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Dislocations in the ductile B2 YAg intermetallic compound

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ABSTRACT

The Burgers vectors of dislocations in plastically deformed, polycrystalline B2 YAg intermetallic compound were determined by transmission electron microscopy using the $\mathbf{g}\cdot\mathbf{b}=0$ analysis. Both ⟨0 0 1⟩ and ⟨1 1 1⟩-type dislocations were observed in specimens that had been deformed in tension; the ⟨0 0 1⟩ dislocations were more abundant. An active ⟨1 1 1⟩ slip direction satisfies the von Mises requirement of five independent slip systems that are necessary for a polycrystal to undergo a general homogeneous strain. Thus, ⟨1 1 1⟩ slip in YAg appears to be a key contributor to the high ductility and high fracture toughness previously reported for polycrystalline YAg.

1. Introduction

Over the past few decades, B2 intermetallic compounds have attracted considerable attention because some of them possess desirable combinations of low density, good oxidation resistance, and high strength at elevated temperature. However, their engineering use has been limited by the generally poor ductility and low fracture toughness of polycrystalline material at ambient temperature [1]; this low ductility results from the inability of their active slip systems to satisfy the von Mises criterion [2]. A family of ductile intermetallic compounds with composition RM (where R is a rare-earth element and M is a Group 2 or 8–13 element) has recently been discovered to have remarkably high ductility [3]. These RM compounds are "line-compounds" with the exact 1:1 stoichiometry. Over 120 such compounds exist; of the 15 tested to date, most exhibit good ductility. The most ductile composition tested, YAg, tolerates cold rolling to 88% reduction in thickness and shows more than 20% elongation in polycrystalline specimens tensile tested at room temperature in room air of normal humidity [4]. The fracture toughness (K_{IC}) value of YAg has been reported as 19.1 MPa $m^{1/2}$, which is nearly as high as the K_{IC} values for several precipitation hardened commercial aluminum alloys and is much larger than that of the well-studied NiAl B2 intermetallic (5.1–6.4 MPa $m^{1/2}$) [5].

Slip line analysis of single crystal tensile test specimens has shown that the slip systems operating in RM compounds are {1 1 0} ⟨0 0 1⟩ (YAg, YCu, and DyCu), {1 0 0} ⟨0 0 1⟩ (YAg and YCu), and {1 1 0} ⟨1 1 1⟩ (DyCu) [4,6,7]. Of these, the {1 1 0} ⟨0 0 1⟩ and {1 0 0} ⟨0 0 1⟩ are common in B2 intermetallics, but the {1 1 0} ⟨1 1 1⟩ system is usually seen only in B2 compounds with low ordering energies (e.g., CuZn). According to the von Mises criterion for polycrystalline ductility, a B2 material deforming only by {1 1 0} ⟨0 0 1⟩ and {1 0 0} ⟨0 0 1⟩ slip has only three of the five independent slip modes required by the von Mises criterion and would not be expected to show high tensile ductility. However, if ⟨1 1 1⟩ dislocations move in such materials, the required five independent slip modes are available [2], and this would explain the unusually high ductility of these materials. So far only a few prior reports address the dislocation behaviors in B2 RM materials [3,8]. In this letter, we report the dislocation structures observed via transmission electron microscopy (TEM) in polycrystalline YAg specimens deformed in tension.

2. Experimental procedure

The YAg ingot was made by arc-melting equi-molar amounts of Y and Ag several times in an Ar atmosphere. The Y and Ag metals used in this study had a purity of 99.99 wt.% and 99.999 wt.%, respectively. The arc-melted YAg was cold swaged and then annealed in Ar at 500 °C for 1 h. The cylindrical tensile test specimens were machined on a lathe with a gauge section 2.4 mm in diameter and 9.6 mm long. Tensile tests were conducted at room temperature in normal room air with an Instron 1125 machine using a strain rate of $1\times10^{-4}\ s^{-1}$. Slices about 0.5 mm thick were cut by a diamond saw for TEM investigations from a portion of the gauge length of the broken tensile specimens. These slices were mechanically ground and punched into discs 3 mm in diameter, then dimpled before ion milling to perforation. TEM bright field (BF) imaging and selected area electron diffraction (SAED) were performed on a CM30 Philips electron microscope. The Burgers vectors were determined by the standard $\mathbf{g}\cdot\mathbf{b}$ analysis.

3. Results and discussion

The grain sizes of the YAg specimens ranged from about 200 nm to 800 nm as shown in Fig. 1. The inset in Fig. 1 is a SAED pattern along the $[1\bar{1}1]$ zone axis from one of the YAg grains. Indexing

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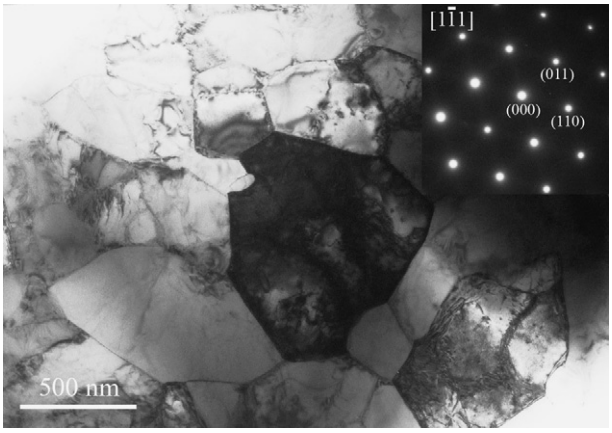

Fig. 1. TEM BF image showing the grain structure of polycrystalline YAg. The inset is a SAED pattern of B2 YAg along the [1 $\bar{1}$ 1] zone axis.

confirms that YAg has the B2 structure with a lattice parameter of 0.362 nm. Fig. 2 shows dislocations in one of the TEM specimens. The dislocations were imaged under different diffraction (**g**) conditions. Table 1 summarizes the electron beam axes, diffraction **g** values, and corresponding dislocation contrast observed. It was determined that dislocations A and E in Fig. 2 are [1 0 0]-type, B and D are [0 1 0]-type, whereas, C is [$\bar{1}$ 1 1]-type. In general the ⟨0 0 1⟩-type dislocations were much more abundant than the ⟨1 1 1⟩-type dislocations. Trace analysis indicates that the slip plane is {1 1 0}. No twins were seen under TEM.

In B2 intermetallic compounds, the {1 1 0} ⟨0 0 1⟩ slip system is often the dominant deformation mode, since {1 1 0} are the most densely packed planes and ⟨0 0 1⟩ are the shortest slip direction vectors [9]. *Ab initio* calculations [10] show that the unstable stacking fault energy [11,12] for slip along the ⟨0 0 1⟩ direction on the {1 1 0} plane for YAg is ~315 mJ/m^2. This suggests that the {1 1 0} ⟨0 0 1⟩ slip mode is easily activated in the RM intermetallic compounds [13]. TEM observations in this study indicated abundant ⟨0 0 1⟩-type Burgers vector dislocations, which is consistent with the *ab initio* calculations. However, as previously stated, ⟨0 0 1⟩-type slip provides only three independent slip systems, so mobile ⟨1 1 1⟩ dislocation is needed to satisfy the requirement for five independent slip systems according to the von Mises criterion for generalized plastic deformation of a polycrystalline aggregate [2].

It is noteworthy that ⟨1 1 1⟩dislocations were observed in these polycrystalline YAg specimens in present study. In B2 crystals a ⟨1 1 1⟩ dislocation has a Burgers vector $\sqrt{3}$ times longer than the Burgers vector for a ⟨0 0 1⟩ dislocation. Energy considerations suggest that slip in the ⟨1 1 1⟩ direction would be more likely to occur by means of two 1/2 ⟨1 1 1⟩ dislocations joined by an anti-phase boundary (APB). Slip in the ⟨1 1 1⟩ direction has been observed in

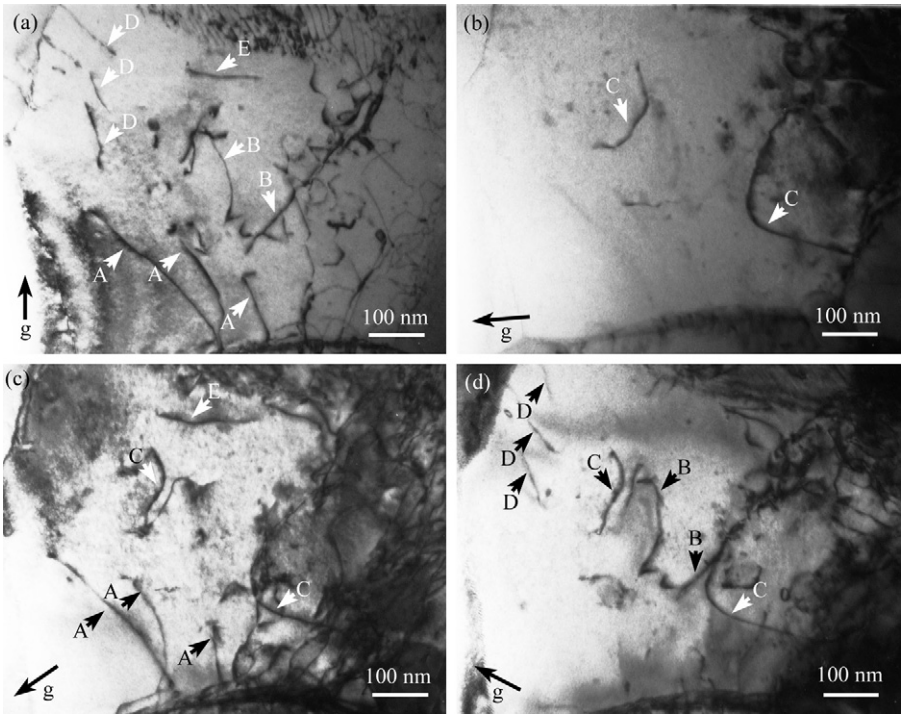

Fig. 2. Bright field TEM images showing dislocations in YAg: (a) beam ≈ [1 $\bar{1}$ 0], **g** = (1 1 0); (b) beam ≈ [1 $\bar{1}$ 0], **g** = (0 0 1); (c) beam ≈ [1 $\bar{1}$ 1], **g** = ($\bar{1}$ 0 1); and (d) beam ≈ [1 $\bar{1}$ 1], **g** = (0 1 1). See the text for the identification of the dislocations marked as A, B, C, D and E.

Table 1
Burgers vector analysis.

Beam	**g**	Dislocation contrast in Fig. 2					Burgers vector in Fig. 2				
		A	B	C	D	E	A	B	C	D	E
[1 $\bar{1}$ 0]	(1 1 0)	V	V	I	V	V	[1 0 0]	[0 1 0]	[$\bar{1}$ 1 1]	[0 1 0]	[1 0 0]
	(0 0 1)	I	I	V	I	I					
[1 $\bar{1}$ 1]	($\bar{1}$ 0 1)	V	I	V	I	V					
	(0 1 1)	I	V	V	V	I					
[1 $\bar{2}$ 0]	(2 1 1)	V	V	I	V	V					

V: visible; I: invisible.

CuZn and FeCo compounds, which all have fairly low ordering energies [14,15]. The calculated APB energy for {1 1 0} 1/2 ⟨1 1 1⟩ in YAg is ∼745 mJ/m^2, which is relatively high, although not quite as high as that of NiAl (∼815 mJ/m^2) [10]. High APB energies make formation of 1/2⟨1 1 1⟩ + APB + 1/2⟨1 1 1⟩ superdislocation pairs difficult. No 1/2⟨1 1 1⟩ + APB +1/2 ⟨1 1 1⟩ superdislocation pairs were observed in the polycrystalline YAg specimens used in this study. It may be that the ⟨1 1 1⟩ dislocations were present in the specimens only after the ⟨0 0 1⟩ dislocations were activated. Although questions remain about how ⟨1 1 1⟩-type dislocations form and move in YAg, it provides a reasonable explanation for the high ductility and fracture toughness of the YAg intermetallic compound.

4. Conclusions

In summary, TEM investigations of the Burgers vector of various dislocations in tensile tested polycrystalline B2 YAg specimens showed ⟨0 0 1⟩ and ⟨1 1 1⟩ dislocations. The ⟨0 0 1⟩ dislocations observed by TEM are consistent with *ab initio* calculations of the low unstable stacking fault energy of the {1 1 0} ⟨0 0 1⟩ slip mode in B2 YAg. The observation of ⟨1 1 1⟩ dislocations is the most important finding of this study because they along with the ⟨0 0 1⟩ dislocations provide the five independent slip systems required for high ductility and fracture toughness in polycrystalline YAg.

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