ROLE OF TWINNING IN BRITTLE FRACTURE: INTERMETALLIC COMPOUNDS

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ABSTRACT

Our current understanding of the role twinning plays in microcrack initiation, polycrystalline ductility, and crack-tip microplasticity in intermetallic compounds is critically reviewed. Microtwinning in γ' phase of Ni-base superalloys under creep conditions and {111} cleavage fracture in Ni_3Al at room temperature are interpreted in terms of the competition between slip/twin transfer and microcrack initiation. Domain and grain boundaries are effective sites for twin nucleation and lead to a measurable ductility of two-phase lamellar Ti-Al alloys. Formation of superlattice intrinsic stacking faults (SISFs) at a crack-tip in Ni_3Al and $(Co,Ni)_3Ti$ makes a contribution of "stacking fault toughening". Twin toughening in Mn-doped Ti-54at.%Al gives more than a seven-fold increase over the critical Griffiths stress intensity factor. Mode-mixity effects of coplanar twinning and/or slip at the tip of a {111} mode-I crack causes unstable crack propagation, leading to "quasi-brittle" or "semi-brittle" shear fracture in many $L1_2$ and $L1_0$ compounds. Unresolved critical issues are discussed, and future research directions are suggested.

KEYWORDS:

Twinning, intermetallic compounds, dislocations, stacking faults, microcrack, quasi-brittle, toughness

INTRODUCTION

The role of twinning in fracture of metals and alloys was reviewed in 1981 by focusing on three crystal-classes of b.c.c., f.c.c., and h.c.p. structure types. In b.c.c. and f.c.c. metals and alloys, the available experimental data show a dichotomy in that deformation twinning can effectively strengthen a material under some circumstances and weaken it under others [1,2]. In h.c.p. metals and alloys, on the other hand, those that deform by both "tension twins" and "compression twins" (with respect to the c-axis) are more ductile than those that deform by only one twin system [3]. Since then, it has been increasingly recognized that twinning plays an important role in brittle fracture of some intermetallic compounds of non-cubic crystal structures [4,5]. In polysynthetically twinned (PST) two-phase TiAl alloys, both heterophase (α_2/γ) lamellar interfaces and lamellar boundaries in γ-phase play crucial roles in propensity of twin nucleation and increase of fracture toughness [6-9]. Possible intrinsic effects of stacking faults, nano-twins, and pseudo-twins (martensites) on toughening by crack-tip microplasticity have been the subjects of many research works dealing with single-phase intermetallic compounds, e.g., Ni_3Al [10], $(Co,Ni)_3Ti$ [11], and TiAl [12]. The purpose of this paper is to review the role of twinning in microcrack initiation, polycrystalline ductility, and crack-tip plasticity and to assess unresolved critical issues regarding the effects of temperature, strain-rate, alloy composition, microstructure, test environment, and neutron irradiation on twinning and fracture.

TWIN NUCLEATION AND CRACK INITIATION

Both twin nucleation and crack initiation require an internal stress concentration and, therefore, share common heterogenous nucleation sites in the microstructure of a given material. Schematic illustrations of Fig. 1 depict a variety of possible cases of slip, twin, and crack initiation at γ_1/γ_2 grain or domain boundaries which act as effective barriers against a dislocation pile-up. In Fig. 1, (a) and (b) indicate that an interface can be a source and a sink of slip/twin dislocations, (c) a site for slip/twin transfer, (d or e) for crack initiation within the grain (or domain) or into the next grain (or domain), and finally (f, g, and h) for microcracking along the interface. When the dislocation initiation, absorption, and transfer at interfaces, (a-c), are prevalent,
this localized microplasticity may lead to a relatively large elongation at failure. On the other hand, when the
conditions for crack nucleation of any one of the latter five cases, (d-h), are satisfied before the localized microplasticity sets in, microcracking will occur, resulting in a relatively low ductility.

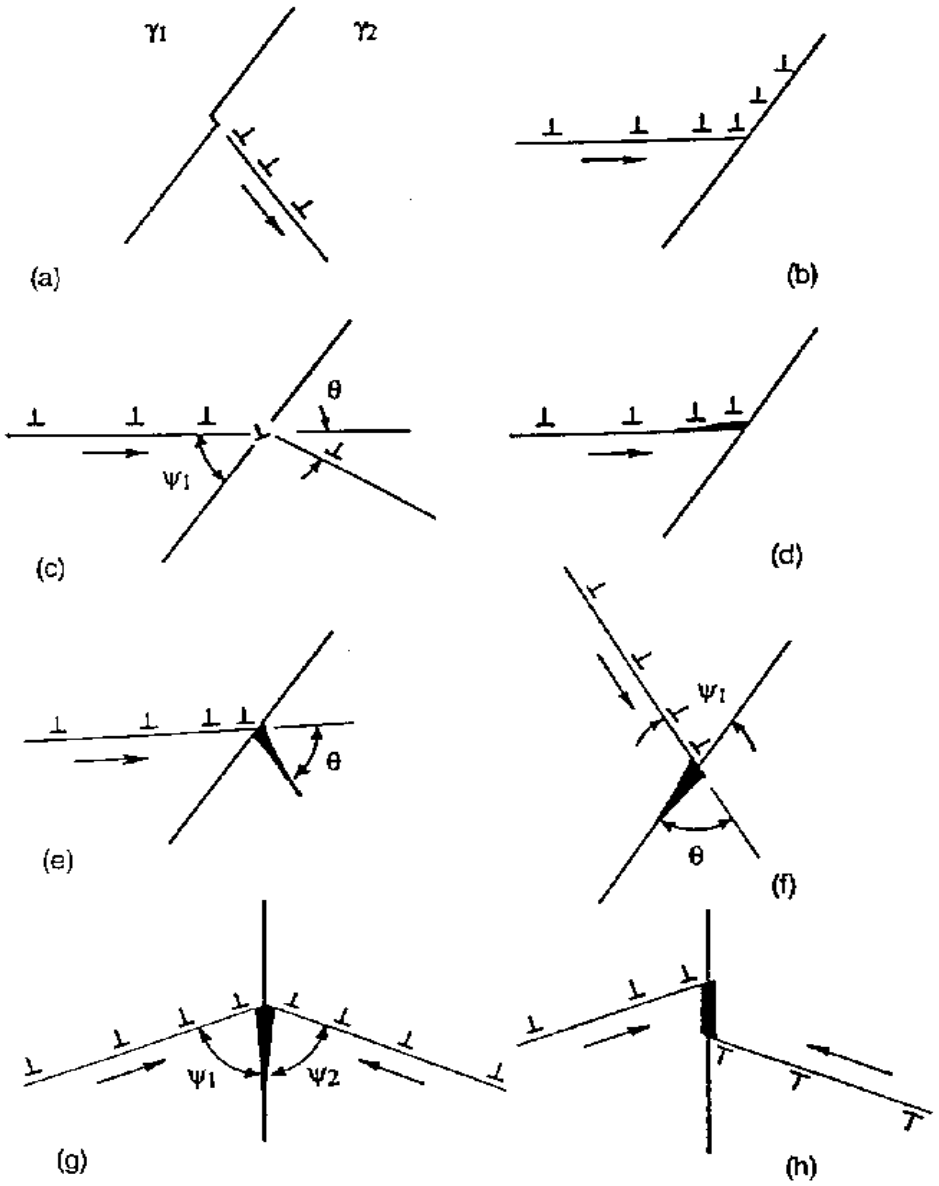

Fig. 1: Various pile-up configurations of slip/twin dislocations against γ_1/γ_2 interfaces

Some special cases of [110] symmetric tilt boundaries in the $L1_2$ structure were investigated earlier using the anisotropic elasticity theory of dislocations and fracture [13,14] and available surface and grain-boundary cohesive energies [15]. The results show that, in the case of Fig. 1(c), the transmission of the

primary slip dislocations across the boundary into the conjugate slip system occurs with a certain degree of difficulty, which is eased by localized disordering. The difficulty of true-twinning in fully-ordered $L1_2$ alloys may also be alleviated by the locally-disordered boundary, especially at elevated temperatures. Microtwinning in γ' phase of Ni-base superalloys under creep deformation condition at elevated temperatures [16] and resulting tension/compression asymmetry [17] may be interpreted with the aid of Fig. 1(c) with γ on the left and γ' on the right where $\psi_1 = 54.7^\circ$ and $\theta = 0^\circ$. Deformation twinning within the localized slip regions resulted in formation of cavities in the twin boundaries [16]. As for Fig. 1 (e) versus (f), cleavage fracture on the (111) plane is predicted, rather than intergranular fracture [13,14]. The available transmission electron microscopy (TEM) data on Ni_3Al are in good agreement with the prediction [10,18].

In PST TiAl alloys, in addition to α_2-γ interfaces, the three different types of intervariant γ_1/γ_2 lamellar interfaces are (1) true-twin boundaries, (2) pseudo-twin boundaries, and (3) 120˚ rotation boundaries [8]. All of these boundaries, especially when they are in a semicoherent form, can act as effective sites for slip and/or twin initiation [7,8]. The role of these lamellar boundaries as dislocation sources, Fig. 1 (a) and (c), may be partly responsible for the measurable ductility reported in two-phase lamellar Ti-Al alloys as compared to single-phase γ-TiAl alloys [19]. The case of slip/twin transfer, Fig. 1 (c), and the four cases of crack initiation, Fig. 1 (e-h), can be discussed in terms of a Hall-Petch type relationship and Stroh mechanism, respectively. Hazzledine and Kad [20] interpreted the anisotropy of yield and fracture stresses reported in PST TiAl crystals [8]. In view of the fact that all the deformation modes in γ-TiAl occur on {111} planes and the ideal cleavage (Griffiths) energy is the lowest on these planes, Yoo et al. [21] pointed out the importance of mode-mixity (I-II or I-III) not only in crack-tip plasticity, but also in microcrack nucleation by stress concentration due to a dislocation pile-up at interfaces.

Additional heterogeneous nucleation sites are extended lattice defects, viz., dislocations and stacking faults. Faulted Frank loops of vacancy and interstitial types in the $L1_0$ structure have {111} habit planes. The so-called radiation-induced ductility (RID) of nearly two-fold increase in tensile elongation at 600˚C reported in two-phase TiAl alloys [22] is attributed to a mechanism that involves additional deformation twins, nucleating during neutron irradiation and growing during tensile deformation after irradiation [23]. Extending the pole mechanism for the $L1_0$ structure [24], we [23] explained the experimental data [22] quantitatively on the basis of (a) the stability of large faulted interstitial-type Frank loops, (b) the pole mechanism facilitated by the interaction of ordinary dislocations and a Frank loop, and (c) the formation of effective twin embryos and the kinetics of twin formation. The recorded data that no appreciable changes in yield strength and work hardening were observed in this experiment [22] can be explained also by the model [23], which requires a moderate stress concentration by a pile-up of about six ordinary dislocations only.

CRACK-TIP TWINNING AND TWIN TOUGHENING

Twinning plays two different roles in crack-tip microplasticity, which may be discussed with the aid of Fig. 2 for fcc-derivative superlattice structures (e.g., $L1_2$ and $L1_0$ types). When a (001)[1-10] mode-I crack is subjected to an uniaxial tension along the [001] direction, shown schematically in Fig. 2(a), crack-tip-blunting type of microplasticity is possible by the formation of two symmetric group of superlattice intrinsic stacking faults (SISF) or nano-twins. Even though crack blunting was not effected, extensive symmetric distribution of SISFs on both sides of a mode-I crack was observed by *post mortem* TEM in $(Co,Ni)_3Ti$ [11]. Extended SISFs trailed by super-Shockley partial dislocations, emitting from a discontinuously propagating crack-tip, were directly observed in stoichiometric Ni_3Al by *in situ* straining TEM [10]. Since the SISF energy of Ni_3Al is 40 mJ/m^2 and the extent of SISF strip is on the order of 1 μm [10], toughening of a (001)[1-10] mode-I crack is energetically feasible in Ni_3Al by stacking fault generation, viz., "stacking fault toughening". In case of $(Co,Ni)_3Ti$, however, extensive faulting at the crack was attributed in part to hydrogen in the test environment [11].

In the case of the $L1_0$ structure, the two symmetric twins in Fig. 2(a) are "tension twins" of the complementary (anti-twinning) type [5,10]. This was experimentally confirmed in Mn-doped Ti-54at.%Al single crystals by Phan-Courson [12]. Using the twin boundary energy of 60 mJ/m^2 and the (001) cleavage energy of 5.6 J/m^2 [6,8], the calculated values for stoichiometric TiAl at 0 K, 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.

Figure 2 (b) or 2(c) shows the case when the mode-II or mode-III component of an external loading is mixed with a (111)[1-10] mode-I crack. According to the compilation of cleavage energies calculated for transition-metal aluminides and silicides [25], the cleavage energy of {111} habit planes is lower than that of the (001)

plane in both Ni_3Al and Ni_3Si [10], and it is the lowest (4.4 mJ/m^2) among the four low index planes in TiAl [21]. Since the (111) plane is also twinning plane or slip plane, coplanar deformation twinning or ordinary slip can occur, as indicated in Fig. 2 (b) or (c), so as to shield the crack-tip shear stress field. Because the stress field corresponding to the Mode-I component is not relaxed by the crack-tip twinning or slip, this type of coplanar microplasticity concentrated on the (111) habit plane may induce an unstable crack propagation, leading to {111} translamellar fracture as observed in Ti-rich TiAl alloys [7,8]. This may explain quasi-brittle, or semi-brittle, shear fracture as observed in Ni_3Al and Ni_3Si [10].

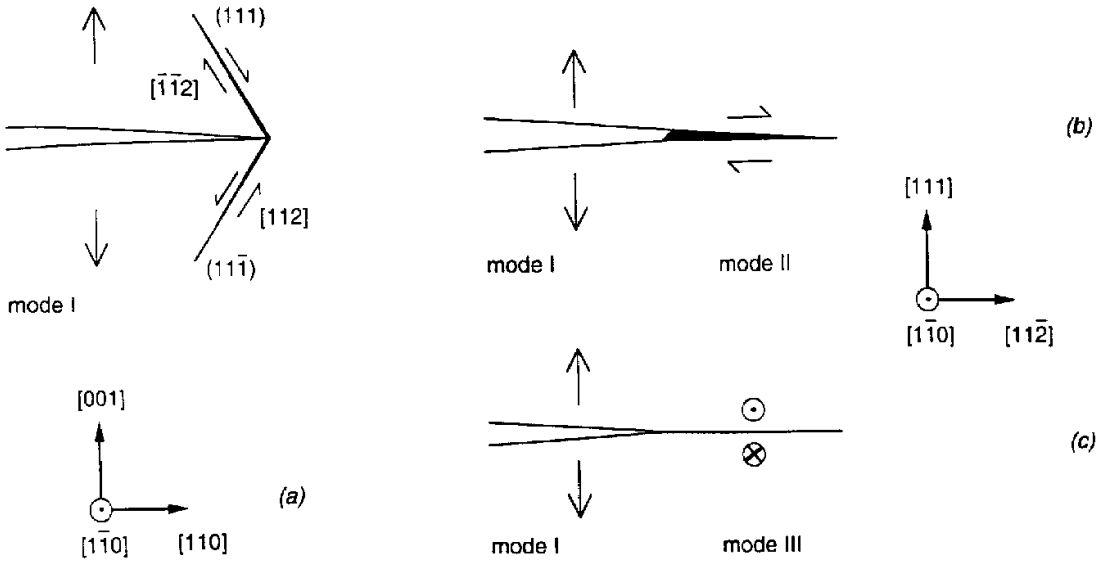

Fig 2: Crack-tip microplasticity by twinning and slip: (a) two symmetric twins, (b) coplanar twinning (edge character), and (c) coplanar slip (screw character)

Fracture toughness of binary Ti-54at.%Al single crystals at room temperature is $K_{IC} \approx 1$ MPa-√m [26], essentially equal to theoretical stress intensity factors of k_{IG}, Griffith values [21]. Increases in provisional K_{IC} value to $K_Q > 7$ MPa-√m in Mn-doped single crystals [12] and $K_Q = 10$ MPa-√m in polycrystals [27] are attributed to crack-tip twinning and intergranular microcracking, respectively. According to the description of a plastic zone by Cherpanov [28], the former occurs in the "superfine structure" at the atomically sharp tip of a slit crack, and the latter in the "fine structure" beyond the transition region.

In two-phase multicomponent TiAl alloys, fracture toughnesses are reported to be reasonably good, e.g., K_Q = 10-32 MPa-√m with duplex microstructures [27], K_Q = 25-43 MPa-√m with lamellar microstructures [29], and $K_Q > 50$ MPa-√m with fine lamellar microstructures [30]. The presence of various lamellar interfaces and grain boundaries strongly influences the crack-tip plasticity, because of its orientation dependence, and therefore affects translamellar and interfacial microcracking in the crack-tip process zone in a complex manner. From a broad perspective viewpoint of two-phase microstructure, fracture toughness may result from various mechanisms such as, ductile-phase blunting, ductile-phase bridging, ligament toughening, and twin toughening [29]. One area yet to be explored is whether synergistic toughening effects can be obtained by combining some of these mechanisms.

The recent study of crack-initiation and "small-crack" growth during the ambient-temperature fatigue of a multicomponent γ-TiAl based alloy [31] showed that crack initiation resistance in the duplex microstructure was observed to be superior to that in the lamellar microstructure. Such a small crack effect is typically seen when its size is comparable to the characteristic dimensions of the microstructure [32]. This result is contrary to that of their earlier work on large cracks in the same alloy. In view of the discussion of twin

nucleation and crack initiation (Fig. 1), it appears that microcrack initiation by means of the possible mechanisms of Figs. 1 (d-h) might have been as effective as twin nucleation mechanism by either Fig. 1(a) or 1(c) in the lamellar microstructure of this particular alloy. A quantitative assessment of the specific contribution of twinning and microcracking in the fracture toughness of two-phase alloys is yet to be made.

DISCUSSION

In the main, our mechanistic understanding of the competition between slip/twinning and microcracking at various interfaces has been attained based on energetic aspects of a dislocation pile-up model under a static equilibrium condition. This model cannot be applied to treat dynamic aspects of a stress concentration, which may strongly influence the effect of temperature and strain rate on yield stress and fracture strain of polycrystals or multilayered materials. A preliminary analysis indicated that the kinetics of dislocation reactions at an interface resulting from the leading dislocation of a pile-up are far more important than any energetic factors involved [33]. In other words, how effectively the reaction products move away from the site of intersection, Fig. 1 (b) and (c), seems to be crucial to whether or not the following dislocations can be incorporated into the interface. Pestman et al. [34] investigated atomic processes of slip interactions with a tilt boundary in f.c.c. and $L1_2$ crystals using a computer simulation method and found that the interaction in ordered compounds showed similarities to that in f.c.c. metals.

A few atomistic simulation results showing nano-twinning at the tip of a mode-I crack have been reported, viz., the two cases of {11-2}<111> twinning, equivalent to Figs. 2(a), and 2(b) in bcc crystals [35,36], and transonic twin formation in the forward direction [37]. No computer simulation result of crack-tip twinning in intermetallic compounds has been reported. The only experimental evidence of twin toughening in single-phase intermetallic compound was given in Mn-doped γ-TiAl by Phan-Courson [12]. By using PST TiAl crystals, the anisotropy of fracture toughness was measured in the three principal orientations [38,39], but the specific contribution of twinning was not determined. The paper entitled "twin toughening in titanium aluminides" by Deve and Evans [40] reported that twinning occurred within a process zone and crack bridging ligaments, with about equal contributions arising from the process and bridging zones.

Most of the creep strength and ductility data of titanium aluminides published in the past decade are on multicomponent alloy systems having many different microstructures. It is, therefore, difficult to understand the mechanistic role of twinning in creep flow and fracture behavior in these alloys at elevated temperatures. To list a few outstanding problems in two-phase TiAl alloys: the intrinsic effect of aluminum content on deformation twinning and fracture, effects of interfacial sliding and true-twinning parallel to the lamellar boundaries on creep strength and ductility, mechanistic role of enhanced twin nucleation in the radiation-induced ductility (RID), solute effects (e.g., Nb, V, Mn, etc.) on twinning propensity and enhanced cleavage strength, and environmental effects (O, H) on twinning and fracture remain unresolved issues.

As we seek tougher and stronger intermetallic alloys with ultra-high melting temperatures for structural applications, which have mostly non-cubic crystal structures, twinning as a deformation mode would play an important role in maintaining their integrity throughout processing, handling, and deforming. In the past two decades, there has been a significant advance in our mechanistic understanding of the role twinning plays in brittle fracture of intermetallics, e.g., Ni-base $L1_2$ alloys and TiAl-base alloys. More effort in experimental and theoretical interdisciplinary research at multi-levels of length and time scales is needed, particularly in the evolution of internal stress concentration and kinetics of twin nucleation and/or microcrack initiation.

SUMMARY

A critical review is given on the role twinning plays in brittle fracture of intermetallic compounds, and the highlights are:

1. Tension/compression asymmetry of creep strength in Ni-base superalloys was attributed to deformation twinning in γ' phase, and cavity formation was observed to occur at twin boundaries.
2. {111} cleavage fracture at <110> tilt boundaries in the $L1_2$ structure was predicted based on the available surface and interfacial energies, and was confirmed by TEM observations in Ni_3Al.
3. Formation of extensive SISFs at an advancing crack-tip, reported to occur in Ni_3Al and $(Co,Ni)_3Ti$, may give rise to the so-called "stacking fault toughening."
4. Grain and domain (including true-twin) boundaries are effective sites for twin nucleation, and also for microcrack initiation, in two-phase γ-TiAl-based alloys.

5. Twin toughening in Mn-doped Ti-54at.%Al single crystals was reported to be $K_Q > 7$ MPa$\sqrt{m}$, a factor of about 7 larger than Griffith stress intensity factor.
6. Mode-mixity of coplanar twinning and/or slip is a cause for unstable crack propagation which leads to quasi-brittle shear fracture, observed in many $L1_2$ and $L1_0$ compounds.

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