COMPOSITION DEPENDENCE OF X-RAY ELASTIC CONSTANTS
OF TITANIUM ALUMINIDE INTERMETALLIC COMPOUNDS

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ABSTRACT

X-ray stress measurement was applied to two-phase TiAl intermetallic compounds consisting of
Ti₃Al (α₂) and TiAl (γ) phases. X-ray Elastic constants in both phases of various aluminum
compositions were measured. As compared with mechanically determined elastic constants, the
X-ray elastic constants showed microstructure dependence. The microscopic stress-states of these
two-phase TiAl alloys are discussed.

INTRODUCTION

Extensive studies on microstructures and mechanical properties of two-phase TiAl intermetallic
compounds have been reported recently [1]-[5]. The two-phase TiAl alloys consist of Ti₃Al (α₂)
and TiAl (γ) phases, and can be obtained when Ti is in slight excess than Al in the mixture.
They can be also controlled to various microstructures with the aluminum composition and
appropriate heat treatment. The X-ray diffraction method is useful to evaluate not only
macro-stress but also phase stress and micro-stress of such alloys. However, there are no reports
concerning the microscopic stress-state of these alloys.

In this paper, the X-ray stress measurement method was applied to thesce two-phase TiAl alloys.
As compared with mechanically determined elastic constants by a strain gage, the X-ray elastic
constants showed microstructure dependence. This fact suggests that the microscopic stress-state
of the two-phase TiAl alloy changes with the aluminum composition because of their various
microstructures.

EXPERIMENTAL PROCEDURE

Specimens

The α₂+γ two-phase TiAl alloys of aluminum composition of 42, 43, 44, 45, 46, 47 and 48
mol% were argon arc-melted. They were subjected to several heat treatments (Refer to Fig.1 and
Table 1) to produce different types of microstructures. Figure 2 shows microstructures obtained
by an annealing followed a furnace cooling. The Ti-42mol%Al alloy exhibits fully lamellar
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Fig. 1. The central portion of the Ti-Al binary phase diagram [1]. Arrows indicate heat treatment temperature and process of each alloy.

Table 1. Heat treatment condition and microstructure of each alloy.

<table>
<thead>
<tr>
<th>Alloy (mol%Al)</th>
<th>Heat treatment</th>
<th>Microstructure</th>
</tr>
</thead>
<tbody>
<tr>
<td>42</td>
<td>1150°C/24h/FC1</td>
<td>Lamellar</td>
</tr>
<tr>
<td>44</td>
<td>1200°C/24h/FC1</td>
<td>Widmanstätten</td>
</tr>
<tr>
<td>46</td>
<td>1200°C/24h/FC1</td>
<td>Duplex</td>
</tr>
<tr>
<td>48</td>
<td>1200°C/24h/FC1</td>
<td>Near-γ</td>
</tr>
</tbody>
</table>

*FC1: Furnace cooling at the rate of -30°C/min to 1050°C and then -10°C/min.

Microstructure with about 60 μm grain size. Ti-44 and 46mol%Al alloys exhibit a fine equiaxed lamellar structure (Widmanstätten state) with about 30 μm grain size and an α2/γ + γ duplex structure with about 80 μm grain size, respectively. The Ti-48mol%Al alloy exhibits a near-γ structure with about 80 μm grain size.

Specimens for X-ray stress measurements were cut from the ingots using a wire electrodischarge machine. The dimensions of these specimen were thickness x width x length, 4.0 x 8.0 x 60 mm³. The specimen surfaces were emery-polished followed by electropolishing.

**X-Ray Stress Measurement**

In X-ray stress measurement, the X-ray strain \( \varepsilon (\phi) \) of \( \phi \)-direction shown in Fig. 3 was obtained from \( \alpha_2\)-Ti₃Al (203) reflection by V-K \( \alpha \) X-rays and \( \gamma\)-TiAl (311) reflection by Cr-K \( \alpha \) X-rays. The crystal structure of \( \alpha_2 \) and \( \gamma \) are tetragonal and hexagonal, respectively. Seven X-ray strains at \( \phi = 0, 18, 27, 33, 39, 45 \) and 51 directions were measured using a side inclination method with a scintillation counter. The tube voltage and tube current were 30kV and 10mA, respectively. The X-ray irradiation area was limited to 8 x 15 mm² by masking the rest of the specimen surface by a standard vinyl tape consisting of the chloridization vinyl.
X-ray elastic constants were determined by the $\sin^2 \phi$ method based on the assumption of an elastic isotropic body. In this case, the relationship between an applied stress $\sigma_A$ and an average lattice strain in the direction of $\phi$ $\epsilon(A)$ is written as:

$$\epsilon(\phi) = \left( \frac{s_2}{2} \right) \sigma_A \sin^2 \phi + s_1 \sigma_A$$

(1)

Where, $s_1$ and $s_2$ ($E_X$ and $\nu_X$) are X-ray elastic constants expressed as:

$$s_1 = \frac{-\nu_X}{E_X} = \frac{\partial \epsilon(0)}{\partial \sigma_A}$$

(2)

$$s_2 = \frac{1 + \nu_X}{E_X} = \frac{\partial^{\left[ \frac{\partial \epsilon(\phi)}{\partial \sin^2 \phi} \right]}}{\partial \sigma_A}$$

(3)

The strain $\epsilon(\phi)$ is related with the diffraction angle $2 \theta(\phi)$ by the following equation on the basis of the Bragg's law.

$$\epsilon(\phi) = -\frac{\cot \theta_0}{2} \{ 2 \theta(\phi) - 2 \theta_0 \}$$

(4)

Where, $2 \theta_0$ is the diffraction angle in the non-strained state. The applied stress $\sigma_A$ was estimated by multiplying the mechanically determined Young's modulus $E_M$ by the applied strain $\epsilon_A$ detected by a strain gage. The X-ray elastic constants can be determined experimentally from $2 \theta - \sin^2 \phi$ diagrams. Variations of the gradient $M$ and intercept $2 \theta(0)$ of the $2 \theta - \sin^2 \phi$ diagram with applied strains give $s_2$ and $s_1$, respectively. In this study, four applied strains of $\epsilon_A = 0, 300, 600, 900$ were applied to specimens by a four point bending jig.

**RESULTS AND DISCUSSION**

**Mechanical Elastic Constants**

Figure 4 shows mechanically obtained elastic constants (Young's moduli) of the $\alpha_2 + \gamma$ two-phase TiAl alloys of Ti-42, 44, 46 and 48mol%Al. Young's moduli of $\alpha_2$ and $\gamma$ single-phase alloys are also shown. Aluminum compositions of these single-phase alloys are 27 and 53mol%, and they were annealed at 1100°C for 24h. These Young's moduli were obtained from four point bending tests, where the strains were detected by a strain gage. The lines in Fig.4 are also variations of Young's moduli estimated under Voigt (strain constant model) and Reuss
Fig. 4 Young's moduli of TiAl alloys. Symbols: Two-phase alloys and single-phase alloys of present study (●). Single-phase alloys of ref.[7] (☐). Variations of young's modulus with aluminum composition estimated under Voigt condition (-----) and Reuss condition (-----) from $\alpha_2/\gamma$ volume.

**X-ray Elastic Constants**

Figure 5 shows $2\theta$ -sin$^2$ $\phi$ diagrams of Ti$_3$Al (2023) and TiAl (311) reflections of the Ti-44mol%Al alloy, and Fig.6 shows the gradient M and intercept $2\theta$ (0) of the $2\theta$ -sin$^2$ $\phi$ diagram vs. applied stress $\sigma_A$ plots. The applied stress $\sigma_A$ was obtained by multiplying the mechanically determined Young's modulus $E_M$ by the applied strain $\varepsilon_A$. These $2\theta$ -sin$^2$ $\phi$ diagrams are not linear because of texture in both phases of the alloy. However, the gradient M and intercept $2\theta$ (0) are linearly related with the applied stress $\sigma_A$. X-ray elastic constants were determined from these linear lines by the procedure described before.
Influence of Microstructures on X-Ray Elastic Constants

Several different heat treatments were employed to make clear the influence of microstructures on X-ray elastic constants. Figure 7 shows X-ray elastic constants with aluminum composition. The figure also shows the relationship between the X-ray elastic constant and Young’s modulus by its upper axis. The broken line shows that the X-ray elastic constant equals to Young’s modulus. Table 2 shows relationships between the X-ray elastic constant and the microstructure with the aluminum composition.

As compared with Young’s modulus obtained by a strain gage, the X-ray elastic constants showed microstructure dependence in both phases. Though Young’s modulus of γ phase was larger than that of α2 phase, the X-ray elastic constants of γ phase were smaller than those of α2 phase in any aluminum composition. The X-ray elastic constants of α2 phase also agreed with Young’s modulus at high aluminum composition, and the γ phase agreed at low aluminum composition.

These results show that the microstructures influence on the X-ray elastic constants. In the case of fully lamellar structure, X-ray values close to mechanical values are obtained from γ phase. On the contrary, the X-ray values of near-γ structure is close to the mechanical values in α2 phase. For duplex structure, on the other hand, the X-ray values are lower than the mechanical values in γ phase and higher in α2 phase.

Microscopic Stress State of (α2 + γ) Two-Phase TiAl Alloys

X-ray elastic constant is determined from the measurement of lattice strain averaged over the selected crystals satisfying Bragg’s condition,
Table 2 X-ray elastic constants of Ti₃Al (2023) and TiAl (311) reflections in two-phase TiAl intermetallic compound in this study.

<table>
<thead>
<tr>
<th>Alloy (mol%Al)</th>
<th>Yong’s modulus E_M (GPa)</th>
<th>X-ray elastic Constant</th>
<th>Microstructure</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>α₂-phase</td>
<td>γ-phase</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Eₓ(GPa)</td>
<td>νₓ</td>
</tr>
<tr>
<td>42</td>
<td>158</td>
<td>183.0</td>
<td>0.279</td>
</tr>
<tr>
<td>43</td>
<td>(160)*</td>
<td>189.5</td>
<td>0.191</td>
</tr>
<tr>
<td>44</td>
<td>162</td>
<td>177.9</td>
<td>0.158</td>
</tr>
<tr>
<td>45</td>
<td>(164)*</td>
<td>190.6</td>
<td>0.316</td>
</tr>
<tr>
<td>46</td>
<td>167</td>
<td>139.8</td>
<td>0.200</td>
</tr>
<tr>
<td>47</td>
<td>(168)*</td>
<td>178.5</td>
<td>0.368</td>
</tr>
<tr>
<td>48</td>
<td>171</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

* Values estimated by using the variation of Yong’s modulus under Voigt condition
* Volume fractions were estimated by the lever rule at the lowest temperature in Fig.1

whereas the mechanical elastic constants are an average value over whole crystals. If strain is not uniform throughout the aggregate, it is expected that there is a difference between Yong’s modulus and the X-ray elastic constant. In γ phase, the good agreement between both elastic constants in fully lamellar structure suggests that they deform under the Voigt assumption that strain is uniform throughout the aggregate. On the other hand, the difference of elastic constants in near-γ structure suggests that the deformation shifts toward the Reuss assumption that stress is uniform from the Voigt assumption. In α₂ phase, the good agreement between both elastic constants was admitted in near-γ structure contrary to γ phase.

CONCLUSIONS

The results obtained are summarized as followed:
1) The X-ray elastic constants of α₂+γ two-phase TiAl intermetallic compound are obtained from αγ-Ti₃Al (2023) reflection by V-K α X-rays and γ-TiAl (311) reflection by Cr-K α X-rays.
2) Microstructures of α₂+γ two-phase TiAl alloys influence X-ray elastic constants.
3) These results suggest that the deformation in α₂+γ two-phase TiAl alloys changes according to the microstructures.

REFERENCES