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Twinning and mechanical behavior of titanium aluminides and other intermetallics

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Based on the recent studies of deformation twinning in ordered intermetallics, the general background on slip-twinning-microcracking relationships is established. Specific roles of deformation twinning in the generalized plasticity of polycrystals and the crack-tip microplasticity are discussed in terms of the local strain compatibility by invoking both 'tension' and 'compression' twins. Special examples are given for γ-TiAl, other $L1_0$ alloys, and Ti_3Al of the $D0_{19}$ structure. Effects of composition, microstructure and temperature on defect properties that are relevant to the propensity of deformation twinning are discussed. © 1998 Elsevier Science Limited. All rights reserved

Key words: A. titanium aluminides (based on TiAl), B. mechanical properties, C. twinning, D. defects: twin dislocations, dislocation mobility.

INTRODUCTION

Crystallographic elements of twinning, atomic shuffling, and twin-slip conjugate relationships in superlattice crystal structures were discussed by Christian and Laughlan[1] and Yoo,[2] and possible roles of twinning in mechanical behavior of ordered intermetallic compounds were briefly reviewed by Yoo *et al.*[3] and Fujiwara *et al.*[4] Specific discussion on the role of twinning in brittle fracture of titanium aluminides was given by Yoo *et al.*[5,6] During the past decade, as research and development activities on titanium aluminides as high-temperature structural materials were intensified, the important role of transformation twinning in processing-microstructure-properties relationships of two-phase TiAl–Ti_3Al alloys have been widely recognized, but specific mechanistic understanding of the role that deformation twinning plays in mechanical behavior of these alloys is still incomplete.[7–9] As materials technology demands tougher and stronger materials, which often possess limited operative slip systems, mechanistic understanding of deformation twinning could provide an enhanced capability for controlling the processing and mechanical behavior of advanced materials.

The purpose of this paper is twofold. First, after giving a general background on slip-twinning-microcracking relationships, the role of deformation twinning in the generalized plasticity of polycrystals and in the crack-tip microplasticity is discussed from the geometrical and energetics viewpoints. Second, critical issues on the effects of composition, microstructure and temperature on the propensity of deformation twinning are assessed.

CRYSTALLOGRAPHY OF TWINNING AND INTERNAL STRESS

Figure 1(a) and (b) shows the primary and complementary (anti-twinning) modes of true-twin (order twinning) systems in the $L1_0$ (face-centered tetragonal) structure. Twinning shears as functions of the axial ratio, $\lambda = c/a$, are plotted in Fig. 2 for the primary and complementary modes of $(111)[11\bar{2}]$ true-twin, $g_P = (2\lambda^2-1)/\lambda\sqrt{2}$ and $g_C = \sqrt{2}/\lambda$, respectively, and the $(011)[01\bar{1}]$ transformation twin with $g_T = \lambda - 1/\lambda$. The dashed curves in Fig. 2 are for the $(111)[2\bar{1}\bar{1}]$ pseudo-twin (forbidden twinning) system. The integer q given in Fig. 2 denotes the number of K_1 lattice planes

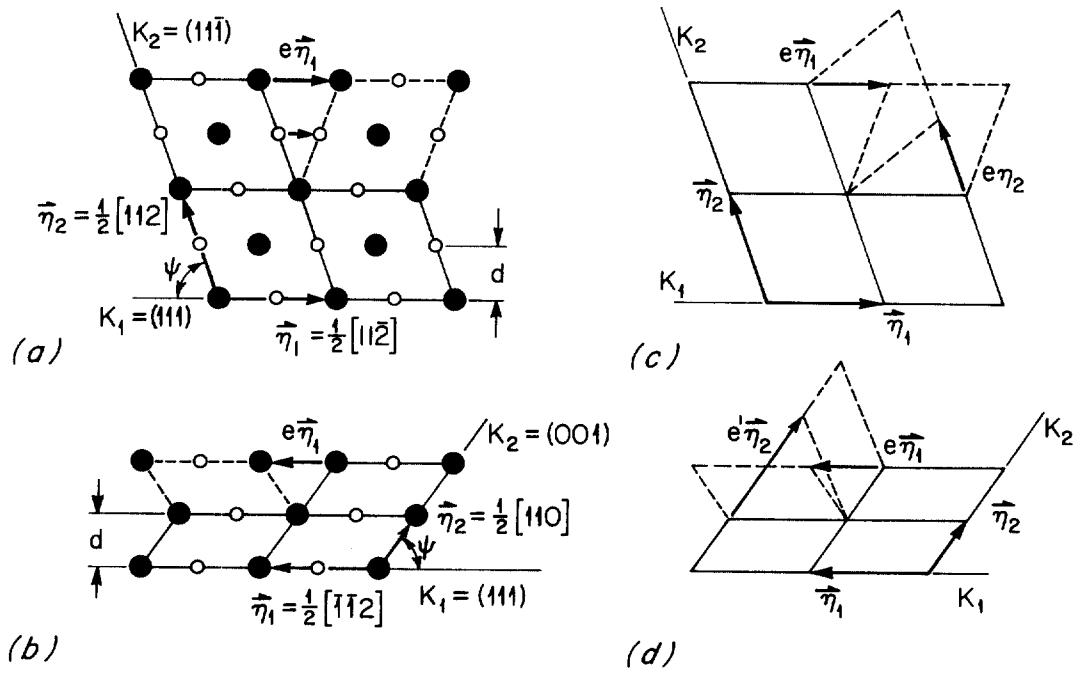

Fig. 1. Twinning in the $L1_0$ structure: (a) primary (twinning) system, (b) complementary (anti-twinning) system, (c) crystallographically-equivalent conjugate twin system,and (d) non-equivalent twin-slip conjugate system.

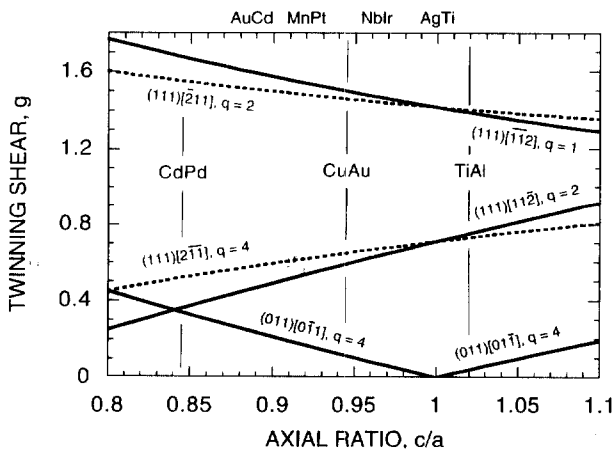

Fig. 2. Variation of twinning shear with the axial ratio in $L1_0$ compounds.

intersected by the η_2 vector. When $q > 2$, some atom shuffling is required. On the $K_1 = (111)$ plane, the Burgers vector of a unit twin dislocation for the primary twinning is $\mathbf{b}_t = [11\bar{2}]/6$, and that for the anti-twinning case is $\mathbf{b}_c = -2\mathbf{b}_t = [\bar{1}\bar{1}2]/3$. While the coherent twin boundary energy for the two cases are the same (calculated to be rather low, $\Gamma_T = 50$–$60\,\mathrm{mJ/m^2}$, for TiAl[10,11]), the twinning shear of the former is about one-half of that for the latter when $\lambda \approx 1$.

Figure 1(c) shows that the primary and its conjugate (reciprocal twinning) twin systems are crystallographically equivalent. Under an appropriate internal stress system, therefore, the conjugate twinning pair may give rise to a pure shear, resulting from an algebraic average of two simple shears indicated by the dashed prisms in Fig. 1(c). In contrast, the slip-twin conjugate relationship of (001)[110]/2 and (111)[$\bar{1}\bar{1}$2]/2 for the $L1_0$ structure is illustrated in Fig. 1(d). Because of the large magnitude of twinning shear ($g_C > 1{\cdot}2$ for $\lambda < 1{\cdot}1$), deformation by the complementary or anti-twinning is not expected to occur unless it is needed at a site where a large amount of strain incompatibility must be relieved, such as at a twin–twin intersection or a crack tip.

Several micromechanical models for the plastic deformation of polysynthetically twinned (PST) crystals and polycrystalline TiAl-Ti_3Al alloys with the fully lamellar microstructure have been proposed recently,[12–16] which include the role of deformation twinning. As shown by the solid curves in Fig. 2, while the primary twin system occurs under a compressive stress along the c-axis (thus, primary twins may be called 'compression twins'), complementary twins in anti-twinning direction may be called 'tension twins.' Similarly to the twin systems in hcp and $D0_{19}$ structures,[2,6] the solid curves in Fig. 2 of compression (tension) twins show positive (negative) slopes with increasing λ, and the opposite for the dashed curves of pseudo-twins. Recently, systematic transmission electron microscopy (TEM) examinations were made on deformation microstructures of PST crystals of five orientations deformed in tension and compression at a wide range of temperatures,

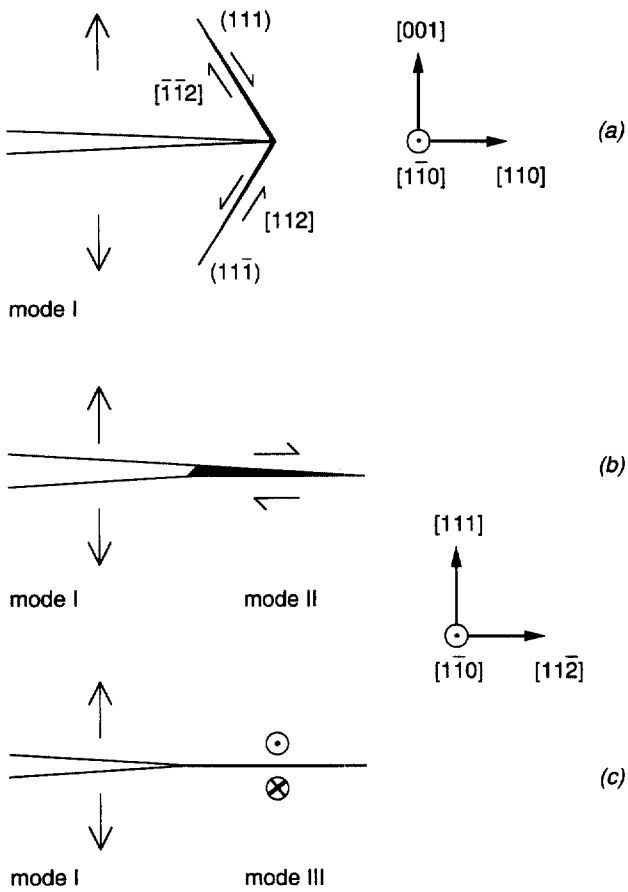

Fig. 3. Crack-rip microplasticity by twinning and slip in the $L1_0$ structure: (a) two symmetric tension twins, (b) coplanar primary twinning (edge type), and (c) coplanar ordinary slip (screw type).

and the operative deformation modes (ordinary slip, superlattice slip, and deformation twinning) in six orientation variants were determined.[17] The results of this work indicate that the relative ease of each deformation mode is involved with some factors beyond Schmid factors, indicating an important role of the internal stress field in plastic deformation of two-phase alloys.

Both twin nucleation and crack initiation require internal stress concentration by a pileup of slip dislocations. A comparison analysis of these competitive processes may be studied with the aid of Hall-Petch and Stroh models or a dislocation model for twinning and fracture as was applied to h.c.p. metals.[18,19] Once nucleated, slip-twin and/or twin–twin interaction may cause the nucleation of a microcrack, or crack extension can be halted by slip and/or twinning at the crack-tip. In bcc metals and alloys, it has been experimentally observed that deformation twinning can effectively strengthen a material under some circumstances and weaken it under others.[20] In two-phase TiAl-based alloys, on the other hand, deformation twinning appears to play beneficial role in both strengthening and toughening of the alloys.[7–9]

TWIN NUCLEATION AND GROWTH

The important factors that control the nucleation of deformation twins are heterogeneous nucleation sites, formation energetics of twin embryos, and growth kinetics of twin nuclei. Bulk, defect, and planar-fault properties that are relevant to twin nucleation in titanium aluminides were summarized recently.[21] In the case of TiAl, the coherent interfacial energy of a true-twin boundary ($\Gamma_T = 60\,\mathrm{mJ/m^2}$) is lower than that of a pseudo-twin boundary ($\Gamma_P = 270\,\mathrm{mJ/m^2}$) by a factor of 4·5.[22] This indicates that the nucleation of a true twin is not too difficult in TiAl, as compared to that of a pseudo twin, at a site of stress concentration.

Potential sites for twin nucleation in single-phase alloys are grain boundaries, transformation twin boundaries, dislocations, surfaces, and crack tips. Dislocation mechanisms for deformation twinning in the $L1_0$ structure have been reviewed elsewhere.[21,23] Grain boundaries are the most potent sites for twin nucleation in polycrystalline alloys, for example, in TiAl,[24–26] FePt[27] and Ti_3Al.[28] In two-phase TiAl–Ti_3Al alloys, it is now well established that deformation twins in γ-TiAl phase are readily nucleated at a variety of homo- and heterophase interfaces, such as γ/γ and γ/α_2 lamellar interfaces, and grain boundaries, even at slow strain-rate and/or elevated temperatures.[7–9]

The $\{20\bar{2}1\}\langle 10\bar{1}4\rangle$ twin system was found to be the most active twin mode in Ti-34Al polycrystals compressed at 1073–1373 K.[28] This compression twin has not been identified in α_2 lamellae, so far, when the two-phase lamellar microstructure is compressed perpendicular to the interfaces.

Once nucleated, the increase in twinned volume takes place by its lengthening in the η_1 direction and thickening in the direction normal to the K_1 plane. The former results from propagation of twin dislocations at the incoherent twin boundary, while the latter from acquiring additional twin dislocations either by the interaction with slip dislocations, or by the nucleation of partial dislocation loop(s) with the aid of an internal stress concentration. The relative mobility of twin dislocations can be estimated by using the ease of gliding parameter,[29] $\zeta/b = K_e S_{66}/2g$, where K_e is the energy factor and S_{66} is the reduced elastic compliance referred to the edge type of a twin dislocation. The

larger the value of ζ/b, the higher the mobility of a twin dislocation will be.

There have been many *in situ* TEM, *post mortem* TEM and high resolution electron microscopy (HREM) investigations of twin–twin interactions in TiAl-based alloys. With an exception of the observation of microcracking at the sites of twin intersections in creep-deformed Ti–54Al polycrystals,[30] most of the investigations[31–38] revealed a variety of localized deformation processes (subsidiary twins, basal or cube slip, nano-twins, twin thickening, and formation of 9R structure, etc.). There are two classes of twin intersections.[32–34] At high temperatures, accommodation shear in type-I intersection (about the $<1\bar{1}0]$ zone axis) occurs via $(001)<110]/2$ slip.[33] According to Fig. 1(d), this suggests a geometrical necessity for anti-twinning (or complementary) to occur at the twin intersection. Though it was recently reported from the HREM investigation that what appeared to be a 9R structure was often caused by overlapping twin-related crystals,[39] it is possible to form a deformation-induced 9R structure by an anti-twinning operation on every third plane in the twinned crystal.[31]

DUCTILITY AND TOUGHNESS

The role of twinning in ductility of polycrystalline materials can be discussed in terms of geometrical factors (λ and g) and energy factors (Γ_T,K_eS_{66}, and G_c), where G_c is the cleavage energy. It is desirable to have both tension and compression twin systems available in a given material so as to undergo a generalized deformation without much strain incompatibility. Titanium of the hcp structure is an outstanding case in point.[6] In CdPd of the $L1_0$ structure, the axial ratio ($\lambda=0{\cdot}845$) gives a rather low twinning shear, $g_P \approx g_T \approx 0{\cdot}35$, for both the primary twin (compression) and the transformation twin (tension) as shown in Fig. 2. As the axial ratio increases beyond that of TiAl ($\lambda=1{\cdot}02$), twinning shear of the complementary twins, g_c, decreases steadily and it eventually crosses $g_P=2/\sqrt{3}$ at $\lambda=\sqrt{3/2}$. Alternatively, if the direction of the transformation twinning can be reversed for TiAl, i.e. from compression twin ($\lambda>1$) to tension twin ($\lambda<1$) in Fig. 2, then a generalized plasticity is promoted, provided that the atomic shuffling ($q=4$) associated with the motion of a zonal twin dislocation[40] is not too difficult. The K_eS_{66} values calculated for $(011)[01\bar{1}]$ twinning in Ti-56Al at 300 and 1273 K are, respectively, 1·75 and 1·95, which are larger than those corresponding values (1·56 and 1·68) for true twinning. Whether a γ-TiAl-based ternary alloy system with $\lambda<1$ exists or not is still an open question.

The role of twinning in crack-tip microplasticity may be discussed with the aid of Fig. 3. When a $(001)[1\bar{1}0]$ mode-I crack is subjected to an uniaxial tension along the [001] direction, as shown in Fig. 3(a), crack-tip blunting by two symmetric tension twins of the complementary (anti-twinning) type is possible.[41] Using $\Gamma_T=60\,\mathrm{mj/m^2}$ and the (001) cleavage energy of $G_c=5{\cdot}6\,\mathrm{J/m^2}$ for TiAl,[10,42] one can estimate the length of the tension twins to be $l \geq 10\Delta a$, where Δa is the width of an incremental crack extension. In the case of a $(110)[1\bar{1}0]$ mode-I crack, the basal slip of $(001)[110]/2$ can also induce crack-tip blunting.[3] On the other hand, when the mode-II or mode-III component of an external loading is mixed with a $(111)[1\bar{1}0]$ mode-I crack (see Fig. 3(b) or (c)) of the lowest cleavage energy ($G_c=4{\cdot}4\,\mathrm{J/m^2}$ for TiAl[42]), coplanar deformation twinning or ordinary slip at the crack front will occur, so as to shield the crack-tip shear-stress field. Since the stress field corresponding to the mode-I component is not relaxed by the crack-tip twinning or slip, this type of microplasticity concentrated on the (111) habit plane may induce an unstable crack propagation, leading to {111} translamellar fracture in Ti-rich TiAl alloys.[43] Such an unstable crack propagation may then lead to quasi-brittle, or semi-brittle, shear fracture as observed in Ni-base aluminide and silicide of the $L1_2$ structure.[44]

COMPOSITION, MICROSTRUCTURE, AND TEMPERATURE

On the relative importance of alloy composition, microstructure, and temperature in deformation twinning, diverse opinions have been reported in the literature as were discussed earlier.[21] For instance, the incidence of deformation twinning in γ-TiAl was reported to increase as the temperature was raised above 973 K, rendering an increased ductility and a sharp decrease in yield stress at elevated temperatures.[45,46] The apparent critical resolved shear stress (CRSS) for twinning in Ti-56Al single crystals was measured to be rather low, about 200 MPa at 1000 K and 100 MPa at 1200 K.[46] This experimental data was interpreted based on a dislocation model using reasonable values of a local stress concentration

and a vacancy supersaturation at elevated temperatures.[47] The increase in the number density of deformation twins in lower Al alloys of Ti–(48–52)Al polycrystals, at any given temperature, was attributed to a microstructural effect,[24] e.g., the fine grain size, rather than intrinsic effects of Al content. Our understanding of the off-stoichiometry effect on superlattice intrinsic stacking fault (SISF) and twin boundary energies is not clear. The atomistic simulation study of dislocation core structures using empirical interatomic potential[48] and the compression experiment along the *c*-axis using Ti–51Al and Ti–54Al crystals[49] suggest that both SISF and twin boundary energies increase with increasing Al concentration. On the other hand, TEM analyses by Morris *et al.*[50] and Sriram *et al.*[51] showed just the opposite dependency, and theoretical estimates by Rao *et al.*[52] indicated a very weak composition dependence.

During primary creep of Ti–54Al based alloy, the lamellar microstructure (γ/γ interface spacing) was refined due to the formation of deformation twins parallel to the lamellar interface, which leads to increased creep strength.[53] With ultra-fine grain size and lamellar spacing, relatively high fracture toughness ($K_Q \geq 50\,\mathrm{MPa}\sqrt{\mathrm{m}}$) and high yield strength ($\sigma_y \approx 1\,\mathrm{GPa}$) have been measured in fully lamellar Ti–47Al–2Cr–2Nb alloys at temperatures below 1000 K.[54] During creep deformation of such alloys, deformation twinning occurred across the γ lamellae as a stress-relief mechanism from pileups of interfacial dislocations on γ/α_2 boundaries.[55] Recently, an excellent combination of tensile elongation ($\varepsilon > 7\%$) and yield strength ($\sigma_y > 700\,\mathrm{MPa}$) was obtained in a Ti–40Al–10V alloy at temperatures below 750 K, by refining the grain sizes of γ, α_2 and β phases to the order of a few microns.[56] According to their preliminary TEM analysis,[56] the enhanced ductility of this three-phase alloy is attributable to pseudo-twinning or martensitic transformation in β-phase.

The absence of twinning in the α_2 phase of two-phase TiAl alloys may be attributed either to an intrinsic effect due to the difficulty associated with the interchange shuffling necessary for the $D0_{19}$ structure,[1,6] or to an extrinsic effect due to the presence of interstitial impurities.[2] It was recently reported that when Ti–47Al–2Cr–2Nb was stressed at hard orientations (i.e., either parallel or normal to the γ/α_2 interface), $\langle 11\bar{2}6\rangle/6$ dislocations were generated at the interfaces, and no twinning was observed in α_2 phase.[57] Since the oxygen content in α_2 phase can be as high as 20 000 ppm even when the average oxygen content in the two-phase alloy is only 600 ppm,[58] this level of oxygen may be expected to hinder twinning process.

SUMMARY

While various types of interfaces are the preferential sites for twin formation in $L1_0$ compounds, 'compression twins' of the $(111)[11\bar{2}]$ type alone are not sufficient to render a contribution to the generalized plasticity of PST crystals and γ-phase polycrystals. In order to enhance both the ductility and fracture toughness, 'tension twins' of either the $(111)[\bar{1}\bar{1}2]$ anti-twinning type, or the $(011)[0\bar{1}1]$ transformation twinning type (with $\lambda < 1$), are desirable in ternary or quaternary $L1_0$ alloys. Much more work is needed to understand the effects of composition and temperature on defect properties that are relevant to twin formation in $L1_0$-type and other intermetallics.

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