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An analytical dislocation multiple-pile-up model for the yield stress of fully lamellar TiAl alloys

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Abstract

An analytical dislocation multiple-pile-up model is proposed to relate the yield stress of lamellar materials to lamellar thickness, d_{LM}, and grain size, d_{GB}. A simple analytical formula is derived, which gives a good correlation with the experimental results for relatively thick lamellae.

1. Introduction

Lamellar structures are one of the typical structures presented in composites or alloys. For example, fully lamellar TiAl alloys consist of so-called polysynthetically twinned (PST) crystals, and the PST crystals themselves contain a series of well-oriented lamellae of TiAl (γ) and Ti_3Al (α_2) (figure 1). According to experimental investigations [1, 2], the average thickness of the lamellae and the strengths of different interfaces in such systems strongly affect the mechanical properties of the material. For fully lamellar TiAl alloys, there are two or three pertinent microstructural length scales, namely the average grain size, the average lamella thickness, and the average domain size, which are key factors in controlling their overall mechanical behaviour. Because of their potential applications in high temperature environments, the intermetallic γ-TiAl-based materials have been extensively studied in the past decade (see, e.g., [3] for a review). The multiple scales presented in the fully lamellar TiAl alloys imply that a careful design is necessary in order to achieve an optimal microstructure. Schlögl *et al* [4] and Fujiwara *et al* [5] examined the dependence of the yield stress on loading orientation. Grujicic and Zhang [6] and Kad *et al* [7, 8] proposed a numerical method using dislocation theory to analyse the yield and deformation of TiAl polycrystals. The influence of the specified domain structures of the γ-phase on the overall mechanical properties was also examined by Schlögl *et al* [9].

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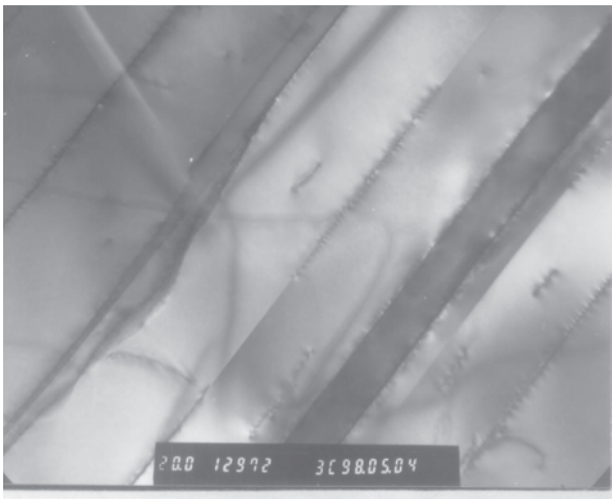

Figure 1. Transmission electron micrograph of PST.

For common polycrystalline materials composed of single-phase grains, which only have one length scale: the average grain size, the Hall–Petch relation [10, 11] gives a good approximation for the dependence of yield stress on grain size, which is expressed in the following form: $\tau_y = \tau_0 + k_{HP} d_{GB}^{-1/2}$, where d_{GB} is the average grain size. For fully lamellar TiAl polycrystals, the experimental results [12] showed that the dependence of the yield shear stress, τ_y, on the average lamellar thickness, d_{LM}, roughly satisfies the Hall–Petch relation. In a similar attempt to this paper, Dimiduk *et al* [12] proposed the following Hall–Petch-like formula for the yield stress of fully lamellar TiAl alloys, and the two length scales are included:

$$\sigma_y = M \left\{ \tau_0 + \left[\frac{4\tau_{LM} G b}{\alpha \pi d_{LM}(d_{GB})} \right]^{1/2} + \left[\frac{(2-\nu)\pi \tau_{GB} G b}{2(1-\nu) d_{GB}} \right]^{1/2} \right\}, \tag{1}$$

where M is the Taylor factor, α is 1 for screw dislocations and $(1 - \nu)$ for edge dislocations, d_{LM} and d_{GB} are the average lamellar thickness and the average grain size as above, τ_0 is the shear stress to move a dislocation through a single crystal of the layered material, G the shear modulus, b the Burgers vector, and τ_{LM}, τ_{GB} are the strengths of the lamellar interface and the grain boundary, respectively. Based on their experimental results, they determined the corresponding parameters. At present, however, an analytical investigation based on a direct dislocation pile-up model has not been made, due to the two length parameters involved. Sun [13] advanced a dislocation pile-up model to study the dependence of yield stress on lamella thickness and grain size by a numerical method. In this paper, based on a numerical simulation, we will propose an analytical dislocation multiple-pile-up model to relate the yield stress of full lamellar TiAl polycrystals to the sizes of the lamellae and the PST grains, respectively.

2. Numerical simulation

Sun [13] has examined dislocation pile-up in a lamellar structure, corresponding approximately to the hard deformation mode for PST crystals. The main idea of his calculation is the following: first impose a very small stress as the net external stress, which makes the dislocation source emit the first dislocation towards the grain boundary; this first dislocation will stop at the first lamellar interface. Check the source stress (applied stress and back stress due

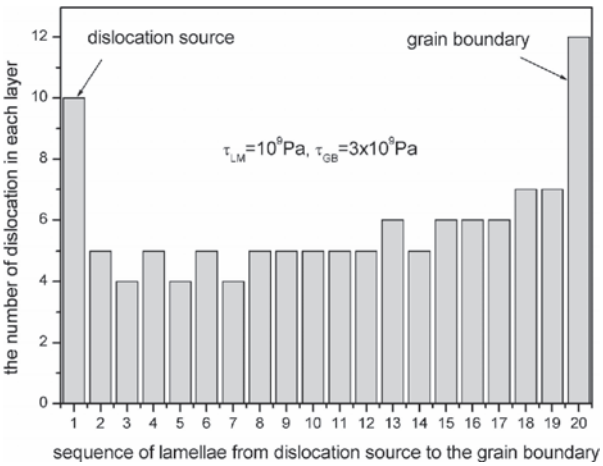

Figure 2. Number of dislocations in each layer at the yield stress ($\tau_{LM} = 10^9$ Pa, $\tau_{GB} = 3\times10^9$ Pa).

to the dislocations): if it is greater than zero, a new dislocation will be emitted; if not, a small increment is added to the applied stress. When the dislocation is within a distance b on either side of a barrier (lamellar interface, grain boundary), the barrier will exert an equilibrium force $\tau_{LM}b$ or $\tau_{GB}b$ on the dislocation. In this paper, we will first follow the numerical method proposed by Sun [13], but with a slight modification made for the leading dislocation within a distance b from the barrier. We suppose this leading dislocation is subjected to a repulsive stress from these barriers, and this repulsive stress can vary from 0 to $\tau_{max} = \tau_{LM}b$ or $\tau_{GB}b$, determined from the equilibrium state of this dislocation instead of a constant stress $\tau_{LM}b$ or $\tau_{GB}b$ in Sun's model. The following material parameters are used in our simulation: $G = 10^{11}$ Pa, $\nu = 0.3$, $b = 0.2$ nm, $d_{LM} = 1.1\,\mu$m, where G, ν, b are shear modulus, Poisson's ratio and Burgers vector, respectively. Various interface strengths and grain boundary strengths are examined; due to the limited computational time, we examined only 20 lamellar layers. Figure 2 shows the number of dislocations in different layers for $\tau_{LM} = 10^9$ Pa, $\tau_{GB} = 3 \times 10^9$ Pa at the moment when the grain boundary is defeated.

If we take the strength values for the lamella and grain boundary as estimated by Dimiduk *et al* [12] from their formula: $\tau_{LM} = 0.015\,G$, $\tau_{GB} = 0.026\,G$, the number of dislocations in different layers are shown in figure 3. We have performed a lot of simulations varying the different parameters, such as the thickness of the lamellae and the strengths of the lamellar and grain boundary, and found that the numbers of dislocations in most layers are almost the same, except the first and last layers, which are the source of emission of dislocations, and the grain boundary.

Based on this observation, in the following we will propose an analytical model to relate the yield stress to the two length scales presented in the fully lamellar TiAl polycrystals.

3. Analytical modelling

In our previous study [14], an analytical approach based on continuum micromechanics and dislocation theory was proposed to predict the yield stress of PST crystals. It was found that the Voigt estimation (constant strain for all lamellar layers) gives better correlation with the experimental results performed by Kishida *et al* [15] than the Reuss estimation (constant stress for all lamellar layers). This suggests that the strain continuity at domain and lamellar interfaces

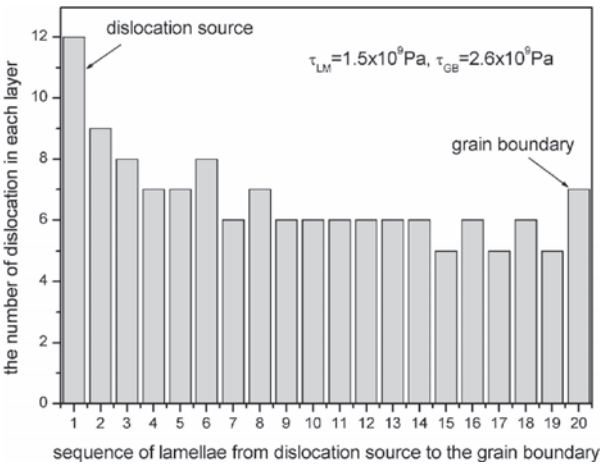

Figure 3. Number of dislocations in each layer at the yield stress ($\tau_{\mathrm{LM}} = 0.015\,\mathrm{G}$, $\tau_{\mathrm{GB}} = 0.026\,\mathrm{G}$).

is one of the important factors in determining the yield stress of a PST crystal. The microscopic plastic strain of each area corresponds to the number of dislocations passing through this area, our previous computation shows that the number of dislocations in each lamella is almost the same; this also agrees with the experimental observation. So in the following, we assume that in each layer there is the same number of dislocations, we will then evaluate the stress needed to defeat the grain boundary.

3.1. The proposed analytical model

In order to proceed with an analytical formulation, the following assumptions are made:

(1) Though the lamellar thickness has a log-normal distribution [12], we assume that all layers have a uniform thickness with an average dimension.
(2) The dislocations in the pile-ups are straight lines with the same Burgers vector and move on a single glide plane across the lamellar interfaces [13], the same assumption as in the numerical computation, corresponding roughly to deformation in the hard mode for PST crystals.
(3) Every layer has the same dislocation pile-up, as demonstrated by the numerical analysis for most layers. This assumption is not applicable for very strong boundaries, where a large single pile-up can be stopped at the grain boundary.
(4) Continuous distribution of dislocations for a single pile-up. In a single pile-up, the head dislocation is locked at the lamellar interface; other dislocations are free, as with case (iii) in the paper of Eshelby *et al* [16].

This model is schematically shown in figure 4.

Now we define a local coordinate system attached to the jth lamella, x' is the distance from the head dislocation in the sub-pile-up of this lamella. The number of dislocations in each lamella can be estimated by the following formula [16]:

$$n = \frac{\pi(1-\nu)d_{\mathrm{LM}}\tau}{Gb} = \frac{d_{\mathrm{LM}}\tau}{2K}, \tag{2}$$

where

$$K = \frac{Gb}{2\pi(1-\nu)}.$$

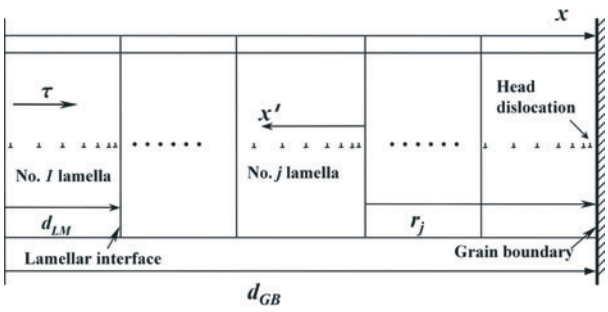

Figure 4. Multiple-pile-up model.

In this local coordinate system, the position of the ith dislocation is evaluated as equation (18) of [16]

$$x_i' \cong \frac{K\pi^2}{8n\tau}(i-1)^2. \tag{3}$$

Equations (2) and (3) are good approximations for a long and isolated dislocation pile-up, but not for small n. When $i = n$, equation (3) cannot give the true distance between the head dislocation and the furthest dislocation, x_n'. Eshelby *et al* [16] estimated the acceptable error caused by equation (3) for $i = n$. Since the furthest dislocation plays an unimportant role in the sub-pile-up of each lamella, equation (3) is suitable for the following analysis. The stress, f_j, acting on the leading dislocation at the grain boundary, by the total sub-pile-up of dislocations in the jth layer is calculated by

$$f_j = \sum_{i=1}^{n} K\frac{1}{r_j + x_i'}, \tag{4}$$

where $r_j = d_{\mathrm{GB}} - jd_{\mathrm{LM}}$. With the help of the continuous assumption for dislocation pile-up [16], f_j can be expressed in the form of an integral as

$$f_j = K\int_0^{d_{\mathrm{LM}}} \frac{1}{r_j + x'}\left(\frac{\mathrm{d}i}{\mathrm{d}x'}\right)\mathrm{d}x' = K\int_0^{d_{\mathrm{LM}}} \frac{1}{r_j + x'}\frac{\tau}{K\pi}\sqrt{\frac{d_{\mathrm{LM}}}{x'}}\,\mathrm{d}x' = \frac{2\tau}{\pi}\sqrt{\frac{d_{\mathrm{LM}}}{r_j}}\arctan\sqrt{\frac{d_{\mathrm{LM}}}{r_j}}. \tag{5}$$

If there are N lamellae in one grain, the stress on the leading dislocation by the $(N-1)$ pile-ups (from the 1st lamella to the $(N-1)$th lamella) is

$$f = \sum_{j=1}^{N-1} f_j = \sum_{j=1}^{N-1} \frac{2\tau}{\pi}\sqrt{\frac{d_{\mathrm{LM}}}{r_j}}\arctan\sqrt{\frac{d_{\mathrm{LM}}}{r_j}}. \tag{6}$$

Due to the large number of lamellae in the grain, and the definition for r_j, we have $\mathrm{d}j/\mathrm{d}r_j = -1/d_{\mathrm{LM}}$. Equation (6) can be expressed in the integral form

$$\begin{aligned} f &= -\int_{d_{\mathrm{LM}}}^{d_{\mathrm{GB}}-d_{\mathrm{LM}}} \frac{2\tau}{\pi}\sqrt{\frac{d_{\mathrm{LM}}}{r_j}}\arctan\sqrt{\frac{d_{\mathrm{LM}}}{r_j}}\left(-\frac{1}{d_{\mathrm{LM}}}dr_j\right) \\ &= \frac{2\tau}{\pi}\left[\frac{2(d_{\mathrm{GB}}-d_{\mathrm{LM}})\sqrt{d_{\mathrm{LM}}/(d_{\mathrm{GB}}-d_{\mathrm{LM}})}\arctan\sqrt{d_{\mathrm{LM}}/(d_{\mathrm{GB}}-d_{\mathrm{LM}})}}{d_{\mathrm{LM}}}\right. \\ &\quad \left. + \ln(d_{\mathrm{GB}}) - \frac{\pi}{2} - \ln(2d_{\mathrm{LM}})\right]. \end{aligned}$$

In fact,

$$d_{\mathrm{GB}} \gg d_{\mathrm{LM}}, \qquad d_{\mathrm{GB}} - d_{\mathrm{LM}} \approx d_{\mathrm{GB}}, \qquad \arctan\sqrt{\frac{d_{\mathrm{LM}}}{d_{\mathrm{GB}} - d_{\mathrm{LM}}}} \approx \sqrt{\frac{d_{\mathrm{LM}}}{d_{\mathrm{GB}} - d_{\mathrm{LM}}}}.$$

The expression for f can then be largely simplified as

$$f = \frac{2\tau}{\pi}\left[2 - \frac{\pi}{2} + \ln\frac{d_{\mathrm{GB}}}{2d_{\mathrm{LM}}}\right]. \tag{7}$$

The stress imposed on the leading dislocation by the dislocations in the last layer is

$$f_N = K\sum_{i=2}^{n}\frac{1}{x_i'} = \frac{\tau}{\pi}\int_{x_2'}^{d_{\mathrm{LM}}}\frac{1}{x'}\sqrt{\frac{d_{\mathrm{LM}}}{x'}}\,\mathrm{d}x' = \frac{\tau}{\pi}\left(-2 + 4\frac{d_{\mathrm{LM}}\tau}{K\pi}\right), \tag{8}$$

where

$$x_2' = \frac{K^2\pi^2}{4d_{\mathrm{LM}}\tau^2}.$$

Now consider when the total stress on the leading dislocation (including the external applied stress) at the yield stress of the polycrystals reaches the strength of the grain boundary, that is

$$\tau + f_N + f = \tau_{\mathrm{GB}}. \tag{9}$$

With the help of equations (7)–(9), we can determine the macroscopic shear yield stress. Then the tensile yield stress can be obtained by multiplying by a Taylor factor M, so that the final expression for the yield stress is

$$\sigma_{\mathrm{y}} = \frac{MK\pi}{4d_{\mathrm{LM}}}\left\{-\left[1 + \ln\left(\frac{d_{\mathrm{GB}}}{2d_{\mathrm{LM}}}\right)\right] + \sqrt{\left[1 + \ln\left(\frac{d_{\mathrm{GB}}}{2d_{\mathrm{LM}}}\right)\right]^2 + \frac{4\tau_{\mathrm{GB}}d_{\mathrm{LM}}}{K}}\right\}. \tag{10}$$

In expression (10), two length scales are present. However, equation (10) does not have traditional $d_{\mathrm{GB}}^{-1/2}$ and $d_{\mathrm{LM}}^{-1/2}$ length dependences. In the following we will apply the model to examine the influence of different parameters.

3.2. Application of the model

The material constants in our computation are taken from Dimiduk [12] and Cao [17–20]: $G = 66 \times 10^9$ Pa, $\nu = 0.33$, $b = \frac{1}{2}\langle 110\rangle = 0.28$ nm, [17, 18], $M = 3$, $\tau_{\mathrm{LM}} = 0.015\,\mathrm{G}$ and $\tau_{\mathrm{GB}} = 0.026\,\mathrm{G}$ [12]. The variation of the yield stress of fully lamellar TiAl polycrystals as a function of the grain and lamellar sizes is shown in figure 5 for $100\,\mu\mathrm{m} \leqslant d_{\mathrm{GB}} \leqslant 1$ mm, $100\,\mathrm{nm} \leqslant d_{\mathrm{LM}} \leqslant 1.5\,\mu\mathrm{m}$.

As shown in figure 5, the yield stress increases as the grain size or lamellar thickness decreases; this trend agrees with experimental observation [12, 17]. Comparisons of the prediction with the experimental results are given by figures 6 and 7.

It is seen from the figures that the proposed model predicts well the trends for the dependence of the yield stress on the grain and lamella sizes. Since in the model we have no parameter to fit, it can be said that the theoretical model can qualitatively predict the yield stress for materials with lamellar microstructure. However, for alloys with $d_{\mathrm{LM}} = 95$ or 160 nm, the theoretical results are 100 MPa larger than the experimental ones. The possible reasons for this will be discussed in the following section.

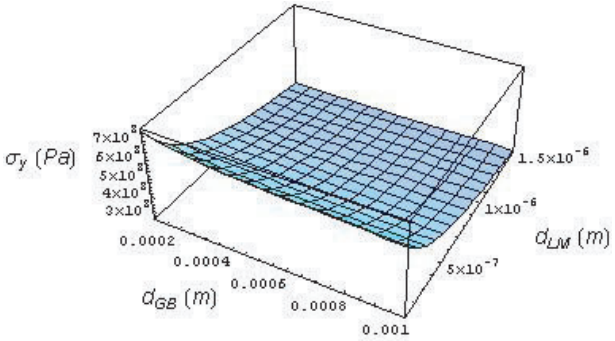

Figure 5. Yield stress as a function of lamellar thickness and grain size.

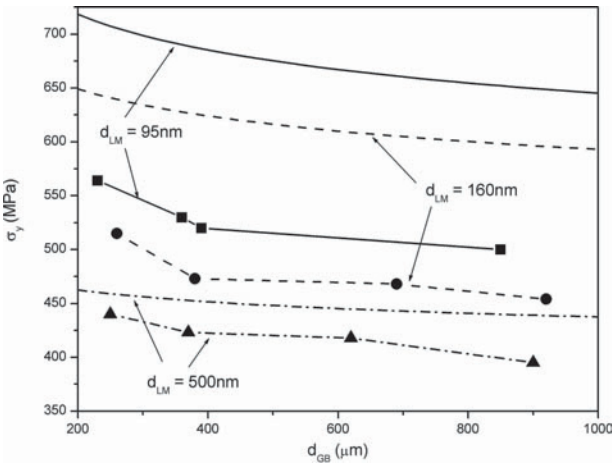

Figure 6. Variation of the yield stress as a function of grain size (prediction and experiment).

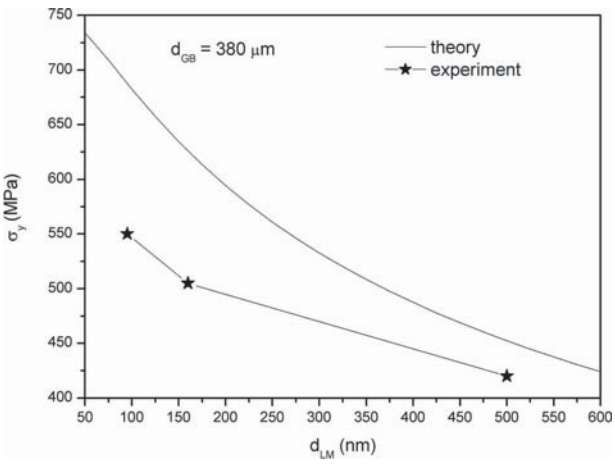

Figure 7. Variation of the yield stress as a function of lamellar size (prediction and experiment).

4. Discussions and conclusion

As illustrated in the comparisons, the proposed model gives good predictions for the dependence of the yield stress on the grain and lamellar sizes. However, a large deviation from the experiment is also found, especially for thin lamellae. Possible reasons for this discrepancy may be: first, when the lamellae are too small, the continuous model of dislocation behaviour is questionable, since when the thickness of the lamella is too small, there are only a few dislocations inside each layer; second, the proposed model only describes deformation in the hard mode in which the dislocations can cross the lamellar boundary, so the yield stresses predicted by our model are larger than the experimental results. Taking into account deformation in the soft mode in which the dislocations glide in the lamellar plane, a better correlation could be expected; third, the lamellae have a log-normal distribution. Our numerical simulation shows that even when the grain size is fixed, different distributions of lamella sizes of different thickness will influence the yield stress; fourth, since a significant fraction of the lamellae are in twin orientation in fully lamellar TiAl alloys, dislocation slip on $\{111\}$ will be deflected at every twin or pseudo-twin $\{111\}$ interface. If we consider a more realistic model, dislocations in the pile-ups are not along a straight line, but are distributed along a zigzag line. This might affect the predicted yield stress.

To conclude, we therefore propose an analytical expression for the yield stress as a function of grain and lamellar sizes, this expression agrees with the experimental results for fully lamellar TiAl alloys for relatively large lamellar thickness.

Acknowledgments

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