THE TEMPERATURE DEPENDENCE OF YIELD STRENGTH IN $L1_2$ INTERMETALLIC COMPOUNDS

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It has been a traditional concept to characterise the temperature dependence of yield strength of metallic systems according to their structure type. However, it has been found quite recently that the $L1_2$ intermetallics family does not obey this general rule. This paper therefore aims at discussing the factors which lead to this discrepancy. Particular attention is paid to the roles of the various planar faults in determining the stable dislocation morphologies and hence in controlling the yield behaviour.

INTRODUCTION

Traditionally, it has been thought that materials with a particular structure type should exhibit a particular kind of yielding characteristic. For example, the temperature dependence of yield strength (TDYS) of most fcc materials is quite athermal, while most bcc's and hcp's exhibit a large and negative TDYS. On this ground is built the concept that in single phase materials the structure is one of the key parameters in affecting the fracture behaviour. For instance, many bcc and hcp metals exhibit a brittle-ductile transition, which is by and large a result of their characteristic large and negative TDYS.

This paper, however, describes the breakdown of such a general rule in the $L1_2$ superstructure. Intermetallic compounds with the $L1_2$ structure have been found to exhibit very different forms of TDYS. As Fig.1 and Table 1 illustrate, Class A $L1_2$'s such as Ni_3Fe exhibit a rather athermal and yet negative TDYS. On the other hand, Classes B and C exhibit respectively a positive and a negative, but both very thermal, TDYS. Regarding the micromechanisms responsible for yielding, Class A and B (in Regions I and II) are found to yield via the <110>{111} octahedral slip systems, while in Class C, the <110>{001} cube system is found to have the lowest critical

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resolved shear stress (CRSS). The picture looks apparently very confusing but fortunately research in the past ten years or so has largely clarified these confusions and it is therefore the aim of the present paper to summarise the most recent view upon which the various forms of TDYS in $L1_2$'s can be rationalised.

The nomenclature of this paper is as follows. Since the $L1_2$ structure is a derivative of the fcc structure, the athermal TDYS with octahedral slip as exhibited by Class A $L1_2$'s, which closely resembles the fcc behaviour, is termed the "normal" behaviour. Class B and C behaviours are therefore regarded as abnormal and to conform with the literature, B (or, strictly speaking, Region II in B) is referred to as the "flow stress anomaly" while C is simply called the "abnormal negative TDYS".

SUPERDISLOCATION STRUCTURES IN $L1_2$

Dissociation of the <110> superdislocation is almost guaranteed to lower the self-energy. For the <110>{111} slip system, two possible schemes are:

$$<110> \rightarrow 1/2<110> + APB\{111\} + 1/2<110> \quad \text{.....(1)}$$

$$<110> \rightarrow 1/3<112> + SISF + 1/3<112> \quad \text{.....(2)}$$

where APB{111} and SISF mean antiphase boundary on the {111} plane and superlattice intrinsic stacking fault respectively. Further splitting (or spreading of the dislocation core) of the superpartials in (1) and (2) is possible and this will affect the Peierls-Nabarro (P-N) stress of the dislocation. In (1), both atomistic calculations (Ref.(1)) and experimental observations (Ref.(2)) suggest that the 1/2<110> superpartials are likely to have low P-N stress. However, the 1/3<112> Shockley superpartials in (2) are expected to have non-planar cores and direct experimental evidence confirms that they are in fact sessile. On the cube plane, <110> superdislocations may dissociate according to

$$<110> \rightarrow 1/2<110> + APB\{001\} + 1/2<110> \quad \text{.....(3)}$$

In the screw orientation, both theory and experiment show that the 1/2<110> cores are non-planar and are thus sessile (Ref.(1)). Similarly, in the edge orientation, experimental evidence suggests that the cores may again be non-planar (Ref.(2)). The influence of these dislocation structures on the TDYS is now discussed.

THE NORMAL TDYS (CLASS A)

The normal TDYS as found in, eg. Ni_3Fe results from the dislocation dissociation according to (1). Because the 1/2<110> superpartials have a low P-N stress, the athermal nature of the TDYS is expected (Ref.(3)).

THE FLOW STRESS ANOMALY (CLASS B)

The progressive elevation of the flow stress in Region II in Fig.1 as temperature increases is due to the thermally activated cross-slip of screw 1/2<110> - 1/2<110> superdislocations from the form in (1) to that in (3). The resultant structure (3), as

mentioned before, is sessile in the screw orientation due to the non-planarity of the 1/2<110> cores on the {001} planes and is therefore termed the Kear-Wilsdorf (K-W) lock. The driving force for cross-slip is due to the difference in the APB energy between the {001} and {111} planes as well as the anisotropy of elasticity which leads to the presence of a tangential interaction between the two 1/2<110> superpartials that aids the cross-slip. A detailed theory which also accounts for other aspects of the flow stress anomaly such as the orientation dependence, tension / compression asymmetry and the small strain-rate dependence of the CRSS has already been given in the literature (Ref.(4)).

The entire form of Class B TDYS can now be summarised. In Region I, temperature is low so that thermally activated K-W lock formation cannot occur. Glide takes place via the <110>{111} system either in the form (1) (eg. as in Ni_3Al) or (2) (eg. as in Co_3Ti). The choice of (1) or (2) in this regime depends of course on the relative energies of SISF and APB{111} as well as on the P-N stress of the 1/2<110> and 1/3<112> partials. In Region II, the higher temperature allows for the formation of K-W locks. As the locking frequency increases while the unlocking frequency stays almost constant (Ref.(4)), the positive TDYS results as the temperature increases. In Region III, the temperature is so high that the <110>{001} system becomes active. The negative TDYS results from the thermally activated breakaway of the Lomer locks which have been found to dominate the microstructure in this regime.

THE ABNORMAL NEGATIVE TDYS (CLASS C)

The abnormal negative TDYS as found in Fe_3Ge or Pt_3Al distinguishes itself from the (normal) negative TDYS in Class A $L1_2$'s or Region I in Class B $L1_2$'s in that in the former cases, cube <110>{001} systems are the easiest systems responsible for slip while in the latter two cases, slip is via octahedral <110>{111} systems. Experimental observations in Fe_3Ge (Ref.(5)) suggest that the dislocations responsible for glide are dissociated according to (3) and the high P-N stress expected for the cube slip system is thought to be responsible for the negative TDYS. However, unlike Region III in Class B behaviour, the 1/2<110> - APB{001} - 1/2<110> superdislocations in Class C are not in Lomer lock configurations and therefore there remains a minor difference between the two behaviours. It may also be considered that in Class C, cube slip is not particularly "easy" but is bound to take place as octahedral slip is prohibited for some reason which is to be discussed in the following section.

WHY DIFFERENT FORMS OF TDYS

The transition from Class A or B to Class C behaviour depends on whether the APB{111}'s are stable. Ngan et al (Ref.(5)) have shown that, very crudely, APB{111}'s will become structurally unstable when

$$\gamma_1 > \mu a / 103 \quad \text{.....(4)}$$

where γ_1, μ and a are the APB{111} energy, shear modulus and the lattice parameter respectively. Thus, $L1_2$'s satisfying (4) will not be able to dissociate according to (1) and since the K-W lock operates only on (1), no flow stress anomaly will be possible.

Dissociation can still take place according to (2) or (3) and both will result in a large and negative TDYS, although (2) will lead to a normal one (with octahedral slip) while (3) will lead to an abnormal one (with cube slip). It should be noted that while Fe_3Ge and Pt_3Al have been found to fall into the latter category of abnormal negative TDYS with (3), no $L1_2$'s have yet been found which exhibit exclusively a normal negative TDYS via dissociation (2).

When (4) is not satisfied, dissociation (1) is possible and will be favourable if it has both the lowest P-N stress and lowest self-energy compared to (2) or (3). Class A or B behaviour will then result depending on whether thermally activated K-W lock formation can occur. Based purely on a positive driving force requirement, this can occur when

$$\gamma_1 / \gamma_0 > \sqrt{3} / (1+f\sqrt{3}) \quad \text{.....(5)}$$

where γ_1 and γ_0 are the APB energies on {111} and {001} planes respectively. f is a quantity which depends on the elasticity anisotropy. $f = 0$ for the isotropic case but $\approx$ 0.62 for Ni_3Al. Thus, $L1_2$'s which do not satisfy both (4) and (5) cannot have a flow stress anomaly and the TDYS will be normal and negative. Alternatively, extensive spreading of the 1/2<110> cores in (1) may also hinder K-W lock formation as is apparently the case in Ni_3Fe in which the flow stress anomaly is absent (Ref.(3)). All the above are delineated in Fig.2, in which in addition to the symbols defined above, γ_S means SISF energy.

CONCLUSIONS

The several possible forms of TDYS in the $L1_2$ family have been introduced and rationalised in terms of the (absolute) planar fault stabilities, (relative) planar fault energies and P-N stresses of the various configurations of the <110> superdislocations.

REFERENCES

(1) Yamaguchi, M., Vitek, V. and Pope, D.P., Phil. Mag., Vol. A43, 1981,pp.1027 -1044. Yamaguchi, M., Paidar, V., Pope, D.P. and Vitek, V., Phil. Mag., Vol. A45, 1982, pp.867-882.

(2) Sun, Y.Q., D.Phil Thesis, University of Oxford, 1990. Sun, Y.Q., Hazzledine, P.M., Crimp, M.A. and Couret, A., Phil. Mag., Vol. A64, 1991, pp.311-330.

(3) Korner, A., Karnthaler, H.P. and Hitzenberger, C., Phil. Mag., Vol. A56, 1987, pp.73-88.

(4) Hirsch, P.B., Phil. Mag., in press.

(5) Ngan, A.H.W., Jones, I.P. and Smallman, R.E., Phil. Mag., Vol. A65, 1992, pp.1003-1020.

TABLE 1 - Classification of TDYS in $L1_2$

Class	TDYS	Examples
A	Region I in Fig.1 Athermal but negative <110>{111} slip	Ni_3Fe
B	All three regions in Fig.1 Regions I & II - <110>{111} slip Region III - <110>{001} slip	Ni_3Al Ni_3Ga
C	Region III in Fig.1 Thermal and negative <110>{001} slip has lowest CRSS	Pt_3Al Fe_3Ge

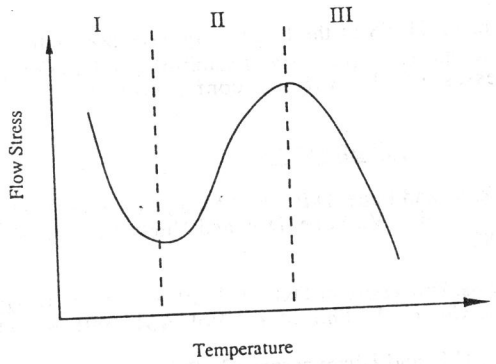

Figure 1 A Generalised Yield Strength vs Temperature Plot of an $L1_2$ Alloy

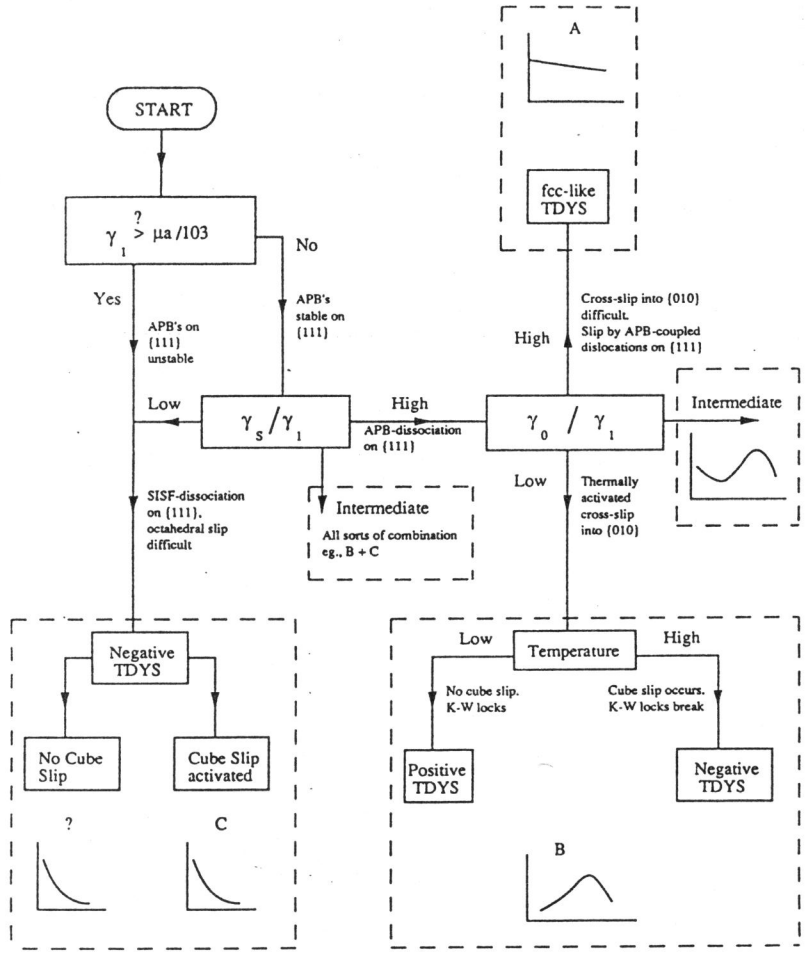

Figure 2 Factors Governing the TDYS of $L1_2$ Compounds