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Fracture behavior of B_2 ordered iron aluminide with Mn addition①

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[Abstract] The microstructure and fracture behavior of B_2-ordered iron aluminides with and without Mn (1.5%, mole fraction) were investigated by tensile tests (TT) and scanning electron microscope (SEM). The results show that the addition of Mn into the alloy can improve tensile properties and plasticity of the alloy and change the fracture behavior of the alloy from transgranular cleavage into intergranular mixed with transgranular cleavage. The theoretical calculation, by computer, indicates that the B_2-ordered Fe-28Al alloy cleaves on {100} planes because of weak bond strength. Addition of Mn into the alloy, whose atoms likely occupy sites I in the unit cell, can increase the cleavage strength of the alloy on {100}, leading to higher fracture strength and plasticity of the alloy after Mn addition.

[Key words] fracture; cleavage strength; iron aluminide
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1 INTRODUCTION

There has been more and more researches on ordered iron aluminides based on the Fe-Al system in recent years. The ordered iron aluminides have excellent oxidation resistance, low cost, rich in material resources and some other advantages, which leads them to many engineering applications[1, 2]. However, the brittleness and lack of ductility at room temperature have been major obstacles to their uses as structural materials. Recently many researches report showed that alloying elements could improve their mechanical properties. For examples, addition of alloying elements such as Cr, Mn, Ce can improve their ductility at room temperature[3~ 8]. Although the changes in grain size, APB energy, and superdislocation structure were suggested to be major effects of ternary additions on the properties of the aluminides and have been studied for years, relatively little attention has been paid to changing valence electron structures such as valence electron and bond strength which cause brittleness in the ordered aluminides.

The iron aluminide Fe-28Al can be in two order structures: the DO_3-order structure which is state below the critical temperature of 540 ℃ and the B_2-order structure between 540 ℃ and 760 ℃. Above 760 ℃ the alloy is of α structure. The B_2-ordered structure in the aluminide could be preserved at room temperature by quenching[9~ 11]. Our earlier studies have shown that the Mn is an effective element for improving cleavage strength and ductility in the iron aluminide of DO_3 structure[3, 5]. The purpose of this paper is to study the mechanism for the effect of Mn addition on the cleavage strength of B_2-ordered FeAl intermetallics by solid valence electron theory[12, 13] as a depiction of valence bonds among Fe, Al and Mn atoms.

2 EXPERIMENTAL

The Fe-28Al and Fe-28Al-1.5Mn alloys (mole fraction) were smelted in a vacuum induction furnace and cast into a mold. After homogenizing at 950 ℃ for 4 h, the alloys were hot-rolled at 950 ℃ and warm-rolled at 650 ℃ from 7.0 mm to 0.7 mm. The tensile samples were punched from the sheets, heated at 800 ℃ for 1 h for recrystallization and then kept at 700 ℃ for 2 h for B_2 ordering, followed by quenching. The tensile samples were tested at room temperature in air at a strain rate of $(3.3\sim 5)\times 10^{-2}$/s on an LX-250 kg tensile tester. The fracture surfaces were examined by DXS-X2 scanning electron microscopy (SEM). The B_2-ordered structure was characterized by Philips CM12 transmission electron microscopy (TEM). The lattice constant of alloys is measured by Rigaku D/max-3BX X-ray diffracetometer.

3 RESULTS

The B_2 superlattice is of BCC structure and the unit cell contains 2 atoms. The coordinates of atom corners are (000) and $(\frac{1}{2}00)$, refereed to the letters I and II, as shown in Fig. 1(a). Al atoms occupy only I site in the B_2 structure, but occupy all sites whose

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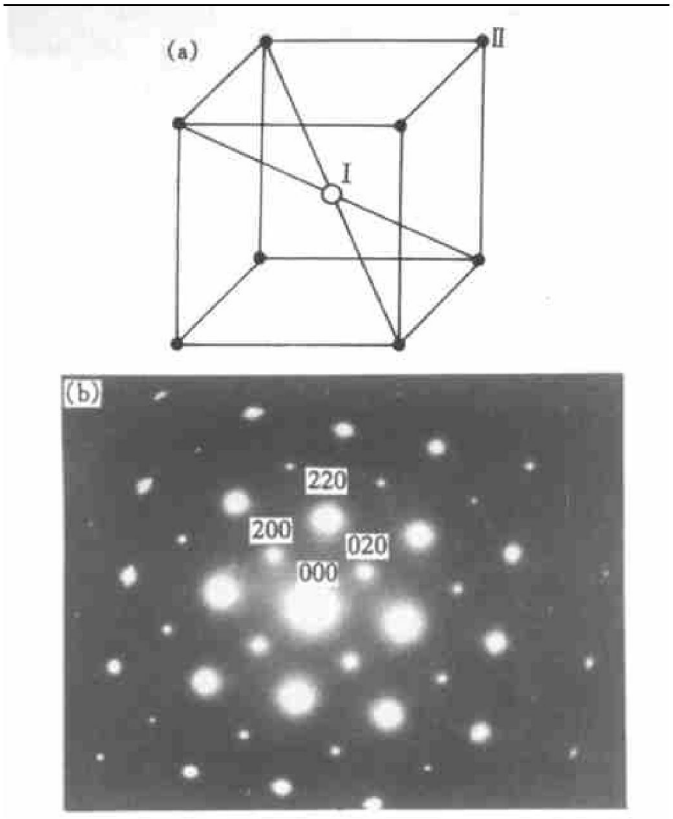

Fig. 1 Unit cell of B_2 structure(a) and electron diffraction pattern of B_2 structure along [100] direction(b)

$h+k+l=4n$ (where n is an integer) and the B_2 superlattice whose $h+k+l=4n+2$. In our investigation, alloys obtain B_2-type ordering structure at room temperature after ordering treatment at 700 ℃ for 2 h and then quenching. Fig. 1(b) shows superlattice in the [001] diffraction patterns. It is shown from Fig. 1(b) that strong fundamental spots are (000), (220) and weak superlattice spots are (020) and (200).

The tensile properties were tested. The results are listed in Table 1, which indicates that B_2-ordered Fe-28Al alloy has lower tensile strength and ductility at room temperature. Addition of Mn into B_2-ordered Fe-28Al alloy can improve fracture strength of the alloy. SEM observes the tensile fracture modes of alloys. The results show that two alloys crack mainly in cleavage mode. It is obvious from Fig. 2(a) that there are many secondary cracks in the Fe-28Al alloy, suggesting easy propagation of crack in this alloy. On the other hand, some intergranular cracks occur in the alloy with Mn addition, as shown in Fig. 2(b).

Table 1 Mechanical properties of two alloys at room temperature

Alloy	σ_b/ MPa	$\sigma_{0.2}$/ MPa	δ/ %
Fe-28Al	485.9	416.9	2.1
Fe-28Al-1.5Mn	521.1	448.3	2.5

The base alloys usually fracture in form of cleavage and(or) intergranular at room temperature, in

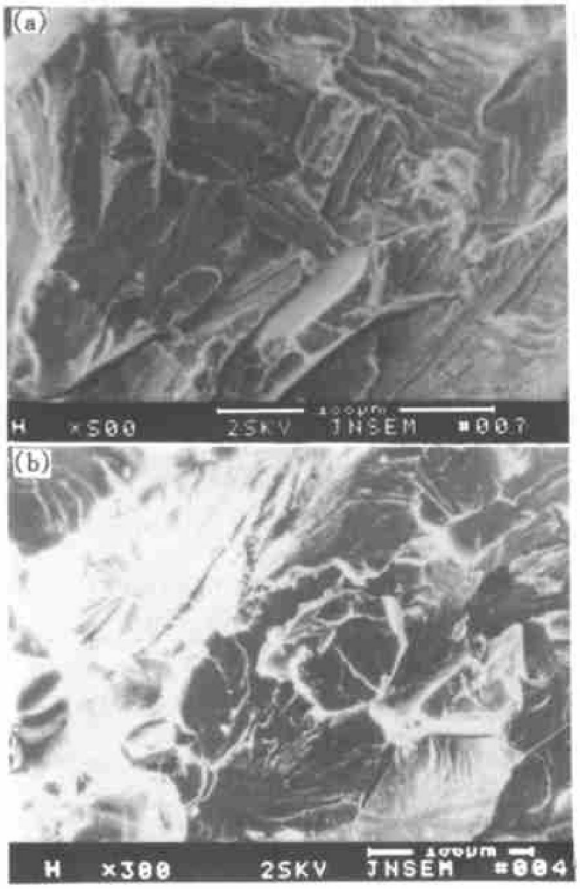

Fig. 2 Fractographs of alloys
(a) —Fe-28Al alloy;
(b) —Fe-28Al-1.5Mn alloy

which the fractures of alloy are dependent on their relative strength to each other. After addition of Mn into the alloy, the fracture mode changes from the trans-granular cleavage to mixed intergranular-trans-granular cleavage accompanying an increase of the fracture strength, which indicates that the Mn addition can increase the cleavage strength and then lead to large plastic deformation in the alloy before fracture. The phenomena could be reasonably explained by theoretical analysis of bond energy strength for the alloys with and without Mn, based on electronic theory [9], which is described as follows.

First, B_2 superlattice is considered for FeAl alloy. There are two kinds of atom site, I and II. Al atoms occupy sites I and Fe atoms occupy sites II. The molecular formula could be shown as $Al^{I}Fe^{II}$, where I and II are atomic sites I and II, respectively. Second, the B_2 unit cell is considered for the Fe-28Al alloy according to comparison of the stoichiometric composition of FeAl. While site II is occupied by Fe atom, site I is partly occupied by Al atom and Fe atom. According to "equicell mode"[12], its equitation formula could be shown as $Fe^{II}Fe_{0.44}{}^{I}Al_{0.56}{}^{I}$, where site I is occupied by equitation formula of 44% Fe atom and 56% Al atom. Its lattice constant is 0.290 90 nm, which is measured by X-ray diffraction

method. The valence electrons and bond strengths of B_2-ordered Fe-28Al alloy, which are in each bond nonignored at room temperature, are mathematically calculated by computer simulation of Fe and Al hybrid atomic states based on valence electron theory[12, 13]. The results are listed in Table 2. In Table 2, I_α is the number of equivalence bonds, n is the number of valence electrons, D_n is the experimental space of each valence bond, and E is the bond strength in each bond. Third for the B_2 unit cell of the Fe-28Al-1.5Mn alloy. Its equitation formula could be shown as $Fe^{II}Fe^{I}_{0.41}Mn^{I}_{0.03}Al^{I}_{0.56}$ where Mn occupies site Ⅰ, or as $Fe^{II}_{0.97}Fe^{I}_{0.44}Mn^{II}_{0.03}Al^{I}_{0.56}$ where Mn occupies site Ⅱ. Its lattice constant is 0.288 37 nm, measured by X-ray
diffraction method. The valence electrons and bond strengths of the two lattices are calculated and shown in Table 3. It is obvious from Table 3 that total energy is 79.708 0 kJ/mol when Mn occupies site Ⅰ and 73.650 0 kJ/mol when Mn occupies site Ⅱ. The stronger the bond, the stabler the state. Those calculated results suggest that Mn atoms are inclined to occupy site Ⅰ. Table 4, which is deduced from Table 3, shows that B_2 Fe-28Al alloy has stronger bonds in ⟨111⟩ directions than those in ⟨100⟩ directions, indicating that the cleavage would take place on {100} planes in the alloy. After addition of Mn into the alloy, the bond strengths are increased in both ⟨100⟩ and ⟨111⟩directions so that the Fe-28Al-1.5Mn alloy has stronger fracture strength than Fe-28Al alloy has. The cleavage would still take place on {100} planes because of stronger bond strength on {111} planes in the alloy after adding Mn. The results of increase in cleavage strength from Table 3 and Table 4 could explain the tensile property results that the Mn addition could improve mechanical properties of the B_2-ordered Fe-28Al alloy.

Table 2 Valence electron and bond strength in B_2 Fe-28Al superlattice

Bond	I_α	n	D_n	E / (kJ·mol^{-1})
Fe^{II}– Al^{I}	8.96	0.479 9	2.497 4	18.630 0
Fe^{I}-Fe^{II}	7.04	0.400 2	2.497 4	16.738 7
Fe^{I}-Al^{I}	5.28	0.162 8	2.883 7	5.100 0
Al^{I}-Al^{I}	3.36	0.195 3	2.883 7	5.678 4
Fe^{II}-Fe^{II}	6.00	0.096 3	2.883 7	5.743 6
Fe^{I}-Fe^{I}	2.64	0.135 8	2.883 7	4.583 6

4 CONCLUSIONS

The theoretical analyses about the cleavage strength for B_2-ordered Fe-28Al alloy and Fe-28Al-1.5 Mn alloy confirm the experimental results that Mn can improve the cleavage strength of the alloy. Besides, the theoretical calculation indicates those Mn atoms likely occupy sites I in the B_2-ordered structure and cleavage would take place on {100} planes in the alloys with and without Mn addition.

Table 3 Valence electron and bond strength in B_2 Fe-28Al-1.5Mn superlattice

Equitation Formula	Bond	I_α	n	D_n	E/(kJ·mol^{-1})
$Fe^{II}Fe^{I}_{0.41}Mn^{I}_{0.03}Al^{I}_{56}$	Fe^{II}-AI^{I}	8.96	0.479 8	2.497 4	19.249 4
	Fe^{I}-Fe^{II}	6.56	0.376 2	2.497 4	16.223 5
	Fe^{I}-Mn^{I}	0.48	0.508 8	2.497 4	17.721 1
	Al^{I}-Al^{I}	3.36	0.195 2	2.883 7	6.061 8
	Fe^{I}-Fe^{I}	2.46	0.150 6	2.883 7	5.403 7
	Fe^{II}-Fe^{II}	6.00	0.096 3	2.883 7	3.743 1
	Al^{II}-Fe^{I}	4.92	0.171 5	2.883 7	5.724 8
	Al^{I}-Mn^{I}	0.36	0.207 0	2.883 7	5.580 6
$Fe_{0.97}{}^{II}Fe^{I}_{0.44}Mn^{II}_{0.03}Al^{I}_{0.56}$	Fe^{II}-Al^{I}	8.96	0.479 9	2.497 4	19.253 4
	Fe^{II}-Fe^{I}	7.04	0.356 1	2.497 4	12.815 9
	Fe^{II}-Mn^{II}	0.36	0.132 5	2.883 7	4.078 2
	Fe^{II}-Fe^{II}	5.82	0.096 3	2.883 7	3.743 6
	Al^{I}-Al^{I}	3.36	0.195 2	2.883 7	6.061 8
	Al^{I}-Mn^{II}	0.48	0.660 3	2.497 4	20.974 1
	Al^{I}-Fe^{I}	5.28	0.144 9	2.883 7	4.036 6
	Fe^{I}-Fe^{I}	2.64	0.107 5	2.883 7	2.686 4

Table 4 Bond strength E in B_2-ordered structure, with and without Mn ($kJ \cdot mol^{-1}$)

Alloy	Mn site	Direction	E_{Al-Fe}	E_{Fe-Fe}	E_{Al-Al}	E_{Al-Mn}	E_{Fe-Mn}	E_{total}
Fe-28Al		⟨111⟩	18.630 0	16.738 7				35.368 7
		⟨100⟩	5.100 0	10.327 2	5.678 4			21.105 6
Fe-28Al-1.5Mn	II	⟨111⟩	19.253 4	12.815 9		20.974 1		53.043 4
		⟨100⟩	4.036 6	6.430 0	6.061 8		4.078 2	20.606 6
	I	⟨111⟩	19.249 4	16.223 5			17.721 1	53.194 0
		⟨100⟩	5.724 8	9.146 8	6.061 8	5.580 6	4.703 3	31.217 3

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