Effects of lamellar thickness on misfit dislocation introduction and mechanical properties of γ/α₂ nano-lamellar TiAl alloys

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Abstract. Stress-strain behavior of lamellar Ti-38Al-3Zr and -3Nb alloys with average lamellar thickness ranging from 10 to 1000 nm were studied at room temperature. Their yield stresses decrease from a high value of coherent lamellar structures to a low value after introducing misfit dislocations onto lamellar boundaries. Their strain hardening rates increase with decreasing lamellar thickness, and then drop to a low level when the misfit dislocations become absent. There is critical thickness of γ lamellae for introduction of misfit dislocations. The thickness decreases with increasing lattice misfit between the constituent phases.

1. Introduction
TiAl Alloys consist of γTiAl and α₂Ti₃Al phases and form a lamellar microstructure. Their yield stresses σₚ increase with decreasing lamellar thickness λ according to the Hall-Petch relation [1-3]:

\[ \sigma_p = \sigma_0 + k\sqrt{\lambda} \]  

where σ₀ is the friction stress, and k is the Hall-Petch slope. Further refinement of their lamellar thickness below 100 nm results in deviation from the Hall-Petch relation [4-6]. Yield stress of polycrystals sometimes exhibits an inverse Hall-Petch relation at very fine grain sizes [7,8].

There is a lattice misfit of 1 to 2 % between the γ and α₂ phases. The misfit is accommodated by elastic deformation (coherent boundary) or by introducing misfit dislocations onto γ/α₂ boundaries (semi-coherent boundary). Hazzledine [9] has predicted a critical lamellar thickness for the introduction of misfit dislocations, and Maruyama et al. [6] have proved the transition from coherent boundaries to semi-coherent boundaries above a critical thickness of γ lamellae. The change in boundary microstructures can affect stress-strain response of lamellar TiAl alloys. The present paper studies how the critical γ thickness for the introduction of misfit dislocations changes with amount of lattice misfit between the constituent phases. Contributions of the misfit dislocation introduction to the lamellar size dependence of yield stress are also studied.

2. Experimental procedure
Ti-38mol%Al-3mol%M (M = Nb or Zr) alloys were used in the present study. The materials used for studying the misfit dislocation introduction were arc-melted and then isothermally forged at 1423 K to nominal strain of 50 %. The other materials for mechanical tests were induction-skull-melted and then hot-extruded at 1473 K to 80 % reduction in area. The alloys were solution treated at 1453 K for 600 s
to produce an $\alpha_2$ single phase state, and then aged in vacuum at 900-1300 K in the $\gamma+\alpha_2$ dual phase field until formation of a fully lamellar microstructure. Since volume fractions of $\gamma$ phase measured by TEM are 31 and 37 % in the Ti-38Al-3Nb and -3Zr alloys, respectively, most of lamellar boundaries are a $\gamma/\alpha_2$ type in the present alloys. The lamellar colony (grain) sizes of the alloys measured by SEM are 75 $\mu$m. Compression tests were carried out at room temperature at a strain rate of $3 \times 10^3$ s$^{-1}$ with specimens of $2 \times 2$ mm$^2$ in cross section and 3 mm height.

3. Results and discussion

3.1. Introduction of misfit dislocation onto $\gamma/\alpha_2$ boundaries

When lamellar boundaries are end on, misfit dislocations make a dot like contrast around them on transmission electron micrographs. Density of misfit dislocations can be measured by counting the dot contrast [6]. Misfit dislocation densities of the two alloys measured by this technique are plotted in Fig. 1 against thickness of the $\gamma$ lamella in which the density was measured. Misfit dislocation is absent in thin lamellae, and in thick lamellae the dislocation density reaches a stationary level $\rho_m$ typical of the material. The curves in Fig. 1 were determined by regression analyses based on the error function so that the curves give the best fit to the data points. The arrows in the figure indicate the points of 0.05$\rho_m$ and 0.95$\rho_m$. During aging $\gamma$ plates precipitate in an $\alpha_2$ matrix. Lattice misfit $\Delta\varepsilon_m$ is accommodated by elastic deformation, and thereby introducing misfit stress $\tau_m$ in $\gamma$ lamellae. The misfit stress is in proportion to $\Delta\varepsilon_m$. Suppose misfit dislocations are introduced by dislocation motion in $\gamma$ lamellae, then the critical thickness $\lambda^*$ of $\gamma$ lamellae for the introduction of misfit dislocations is given by

$$\lambda^* = \frac{G b}{\tau_m} \quad (2)$$

where $G$ is the shear modulus, and $b$ is the length of Burgers vector. The misfit dislocation density $\rho_m$ [m$^{-1}$] necessary to fully accommodate the misfit strain $\Delta\varepsilon_m$ is given by

$$\rho_m = \frac{\Delta\varepsilon_m}{b_m} \quad (3)$$

where $b_m$ is the length of Burgers vector of misfit dislocations. The high $\rho_m$ value of Ti-38Al-3Zr alloy points out a larger $\Delta\varepsilon_m$ value in the alloy. The larger $\Delta\varepsilon_m$ results in the lower $\lambda^*$ value in the Ti-38Al-3Zr alloy.

3.2. Effects of lamellar thickness on mechanical properties

![Figure 1. Changes of misfit dislocation density as a function of thickness of $\gamma$ lamella.](image1)

![Figure 2. Representative stress-strain curves with different average lamellar thicknesses.](image2)
Figure 2 shows representative stress-plastic strain curves of the Ti-38Al-3Nb alloy. The lamellar microstructures were produced by isothermal aging at the temperatures listed in the figure, and their average lamellar thicknesses decrease with decreasing aging temperature. The specimen with the finest thickness (14 nm) has high yield stress but low strain hardening rate, whereas the coarse lamellar material of 257 nm thickness has low yield stress and high strain hardening rate. Their 0.2 % proof stresses increase with decreasing thickness and then reach an upper limit. On the other hand, their 4 % proof stresses take a maximum value at the thickness of 92 nm, and then decrease to a stationary value, indicating the inverse Hall-Petch relation. The lamellar thickness dependence of flow stress varies with location on the stress-strain curves. For more detailed understanding of these variations, we examine the yield stress and the strain hardening rate of the present alloys in Fig. 3.

The yield stress in the present study is defined as follows: A straight line connecting 0.2 % and 0.5 % proof stresses is drawn. The intersection of the straight line and the elastic line gives the yield stress. Strain hardening essentially has no contribution to the yield stress. The strain hardening rate is defined as the average slope of a stress-plastic strain curve between 0.2 % and 0.5 % strain. The yield stress and strain hardening rate are plotted in Fig. 3 against the inverse square root of average lamellar thickness. The arrows in the figure indicate the average lamellar thicknesses that correspond to the γ lamellar thicknesses giving 0.05ρm and 0.95ρm in Fig. 1. The yield stress takes a high value at fine lamellar thicknesses, and then decreases stepwise to a low value after introducing the misfit dislocations. Theories on the Hall-Petch relation, for example the dislocation pile-up model [10] and the geometrically necessary dislocation model [11], assume that grain size dependent flow stress is brought about by grain size dependent strain hardening, and that the yield stress defined in the present study is independent of grain size. This is essentially true in the present study. However, it should be pointed out that the lamellar microstructures without misfit dislocation have a higher friction (yield) stress than those having misfit dislocations, since each lamella is elastically deformed in the former for accommodating the lattice misfit. The yield stress levels of the coherent lamellar microstructures increase with increasing misfit strain.

Suppose dislocations glide within a lamella, leaving dislocation segments on both sides of the lamella, and the dislocation segments cause strain hardening. This model gives the following equation for flow stress:

\[
\sigma = \sigma_0 + 0.4 Mg b \sqrt{2M \varepsilon /b\lambda}
\]  

(4)
where $\sigma_o$ is the lattice friction stress, $M$ the Taylor factor (=3), $G$ the shear modulus (61 GPa), $b$ the length of Burgers vector (0.28 nm), $\varepsilon$ the average plastic strain (0.0035 in Fig. 3(b)), and $\lambda$ is the average lamellar thickness. This equation provides the following expression on strain hardening rate:

$$\frac{d\sigma}{d\varepsilon} = 0.2 M G b \sqrt{2 M / b \lambda \varepsilon}$$

These equations are based on the assumptions that lamellar boundaries are too strong for glide dislocations to pass through, and that annihilation of dislocations cannot occur at the boundaries. In Fig. 3(b), $d\sigma/d\varepsilon$ is proportional to $\lambda^{-1/2}$, supporting Eq. (5). The equation gives the slope of the dashed line, and the line agrees well with the experimental data of the Ti-38Al-3Zr alloy in the coarse lamellar microstructures with misfit dislocations. This good agreement points out that the assumptions, namely strong obstacle and no annihilation of dislocations, hold for the lamellar microstructures with a high density of misfit dislocations. The strain hardening rate of the Ti-38Al-3Zr alloy starts to decrease below 100 nm of lamellar thickness, and increases gradually again below 25 nm. The arrows in the figure point out that the disappearance of misfit dislocations from lamellar boundaries brings about the decrease in strain hardening rate. This finding suggests that lamellar boundaries without misfit dislocations are not sufficient obstacles to dislocation glide and/or to annihilation of dislocations left at the boundaries. The strain hardening behavior of the Ti-38Al-3Nb alloy is similar to that of the Ti-38Al-3Zr alloy. However, the slope of the solid line of the Ti-38Al-3Nb alloy for the coarse lamellar microstructures is lower than the prediction from Eq. (5). This fact points out that a sufficient density of misfit dislocations is necessary to keep strain hardening rate at a high level.

4. Conclusions
(a) The critical thickness of $\gamma$ lamellae for the introduction of misfit dislocations decreases with increasing lattice misfit between the two constitute phases.
(b) Yield stress decreases from a high level of lamellar microstructures with coherent lamellar boundaries to a low level after introducing the misfit dislocations. The yield stress of coherent lamellar microstructures increases with increasing lattice misfit.
(c) Strain hardening rate increases with decreasing lamellar thickness, but drops to lower values after the disappearance of misfit dislocations, namely in coherent lamellar materials. The strain hardening rate increases with increasing lattice misfit.

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