strains when a region of transferred material is constrained by the surroundings.

direction, (Fig. 1) the ordered lattice is extended by one atom plane. However, if the atoms move in the $-x$ direction, and if this direction is maintained during further growth, the requirement that the original coherent interface be a symmetry plane of the disordered matrix leads to the growth of a twin of the ordered phase.

If the original transformation strain is a plane strain (with no displacements perpendicular to the coherent interface), then the reversal of the growth mode, as discussed above, results in a transformation strain of $-\epsilon_{ij}{}^{t}$ and, hence, the total transformation strain over a transformed region is $(1 - 2f)\ \epsilon_{ij}{}^{t}$ where f is the volume fraction of the twinned phase. The total transformation strain can be zero when $f = \frac{1}{2}$. Thus it becomes energetically favourable for the crystal to reverse the direction of atomic displacement frequently (i.e., to twin the crystal) during growth removing some of the transformation strain. This type of growth results in a lamellar twinned microstructure. This process is analogous to Gleiter's proposed mechanism [17] for the growth of annealing twins in fcc metals.

The strain between twinned regions is $2\ \epsilon_{ij}{}^{t}$ and this represents the twinning shear. If the transformation is unconstrained, as in a free surface, the strain observed would be $\epsilon_{ij}{}^{t}$ for one twin and $-\epsilon_{ij}{}^{t}$ for the other. Measurements of surface displacements can, therefore, assist in the determination of transformation strains.

If the transformation strain is not a pure plane strain, then, as Tanner and Ashby [9] have shown, it cannot be fully cancelled by the operation of one twinning system alone. In such cases the residual strain will affect the twin orientation in adjacent domains.

3. A comparison of the predicted features of the model with experimental observations

The twinning plane referred to the disordered phases is [101] for Ll_0 structures (e.g. CuAu, CoPt [3, 5] {101} for DO_{22} (Ni_3V [6]), {100} for Ll_1 (CuPt [7]) and (010) in the monoclinic-to-triclinic ordering of alkali feldspars [8]. In every one of these, the twinning plane is a symmetry plane in the disordered phase.*

Unfortunately, adequate data on the measurements of surface relief on ordered crystals are not available to compare the predicted values of $\epsilon_{ij}{}^{t}$ with the measured ones. The one exception to this is the recent measurement in CuPt by Irani and Cahn [7], who have shown that the twinning shear is small. The amount is of the order of $2\ \epsilon_{ij}{}^{t}$. This measurement helps us in considering whether transformation twins could indeed be mechanical twins. The shears that have been suggested for mechanical twins in ordered alloys are rather high (e.g., ~ 1 for Ni_3V and ~ 2 for CuAu) and if twinning were to occur by this mechanism, then the volume fraction of the twinned material must be small. On the contrary, experimental observations show extensive twinning in the ordered microstructure.

Irani and Cahn interpret their observations by invoking a small shear of approximately $2\ \epsilon_{ij}{}^{t}$ applied to the ordered phase *followed by* a diffusional atomic rearrangement to their correct positions, since this shear does not preserve the crystal structure. It is this associated rearrangement which allows the mechanical shear to be reduced to a feasible value.

Another point of interest is concerned with the twinning systems operating in the ordered alloy during mechanical *deformation*. Experimental results available on CuAu [13, 14] show that twinning systems found operating during plastic deformation are not the ones found during the ordering transformation. This suggests that where strain relief can occur by deformation twinning, other systems with small shears are available and can be energetically more attractive than the transformation twin systems.

Some of the electron microscope observations on ordered alloys also corroborate the proposed growth mechanism involving transformation twins. For instance, the antiphase boundaries are found to be continuous across twinned interfaces [15]. This would be unlikely if the twins were of the deformation type. Another observation is concerned with the presence of twins in growing ordered platelets in the disordered matrix. These platelets are always found to contain very fine twins. This, according to Hunt and Pashley [16], suggests that twinning occurs almost at the advancing interface between order and disorder.

4. Conclusion

We therefore suggest that transformation twinning in ordered structures occurs as "growth faults" during the growth of the ordered structures to minimize the transformation strain, and

*It is interesting to point out that in ferroelectric crystals also, the twinning elements are those symmetry elements lost during the ferro electric transition. See, for instance, Zhludev [12].

not as a result of "self-deformation" by mechanical twinning of the ordered alloys.

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