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X-ray elastic constant determination and residual stress of two phase TiAl-based intermetallic alloy①

GUO Fu-an(郭富安)[1,2], ZHENG R. T.[2], V. Ji[1],
ZHANG Yong-gong(张永刚)[2], CHEN Chang-qi(陈昌麒)[2]
(1. LM3 ESA CNRS 8006, ENSAM, 151 Bd. del'Hôpital Paris 75013, France;
2. Department of Materials Science and Engineering, Beijing University of Aeronautics and Astronautics, Beijing 100083, P. R. China)

[Abstract] To evaluate the residual stress in TiAl-based alloys by X-ray diffraction, X-ray elastic constants (REC) of a γ-TiAl alloy were determined. From these results, the stress state of a given phase in a duplex TiAl-based alloy under a uniaxial tensile loading has been characterized by X-ray diffraction. The results show that the X-ray elastic constants and the microscopic stresses of the given phase are different from the apparent elastic constants and the macroscopic stresses of the alloy. The reason of the different distribution of the alloy was also discussed.

[Key words] TiAl-based alloy; X-ray diffraction technique; X-ray elastic constant; duplex structure residual stress
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1 INTRODUCTION

TiAl intermetallic compound has lower density, higher temperature strength, higher stiffness and better oxidation resistance compared to the conventional high-temperature alloys[1], therefore, it is expected to be a potential light mass heat-resistant material. Extensive studies of effect of the microstructures, and alloying elements on mechanical properties have been carried out worldwide. However, there are still road-blocks to successful use of two-phase TiAl alloys in structural applications, and one of the main barriers is that their room temperature tensile ductility is limited to 2%~3%[2]. Room temperature mechanical properties of two-phase γ-TiAl alloys depend strongly on microstructure[3]. It is well known that residual stress plays an important role in the fracture of the intermetallic compounds. So it is necessary to study the distribution and change of the residual stress in TiAl-based alloys.

TiAl alloys exhibit generally a two-phase microstructure composed of γ-TiAl and a small fraction of α_2-Ti_3Al phase. Owing to the tetragonal crystal structure of γ phase and the hexagonal crystal structure of α_2 phase, there is a lattice misfit between them. Moreover, slip systems and mobility of dislocations in these two phases are different, and mechanical properties of the alloy are in high anisotropy. Therefore, it is expected that deformation is inhomogeneous, and deformation incompatibility across the lamellar interfaces and grain boundaries may occur. Local accumulation and non-uniform distribution of internal strain and stresses introduced by all these effects may be related to brittle fracture behavior, which is a main barrier for the application of the alloys.

X-ray diffraction stress evaluation method is a non-destructive experimental technique well adapted to evaluate the residual stress in the metallic materials. Thus, it can be used to study the distribution and change of the residual stress in TiAl-based alloys. In multiphase materials, however, X-ray diffraction method only allows to measure the mechanical state of one particular phase because the elastic constants of the studied phase are different from that of the aggregate. Therefore, it is necessary to know the elastic constants of the studied phases before measuring the residual stress of the phases by X-ray diffraction. As an example, for a two-phase material, the diffraction method is almost the only in-situ method to determine the radiocrystallographic elastic constants (REC) of each phase. Until now, there is little information about X-ray elastic constants of the two-phase TiAl alloys.

In this paper, Ti-47Al-2Cr-2Nb (mole fraction, %) alloy has been studied. Fine grain duplex microstructures with different volume fractions of lamellar (consisting of lath colonies of γ-TiAl and α_2-Ti_3Al) and equiaxed γ have been obtained. The REC of γ phase is determined in-situ by X-ray diffraction method during an uniaxial tensile test, then the stress of the given phase and their distribution are determined using X-ray diffraction technique. The relations between the stresses and the strain, the peak

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broadening evaluation and the deformation are discussed.

2 EXPERIMENTAL

A two-phase gamma TiAl alloy ingot with the nominal composition of Ti-47Al-2Cr-2Nb was prepared by skull melting and casting. The bulk composition of the ingot was determined to be Ti-47.2Al-2.1Cr-1.96Nb. The ingot was hot isostatically pressed, then isothermally forged at 1 180 ℃ to a pancake. The samples were cut from the pancake and sealed in silica tubes filled with argon for heat treatments. In order to obtain the duplex microstructures with different volume fractions of lamellar grains and equiaxed γ, different temperatures and annealing times were chosen in γ+α field, followed by controlled cooling.

The test specimens were machined from the different microstructure samples. The dimension of the specimens is shown in Fig. 1. The specimens were electro-polished in order to eliminate the surface damage induced by machining. The experiments were conducted using a small tensile device that can be fixed on the sample holder of the diffractometer. A strain gage was applied for the measurement of the strain during the test. The stress in γ phase were determined by X-ray diffraction with the equipment micro-CGR during step-by-step uniaxial tension. For each step of these mechanical tests, the specimen was tensioned to a fixed load and kept constant during the X-ray measurements. Thus the macro-stress and micro-stress of the specimen can be obtained. TiK_α radiation of 25 mA and 25 kV was used for {202} planes of γ phase. The X-ray beam was irradiated on an area of 3 mm in diameter of the specimen. X-ray diffraction stress analysis was carried out in loading direction with different ψ angles. Classic $\sin^2\psi$ method was used for stress determination. The precision of stress analysis and peak are less than 50 MPa and 0.3°, respectively. The macroscopic tensile experiments were conducted by MTS universal testing machine.

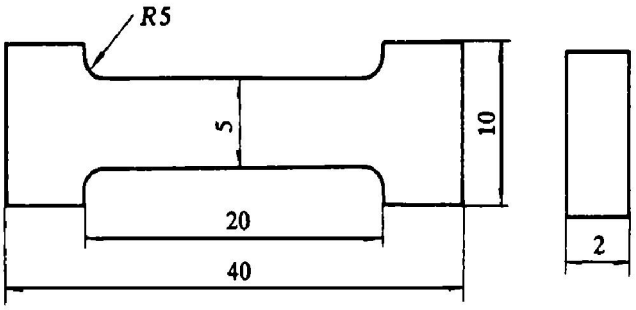

Fig. 1 Dimension of test specimen (mm)

3 RESULTS AND DISCUSSION

3.1 Microstructures and volume fractions of γ and α_2

The microstructures of Ti-47Al-2Cr-2Nb alloy used in the present study are shown in Fig. 2. It can be seen that the microstructures of the four studied specimens are the fine duplex microstructures consisted of equiaxed γ grains and lath colonies (γ+α_2). The volume fractions of lamellar grains were determined by means of quantitative metallography. The volume fractions of γ and α_2 were measured by X-ray diffraction spectrum with a confidence limit of more than 85%. The volume fractions of equiaxed γ and lamellar grains, and the volume fractions of γ and α_2 of the four studied specimens are listed in Table 1.

Table 1 Volume fractions of γ, α_2, equiaxed γ grain and lamellar grains of four studied specimens in Fig. 2

Specimen	Volume fraction/%			
	Equiaxed γ grain	Lamellar grain	γ	α_2
a	80	20	94.2	5.8
b	50	50	94	6.0
c	30	70	92.9	7.1
d	10	90	91.8	8.2

It can be seen from Table 1 that the volume fraction of α_2 phase varies with the different heat treatment conditions. This is in good agreement with that obtained by Kim using other methods[4]. It should be noted that the volume fraction of the phase α_2 in four studied specimens is too small for evaluating the stress in it by X-ray diffraction, and it is hard to give a reliable diffraction peak. Usually, the necessary volume fraction of a phase for X-ray diffraction stress measurement is no less than 20%[5]. So only the REC and the stress in the γ phase have been measured.

3.2 X-ray elastic constants of γ phase

The X-ray elastic constants of γ phase were determined by uniaxial loading experiments as described in Ref. [6]. Specimens *b* and *c* were used for the REC estimation and the confidence limit is 78%. The lattice strain vs applied stress is shown in Fig. 3(a). Fig. 3(b) shows slopes of the straight lines in Fig. 3(a) vs $\sin^2\psi$. ψ is an angle between the loading direction and the normal of the diffracted plane, and it is changeable. The elastic constants determined by X-ray are shown in Table 2.

Table 2 Elastic constants for γ phase

S_1/MPa	$(S_2/2)$/MPa	$E(202)$/GPa	ν
-1.302×10^{-6}	7.701×10^{-6}	156	0.21

S_1 and S_2 are the elastic constants obtained by X-ray diffraction technique for the calculation of the residual stress. E and ν were calculated using Hook's law. We can use the following formulae to calculate E and ν, when the material should be anisotropy.

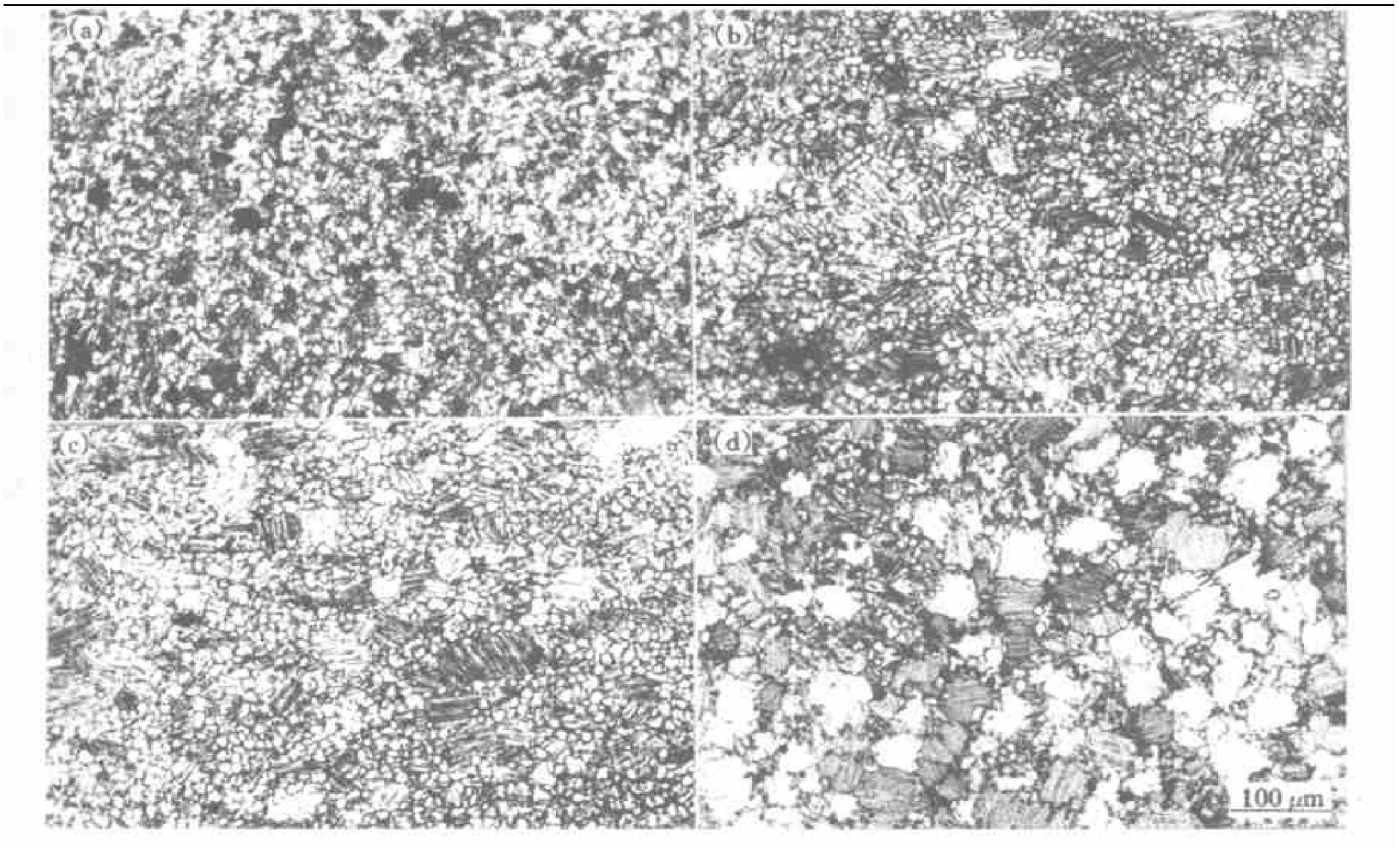

Fig. 2 Microstructures of four studied specimens
(a) —Specimen *a*: 20% lamellar grains+ 80% equiaxed γ grains;
(b) —Specimen *b*: 50% lamellar grains+ 50% equiaxed γ grains;
(c) —Specimen *c*: 70% lamellar grains+ 30% equiaxed γ grains;
(d) —Specimen *d*: 90% lamellar grains+ 10% equiaxed γ grains

$S_1 = -\nu/E$

$S_2/2 = (1+\nu)/E$

It can be seen from Table 2 that the X-ray elastic constants of γ phase show a pronounced difference with that of the macroscopic elastic constants of TiAl alloys (E= 176GPa, ν= 0.23[7]). This is due to the fact that in X-ray diffraction, only those grains obeying the law of Bragg diffraction could contribute to the peaks. This orientation selectivity allows us to measure the anisotropic strain of the grains of a particular orientation relative to the stress axes. So REC retains the anisotropic nature of the crystallites. In addition, the mechanical characteristics of a phase in a multiphase material should be largely influenced by the presence of other phase, so the obtained mechanical properties of this phase can be different from that of the bulk of one phase material.

3.3 Residual stress in γ phase under tensile loading

After determining the X-ray elastic constants of the phase γ, the residual stress in phase γ under uniaxial tensile loading can be measured by X-ray diffraction method. Fig. 4(a) shows the macroscopic tensile stress-strain curves of the four chosen specimens mentioned above. It can be seen that with the increase of volume fraction of lamellar grains, the yield strength and the ultimate strength increase, but the elongation decreases.

Fig. 4(b) shows the stress-strain curves of the γ phase of four chosen specimens evaluated by X-ray diffraction under the uniaxial tension. It can be seen that with the increase of the strain, the stress of γ phase increases, but is less than that of the macroscopic tensile stress at the same strain. The macroscopic yield strength and the ultimate strength of duplex microstructure are higher than that of the phase γ. This indicates that with the appearance of the second phase in the intermetallic compounds, the comprehensive properties can be increased. The improvement of the strength and toughness of TiAl-based alloys through the use of lamellar microstructures is the well-known example[8].

The difference between the residual stress in γ phase and the macro-stress of the alloy is because the elastic constants of the phase γ are different from those of the aggregate, this heterogeneity leads to a localization of the strain fields, they are not compatible in the material and lead to local residual stress.

3.4 Peak broadening

During the tensile testing, the variation of

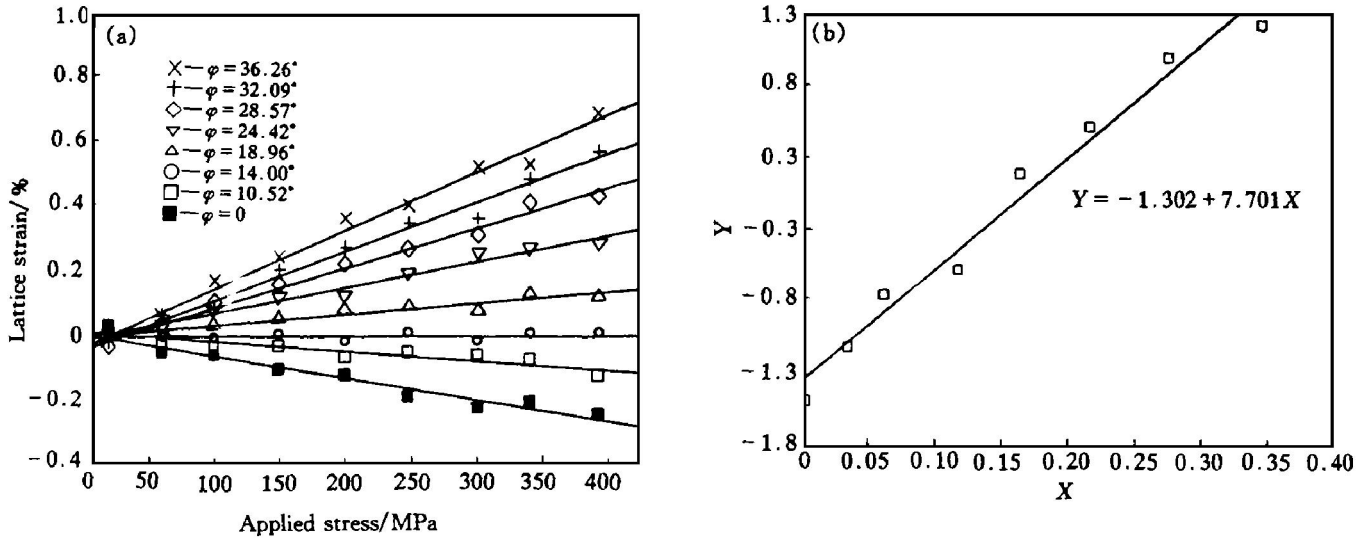

Fig. 3 Variation of strain of studied plane with applied stress (a) and determination of X-ray elastic constant (b) for {202} lattice planes in γ phase
X —$\sin^2\varphi$; Y —Slope of straight lines in Fig. 3(a)

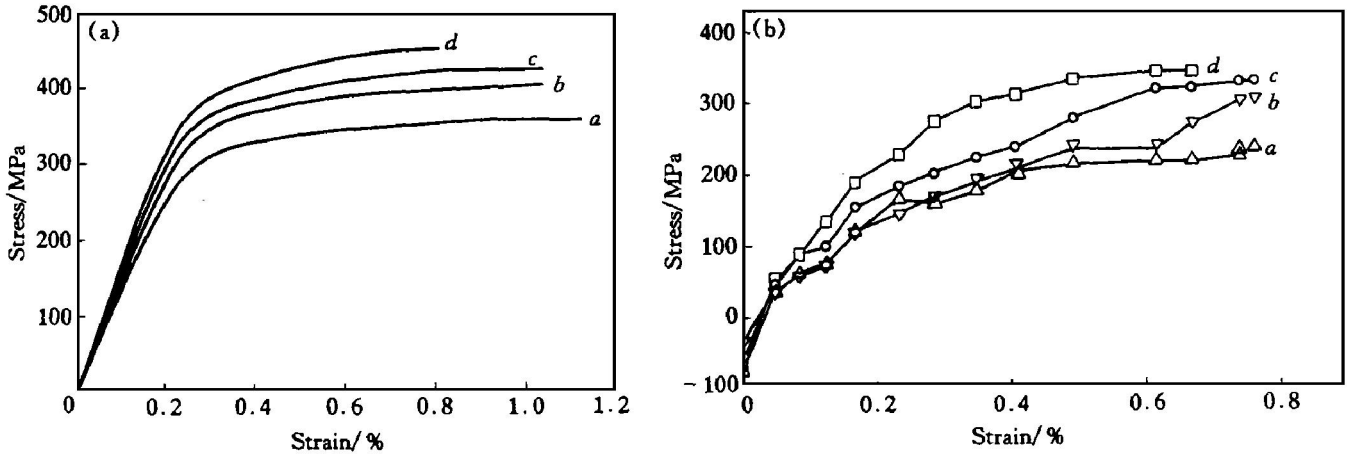

Fig. 4 Macroscopic tensile stress-strain curves of four chosen specimens (a) and stress-strain curves of γ phase of four chosen specimens evaluated by X-ray diffraction under uniaxial tensile stress (b)

diffraction peak width is a phenomenon that concerns with the plastic strain[9]. The values plotted in Fig. 5 are the averaged FWHM (full width at half maximum) evolution vs external applied stress of the four studied specimens.

It can be seen that the width of the X-ray diffraction peaks of the phase γ is increased (broadening) with the increase of the applied stress. This indicates a rapid dislocation multiplication in γ phase. It can be also seen that with the increase of the volume fraction of α_2 and lamellar grains, the broadening of FWHM tends to increase. This may be associated with the elastic anisotropy of γ and α_2 and the plastic strain incompatibility of these two phases. In TiAl alloys, a hexagonal α_2 and a tetragonal γ phase are semi-coherent on their close-packed planes, and the lattice parameter of α_2 is slightly larger than that of γ[10]. In addition, the α_2 has six-fold symmetry,

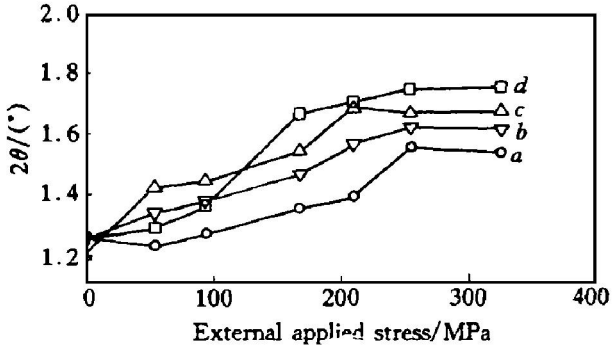

Fig. 5 Relation of peak broadening with applied stress of four chosen specimens

while the γ structure lacks even three-fold symmetry, resulting in a big difference of plastic deformation between these two phases.

4 CONCLUSIONS

1) The tensile properties of two-phase γ-based alloys strongly depend on microstructure. The microstructures with 30% ~ 50% lamellar grains show good comprehensive properties.

2) X-ray elastic constant (156 GPa) and the stresses in γ phase (176 GPa) are different from the macroscopic ones of the alloys, and X-ray diffraction methods can be applied to evaluate the residual stresses of γ phase in TiAl-based alloys, but it requires the elastic constants of the γ phase.

3) The peak broadening indicates that inharmonic residual stress is ubiquitous in TiAl alloy, and it is the reason of incompatible plastic deformation.

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