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SHORT COMMUNICATION

Effect of Vacancies on the Tensile Properties of Fe-40Al Single Crystals in Air and Vacuum

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Tensile tests in both air and vacuum have been performed on Fe-40Al single crystals containing two different vacancy concentrations. It is shown that the room temperature fracture strengths are significantly increased but the elongations are decreased in both test environments at high vacancy concentration. The fracture mechanisms are controlled by the vacancy concentration, with vacancies promoting the fracture along the slip planes.
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INTRODUCTION

It has now been recognized that both the environment and vacancy concentration are two significant factors which affect the mechanical properties of FeAl, see recent reviews [1-4].

The effect of environment on the mechanical properties of FeAl was first found by Liu et al. [5, 6]. They proposed that the observed decrease in the ductility in air compared to vacuum is due to the formation of hydrogen through a surface reaction between Al atoms and water vapor, i.e., $3H_2O + 2Al \rightarrow Al_2O_3 + 6H$. The atomic hydrogen then embrittles the crack-tip region. This environmental embrittlement leads to either transgranular fracture (at low aluminum concentrations) or intergranular fracture (nearer stoichiometric compositions) in FeAl [4, 5, 7, 8], with the cleavage planes being more susceptible to embrittlement than the grain boundaries [5, 6]. For single crystals, it has been shown that the test environment not only affects the elongation but also the crack initiation location [8, 9]. For Fe-40Al single crystals tested in air, fracture initiates at the surface, whereas in oxygen, fracture initiates inside the specimen, with ten times the elongation observed in oxygen compared to air. Fracture toughness tests on stoichiometric FeAl single crystal have shown that fracture propagates along {111} in vacuum but along {100} in air [10]. In contrast, Fe-35Al and Fe-40Al exhibit cleavage on {100} in a hydrogen-free environment [9, 11].

Only recently has it been shown that after annealing at elevated temperature, a large vacancy concentration is easily retained at low temperature in FeAl, and that these vacancies strongly affect the low temperature mechanical properties [1, 12–16]. As calculated by Chang et al. [14] and later confirmed using X-ray analysis by Xiao and Baker [17], both based on a triple-defect model, the room temperature equilibrium vacancy concentration in FeAl alloys increases quickly as the aluminum concentration approaches the stoichiometric composition. It was shown that the hardness is linearly related to the square-root of the vacancy concentration in FeAl [14], in agreement with the parabolic solute-dislocation interaction model [18]. In contrast, results from FeAl single crystals showed that the

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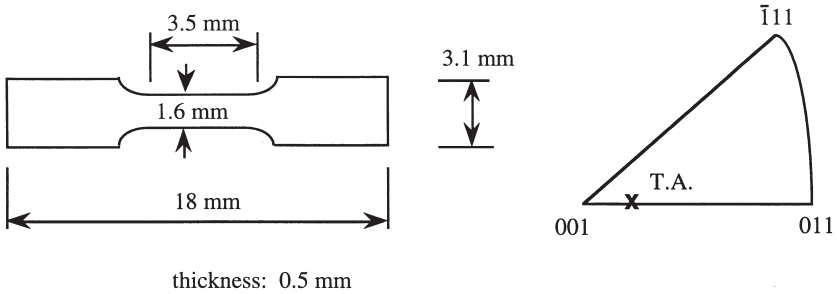

FIG. 1. Schematic showing the dimensions of the tensile specimens and the orientation of the tensile axis (T.A.).

increase in yield stress with increasing vacancy concentration consists of two stages: a fast initial increase followed by a slower increase with increasing vacancy concentration. Also, cross-slip is promoted at high vacancy concentrations [19].

In the present research, tensile tests on Fe-40Al single crystals with two different vacancy concentrations were performed either in air or in a high vacuum in order to investigate the effect of vacancies on the environment embrittlement of this material.

EXPERIMENTAL

A Fe-40Al single crystal was annealed for 16 hrs at 1423 K, followed by slow furnace-cooling, and further annealed at 673 K for 5 days to minimize any retained thermal vacancies [20]. Tensile specimens were cut with the tensile axis at about 8° to [100] direction, see Fig. 1. Some of the specimens were annealed at 1173 K for one hour and air-cooled in order to introduce a high vacancy concentration. Based on previous experimental measurements [19] and thermodynamic calculations [14], the vacancy concentrations are estimated to be $\sim 6.2 \times 10^{-3}$ and $\sim 1.3 \times 10^{-4}$ (in mole fraction) after the anneals at 1173 K and 673 K, respectively.

Before mechanical testing, the specimens were electropolished at 16 V in a 10% perchloric acid-methanol solution at 248 K, then washed in methanol. Tensile tests were performed at room temperature either in air or in ultra-high vacuum ($\sim 10^{-8}$Pa) at a strain rate of $\sim 1 \times 10^{-3}$ s^{-1}. Because of the low compliance of the loading system, the yield point was difficult to define and, thus, is not reported here. The elongations were measured directly from the specimens (after fracture) using an optical microscope equipped with a digital micrometer. Note that the results from two specimens that fractured outside the guage at low stress are not reported here. The fracture surfaces were examined using a JEOL JSM-5310LV SEM operated at 20kV, and slip lines were observed using an optical microscope.

RESULTS AND DISCUSSION

The fracture strengths and elongations for the specimens with different vacancy concentrations tested in different environ-

Table 1 Fracture Strengths and Elongations (in Parentheses) of Fe-40Al Single Crystal Strained under Tension at $\sim 1 \times 10^{-3}$ s^{-1} in Air and in a Vacuum of $\sim 10^{-8}$ Pa

Vacancy concentration (mole fraction)	*Strength, MPa (elongation, %)*	
	Vacuum	*Air*
1.3×10^{-4}	768 (8.7)	471 (0.8)
	706 (6.1)	311 (0.5)
		524 (0.5)
		373 (1.0)
6.2×10^{-3}	1043 (1.7)	714 (0.1)
	895 (4.1)	

ments are shown in Table 1. It is evident that the fracture strengths of the specimens with high vacancy concentration are higher both in air and in vacuum than those of the specimens with very low vacancy concentration tested in the same environment. In addition, the environmental effect on the fracture strength is relatively smaller for the high vacancy concentration specimens. The difference in the fracture strengths in different environments (at a given vacancy concentration) is attributed to the differ-

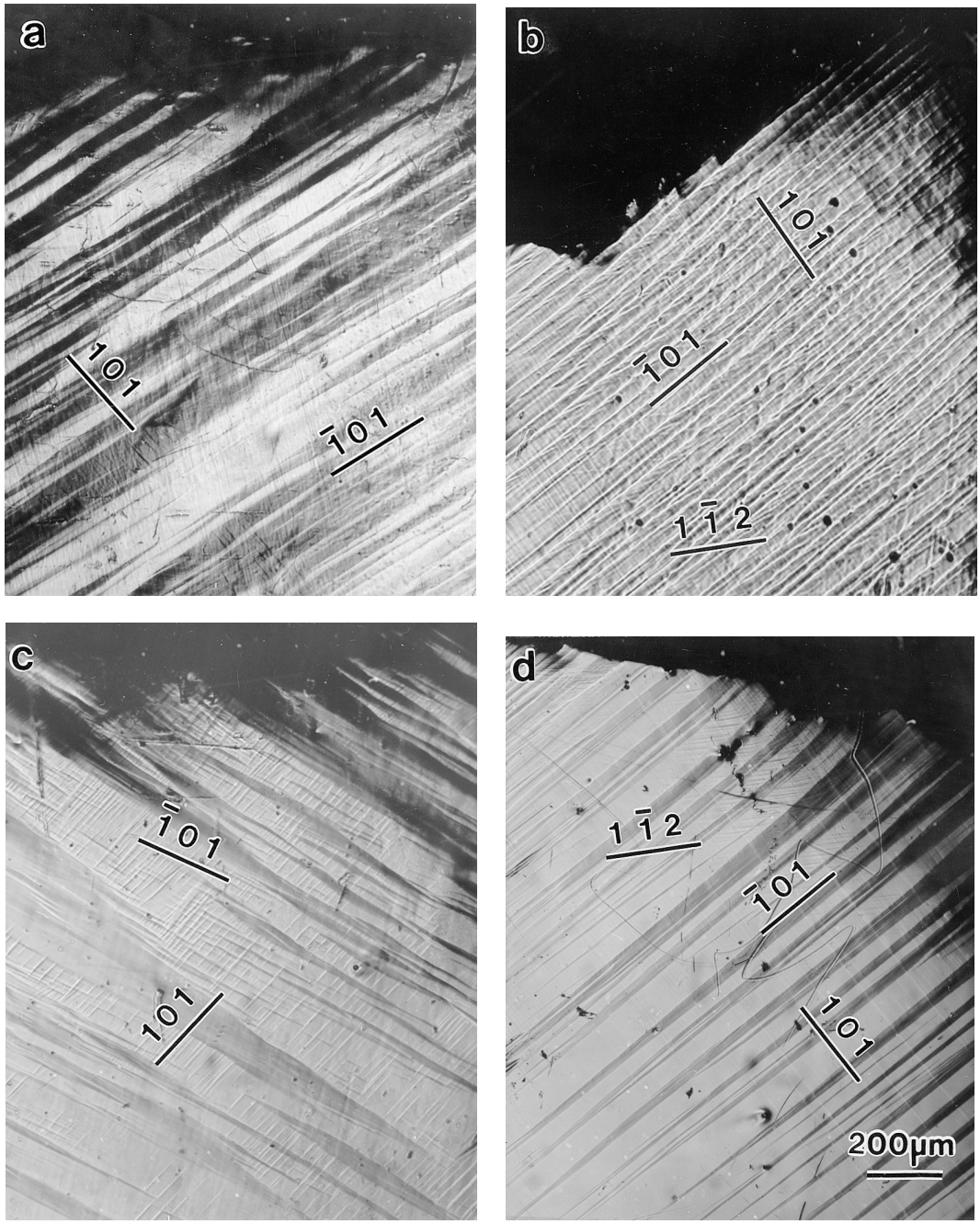

FIG. 2. Slip lines on the specimen surface after test, (a) in vacuum with low vacancy concentration (Cv), (b) in vacuum with high Cv, (c) in air with low Cv, (d) in air with high Cv.

ence in the elongation, as given in Table 1. Increasing vacancy concentration decreases the ductility in both environments.

Since the orientation of the single crystals is very close to the boundary of the stereographic triangle, see Fig. 1, two {110} <111> slip systems having similar Schmid factors can operate during deformation. Consequently, on the faces of the specimens having low vacancy concentration, two sets of slip lines from the two {110} planes with the highest Schmid factors can be identified, see Fig. 2. There are also some weak slip lines on {211} near the fracture surface. In the high vacancy concentration specimens, the slip lines on {110} are finer and more closely spaced. In addition, slip lines corresponding to {211} slip planes are stronger and distributed over the whole gauge section, indicating that slip on {211} planes is

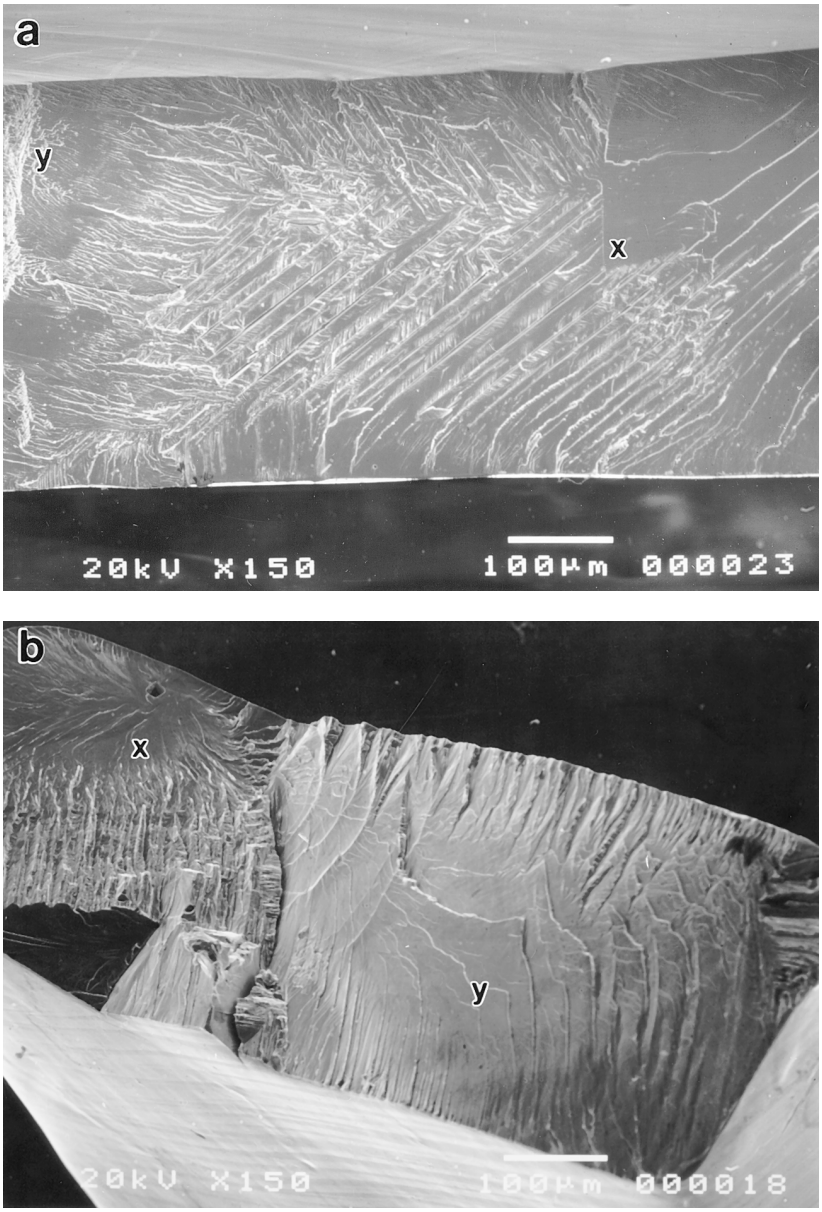

FIG. 3. The fracture surfaces of tensile specimens tested in (a) vacuum with low Cv, (b) vacuum with high Cv, (c) air with low Cv, (d) air with high Cv.

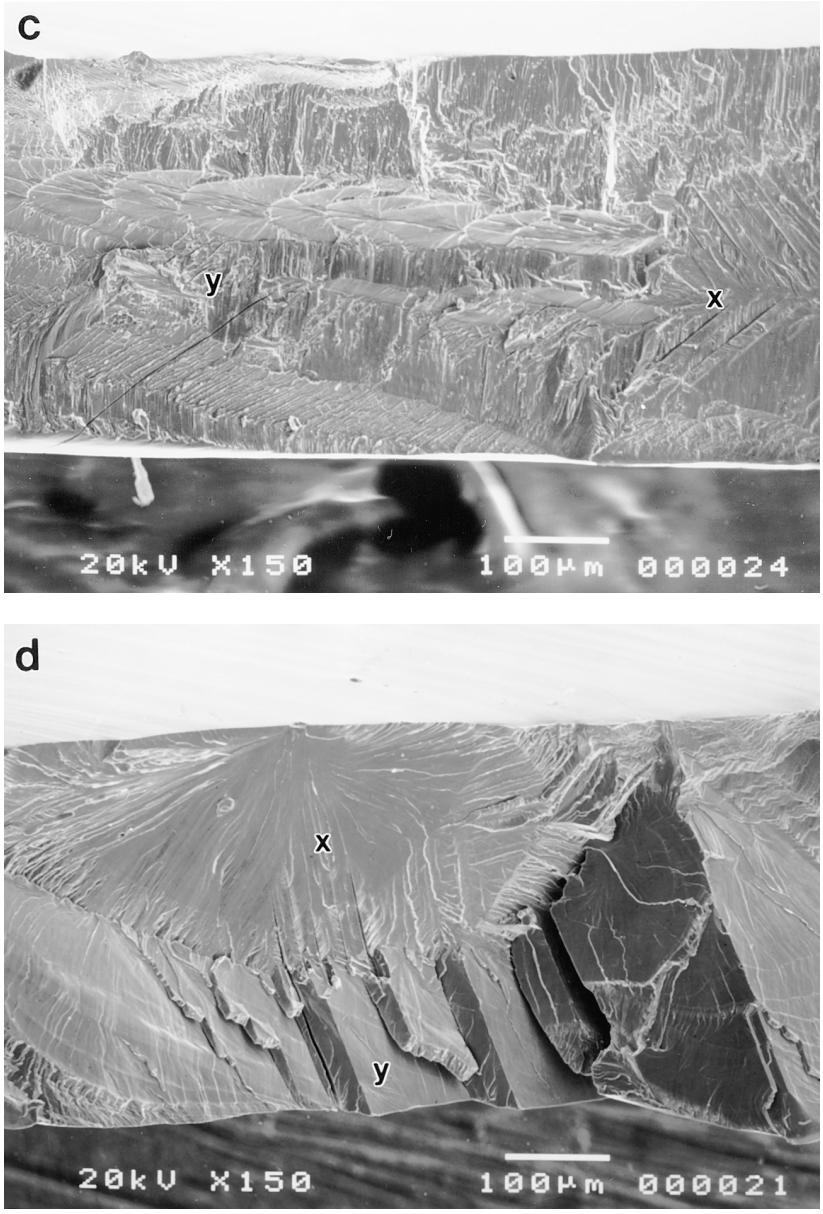

FIG. 3. Continued.

promoted by vacancies. Clearly, plastic deformation is mostly from slip on {110} planes regardless of the testing environment and vacancy concentration. Slip on {211} is activated at high vacancy concentration, but after some prior strain hardening on {110}. The latter observation is in agreement with recent compression studies on Fe-40Al single crystals [19] where {211} slip was only noted at large vacancy concentrations and after the initial operation of {110} slip. In that case, a lower work hardening rate was observed once {211} slip started to operate.

The environment did not appear to have much effect on the fracture mode but the vacancy concentration did, as shown in Fig. 3. The fracture surfaces of the specimens

with low vacancy concentration generally consisted of two different regions, see panels a and b of Fig. 3. In Region X, the fracture plane is approximately perpendicular to the tensile axis, indicating that the cleavage plane is {100}. On this fracture surface there are two sets of orthogonal secondary cracks, which are presumably also on {100}. Region Y has fracture occurring on several different planes. In contrast, at high vacancy concentration, different fracture occurs, as shown in panels c and d of Fig. 3. In addition to the fracture on {100} (Region X), cleavage along the {110} slip planes (Region Y) can be identified from the geometry and the slip traces in which the flat fracture planes are parallel to the {110} slip planes. Cleavage fracture along {100} has previously been observed in FeAl single crystals [8, 9]. Based on the observation of the formation of <100> dislocations, Munroe and Baker [13] suggested that such dislocations are formed through the collision of two <111> superdislocations, and this may be the source of cleavage on {100} planes.

As expected, the elongations are lower in air than in vacuum. However, the present results indicate that cleavage along {110} slip planes is promoted by high concentration of vacancies not by the testing environment. Hydrogen may be transported rapidly by gliding dislocations and, thus, accelerate cleavage fracture by weakening the bonding on the slip plane. Cleavage on the slip plane may be related to the local disordering along the slip plane because of the interaction between vacancies and gliding superdislocations [21, 22]. A recent study by Hirth suggests that dislocation pile-ups lead to the glide plane decohesion [23]. This is due to the non-linear core strain field of screw and edge dislocations that can produce tangential normal stresses in cylindrical coordinates fixed on the dislocation line. In a dislocation pile-up, these core fields generate a stress concentration in the slip plane that favor the formation of an opening Mode I crack [23]. The hardening effect of vacancies (or vacancy clusters) on the slip plane may enhance the dislocation pile-up process.

CONCLUSION

In both air and vacuum, the room-temperature fracture strengths of Fe-40Al single crystals are significantly increased, but the elongations are decreased by introducing a high vacancy concentration. As noted previously [1-4], the test environment also has a significant effect on the elongation. The fracture mode is controlled by the vacancy concentration: with a low vacancy concentration, fracture is through cleavage on both {100} and a variety of other planes, whereas at high vacancy concentration, cleavage occurs mainly on {100} and {110}. The later fracture mode suggests that vacancies promote fracture along the slip planes.

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