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A TEMPERATURE SENSITIVE CRYSTAL PLASTICITY MODEL FOR THE PREDICTION OF HIGH TEMPERATURE MECHANICAL BEHAVIOUR OF MULTI-PHASE TIAL ALLOY

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Abstract. *Intermetallic TiAl alloys for aero-engine turbine blade applications show good thermomechanical properties and excellent creep resistance. These alloys consist of multi-phase intermetallic constituents, mainly of γ-TiAl and α_2-Ti_3Al intermetallic phases, which are arranged in the form of lamellar colonies and globular grains. Characterizing these alloys for room and high temperature behaviour is an ongoing issue that needs to be solved by using a synergic approach of experimental and numerical methods.*

In the recent progress of numerical approaches for the analysis of TiAl alloys, physically motivated crystal plasticity finite element models (CPFEM) have been successfully used to describe room temperature mechanical behaviour and to predict microstructure-property correlations. Unfortunately, not much progress in numerical modelling that is able to characterize this alloy with respect to high temperature mechanical behaviour has been reported. To overcome this lacking, in the present work we propose a temperature sensitive CPFEM model, where the temperature-dependent slip rates of the crystallographic deformation modes are described as a function of history variable and physical material parameters. This model has been verified and validated for multi-phase TiAl lamellar microstructure using the experimental results of fully lamellar PST-TiAl single crystal as published in the literature. Further, for the computational analysis, unit cell based FE models are constructed with representative lamellar microstructure consisting of γ-TiAl and α_2-Ti_3Al lamellar plates. Constitutive behaviour of the phases is described by the proposed crystal plasticity model. A multiscale local-global FE approach has been used to obtain macro-scale homogenized mechanical behaviour of the local microstructure. In this presentation, we will show that our model is able to predict high temperature deformation behaviour of TiAl alloy as observed in the PST-TiAl experiments quite satisfactory. The model successfully captures the temperature sensitive yield behaviour, anisotropic response related to morphological and crystallographic orientation, and rate sensitivity of the slip deformation. Further, we will demonstrate that the activity of crystallographic slip systems can explain the local plasticity in both room and high temperature.

1 INTRODUCTION

Multi-phase TiAl alloys are used in low-pressure turbine blades of aircraft engines where the operating temperature does not exceed 700°C. Recently, considerable amount of research activity is involved in developing new generation of TiAl alloys that may show enhanced thermomechanical properties beyond 700°C temperature. Today, understanding the processing-microstructure-property correlations has become vital to the development of new material with enhanced properties.

For TiAl alloys, the microstructure-property correlations have been explored so far using detailed experiments and microstructure analysis. The experimental results and additional microstructural analysis give somewhat a qualitative picture how the microstructure and properties are correlated. However, the underlying mechanisms of deformation influenced by the local microstructure and available intermetallic phases that influence the macroscopic behaviour remain mostly unknown. Today's material design concepts are based on detail understanding of microstructure-property relationships in a quantitative manner. This requires physics based understanding of the materials deformation mechanisms, which can be obtained by advanced experimental techniques (FIB, nanoindentation) as well as can be explored by advanced numerical modelling techniques incorporating physically motivated materials constitutive behaviour.

To this goal, in past years only limited computational analysis approaches have been proposed for the investigation of TiAl alloy's deformation behaviour. The available models are based on materials micromechanics and micro-macro relationship where the crystal plasticity constitutive models have become a key numerical tool to explore the materials deformation behaviour considering physical microstructural quantities. Only room temperature deformation behaviour was focused. The deformation behaviour at high temperature, which is more relevant for TiAl alloys, has not been systematically investigated so far. Literary study also reveals a lack of proper crystal plasticity models to predict the high temperature deformation behaviour of TiAl alloys.

To overcome this lacking, we propose an extension of crystal plasticity constitutive model applicable to high temperature deformation behaviour. This was done by incorporating the rate sensitivity of the slip deformation as a function of temperature and physical quantities of TiAl alloy, such as, burgers vector, shear modulus of the crystal systems.

In the present work, we have conducted an exploratory numerical investigation to assess the proposed temperature sensitive crystal plasticity model for the room and high temperature behaviour of TiAl alloy. This model will be validated using a single crystal TiAl alloy consisting of multi-phase lamellar microstructure. This type of multi-phase single crystal is known as PST-crystal. For model validation, use of PST-TiAl alloy is ideal, as the fundamental micromechanisms of deformation for various lamellar configurations under various loading histories have been explored through extensive experimental work in past decades.

2 MATERIAL AND METHODS

2.1 Microstructure

The lamellar microstructure of TiAl alloy consists of two intermetallic phases: γ-TiAl with tetragonal crystal structure and α_2-Ti_3Al with hexagonal crystal structure (Figure 1a, b). These phases are arranged parallel to each other in the form of lamellar plates. Between two α_2-lamellar plates many γ-lamellae can be situated. The orientation relationship between these

two phases is as follows: $(0001)_{\alpha 2}$ and $\{111\}_{\gamma}$ planes and the closely packed directions, $\langle 11\bar{2}0\rangle_{\alpha 2}$ and $\langle 1\bar{1}0|_{\gamma}$ are parallel.

The γ-phases contribute to the overall deformation of the macroscopic samples, while, α_2-lamellae is hard to deform. In γ-phases, ordinary, twin, and super dislocations are active which are operative at $\{111\}_{\gamma}$-planes. With respect to available deformation modes of the γ-lamellae, they are divided into γ -matrix and γ -twin lamellae (Figure 1c).

For modelling purpose, the lamellar microstructure is described in a unit cell taking only three representative lamellae phases: α_2, γ-twin and γ-matrix, as shown in Figure 1d. The crystallographic orientation and vol. % of the phases are maintained in the unit cell. In FE model, each phase is defined by 3D linear element. Setting the unit cell periodically side by side, a fully lamellar microstructure is constructed.

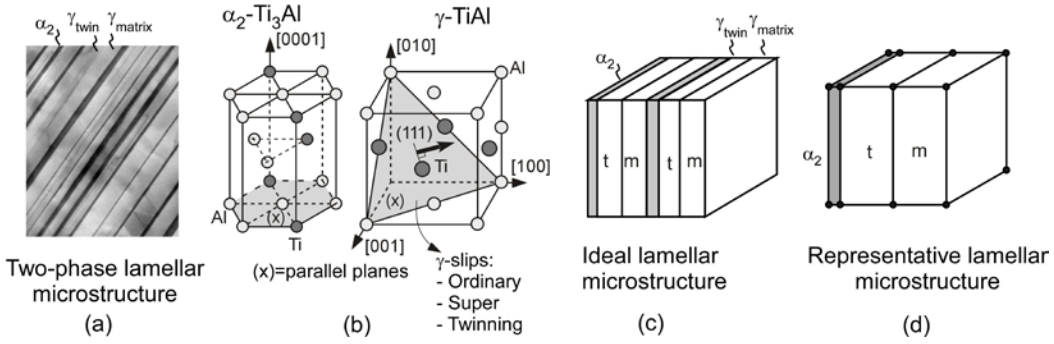

Figure 1: a) Two-phase lamellar microstructure of a PST-TiAl, b) crystal structure of intermetallic TiAl phases, c) simplified lamellar structure with regularly arranged lamellae phases (α_2, γ-matix, γ-twin), d) unit cell of lamellar structure consisting of representative volumes of a γ-matix, a γ-twin and a α_2-lamellae

To understand the mechanical behaviour of the lamellar microstructure, the deformation micro-mechanisms of the intermetallic phases with respect to lamellar orientation have been investigated in detail by many researchers. A clear understanding of these mechanisms has been obtained by analysis of PST-TiAl single crystal (Figure 1a) consisting of various lamellar configurations. Investigating the PST single crystal, very fundamentals of the alloy deformation under room and high temperature behaviour can be obtained. The alloy constituents, microstructural details and the mechanical test data can be used to develop and validate any numerical model and the model parameters influencing the elementary micro-mechanisms can be separately justified, as it will be done in the present work.

2.2 Constitutive behaviour

The constitutive behaviour of the intermetallic TiAl phases is described in a classical crystal plasticity model. In crystal plasticity model the crystallographic slip is taken as the only mechanism for plastic deformation, which occurs due to shearing of slip planes in slip directions. In this model, the shear strain rate $\dot{\gamma}^{\alpha}$ of the slip system α is formulated in terms of resolved shear stress τ^{α} and current strength of the slip systems g^{α} [1, 2]:

$$\dot{\gamma}^{\alpha} = f\left(\tau^{\alpha}, g^{\alpha}\right)$$

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \frac{\tau^{\alpha}}{g^{\alpha}} \left|\frac{\tau^{\alpha}}{g^{\alpha}}\right|^{\frac{1}{m}-1} \tag{1}$$

where, $\dot{\gamma}_0$ is the initial shear strain rate and *m* is the rate sensitivity parameter that controls the rate dependent constitutive behaviour of the material.

The rate sensitivity parameter for the shear strain rate is phenomenological. It generally lies between 0 and 1. Higher values of *m*, i.e. equal to or closer to one, induce viscoplastic response of the material. Lower values results in rate independent deformation of the material.

The evolution equation for the slip system resistance is described by a linear hardening law:

$$\dot{g}^{\alpha} = h_0^{\alpha} \sum_{\beta} q_{\alpha\beta} \dot{\gamma}^{\beta} \tag{2}$$

where, h_0^{α} is the hardening modulus, $q_{\alpha\beta}$ is the slip-plane hardening matrix, which describes the effect of self- and latent hardening. In literature, the values of $q_{\alpha\beta}$ for fcc crystals are in the range of 1.0–1.4. Since $q_{\alpha\beta}$ values for the particular cases of the α_2- and γ-phase have not yet been experimentally estimated, we assume $q_{\alpha\beta}$ = 1.0 for all slip combinations, and do not distinguish between self- and latent hardening.

Twinning is implemented in the UMAT as a unidirectional glide of the partial dislocation and is activated by a set of parameters same as for slip activation.

This classical description of crystal plasticity does not show much sensitivity to strain rate and temperature [3]. As an improvement, Kothari and Anand [3] proposed a physically motivated kinetic equation of shear strain rate on slip systems based on thermally activated dislocation motion [4]. In this approach, the shear strain rate takes the form:

$$\dot{\gamma}_{\alpha} = \dot{\gamma}_0 \exp\left\{-\frac{\Delta F}{k_B T}\left[1-\left(\frac{\tau_t^{\alpha}}{g_t^{\alpha}}\right)^{p}\right]^{q}\right\} sign\left(\tau^{\alpha}\right)$$

$$where \quad \tau_t^{\alpha} = \left[1-\left(\frac{T}{Tc}\right)^{1/q}\right]^{1/p} \quad and \quad Tc = \frac{\Delta F}{k \ln\left(\dot{\gamma}_0 / \dot{\gamma}_0^{\alpha}\right)} \tag{3}$$

Here, k_B is Boltzmann constant, *T* is temperature, $\dot{\gamma}_0$ is the initial strain rate, and $\dot{\gamma}$ is the current strain rate. T_c is the limit temperature beyond which enough thermal energy is present for the barriers to be overcome only by the thermal activation, without the aid of external stresses.

The values of *p* and *q* control the shape of the glide profile. Their values are typically $0 \leq p \leq 1$ and $1 \leq q \leq 2$. ΔF is the activation energy, which is the free energy required to overcome the thermal obstacles during slip deformation without the help of applied stress.

A connection between the physically based formulation of Kothari [3] and the classical power law can be established by defining a physically modified rate sensitivity parameter, *m*, in terms of temperature and activation energy as follows:

$$m = \frac{\partial \ln|\tau|}{\partial \ln|\dot{\gamma}|} = \frac{k_B T}{\Delta F}\frac{1}{pq}\left(\frac{\left(\frac{T}{T_c}\right)^{\frac{1}{q}-1}}{1-\left(\frac{T}{T_c}\right)^{\frac{1}{q}}}\right) \qquad (4)$$

$$where, Tc = \left(\frac{\Delta F}{k_B.\ln\left(\frac{\dot{\gamma}_0}{|\dot{\gamma}|}\right)}\right)$$

The power law equation can be now modified as follows:

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \frac{\tau^{\alpha}}{g^{\alpha}}\left|\frac{\tau^{\alpha}}{g^{\alpha}}\right|^{\frac{1}{m(\dot{\gamma},T)}-1} \qquad (5)$$

Where in classical power law the rate sensitivity parameter is purely phenomenological, in current modification the evolution of shear strain rate depends on materials physical parameter via the rate sensitivity parameter *m*, which is now sensitive to slip strain rate and temperature.

The ΔF should be representative to the investigated material. The activation energy can be written in terms of shear modulus μ of the material and its burgers vector *b* as follows [3]:

$$\Delta F = A\mu b^3 \qquad (6)$$

Depending on the strength of the obstacle, the pre-factor *A* varies from 0.05 to 2.0. Frost and Ashby [5] suggested the range of *A* depending upon the strength of the material obstacles as shown in Table 1. In other words, this pre-factor describes the strength of the material obstacles.

Obstacle Strength	*A*	Description
Strong	2.0	Strong Precipitates, Dispersions
Medium	0.2 - 1.0	Weak Precipitates, Forest Dislocations
Weak	< 0.2	Lattice Resistance, Solution Hardening

Table 1: Characteristics of obstacles

In γ-TiAl alloys, the dislocations glide on {111} planes with the Burgers vectors, 0.283nm, 0.566nm, 0.4905nm [6]. For current calculations, the Burger's vector of 0.283nm is used. The shear modulus, μ for γ-TiAl alloys varies with temperature *T* as follows [6]:

$$\mu = 70.30\text{-}0.0141(T) \qquad (7)$$

For glide profile, the values of *p* and *q* can be taken as 1 for simplicity which yields the *m* equation to the following:

$$m = \frac{k_B T}{\left(A\mu b^3 - k_B T . \ln\left(\frac{\dot{\gamma}_0}{|\dot{\gamma}|} \right) \right)} \tag{8}$$

This modified power law form of viscoplastic formulation taking a physically motivated *m* parameter for temperature sensitivity has not been pursued in any published work. One advantage of using this model is that the framework of the crystal plasticity model need not be changed rigorously but can be easily implemented in the existing code.

This model has been verified for room and high temperature behaviour of PST-lamellar alloy.

2.3 Micro-macro two-scale Model

While the constitutive behaviour of the phases is obtained by the temperature sensitive CPFEM model, the overall mechanical behaviour is calculated from the numerical averaging of stresses and strains over the whole unit cell consisting of intermetallic phases. To obtain the macroscopic behaviour, for example, load vs displacement or stress vs strain curves, as a response to the local deformation micromechanics of the microstructure; a two-scale micro-macro approach is implemented. In this two-scale approach, deformation localization is done via transforming nodal deformation gradient from the macroscopic boundary to the micro-scale unit cell boundary (known as FE^2 approach for micro-macro coupling). After getting stresses on each intermetallic phase due to boundary loading, a volumetric average is performed to obtain overall stress values. At the boundary nodes a reaction force can be derived, which is used to re calculate the macroscopic load-displacement curve (converted to stress-strain curve). The approach is schematically shown in Figure 2, and a detail of this model can be found elsewhere [7,8].

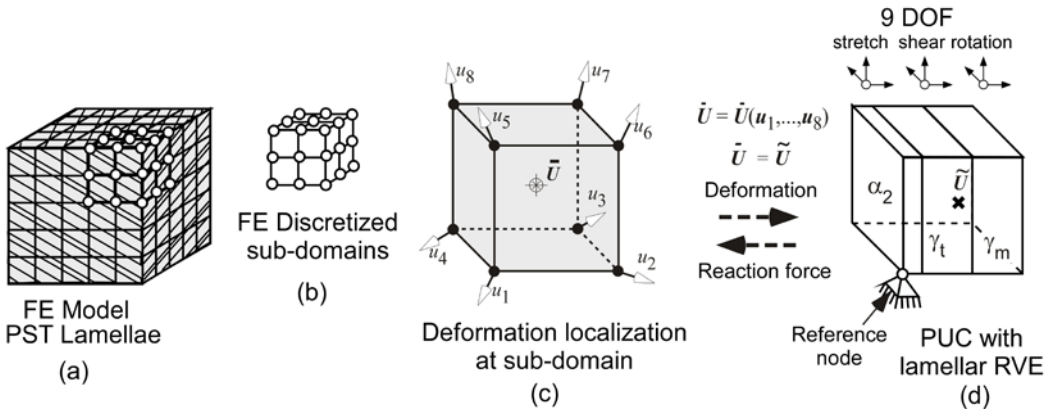

Figure 2: Micro-macro approach for homogenized multi-phase behaviour (a) discretized FE model of a PST-TiAl, (b) a macro-scale subdomain where a micro-scale unit cell is defined, (c) deformation localization at the subdomain, (d) localized deformation is transferred to the unit cell to act as boundary conditions.

In the present case, the microstructure details, e.g. presence of phases, vol. % of the crystallographic orientations or texture, are defined in the unit cell. Further, correlation of the macroscopic sample and the oriented lamellar microstructure is defined by a rotation matrix.

3 SIMULATION AND RESULTS

3.1 Parameter estimation and deformation behaviour

The fundamental parameter set has been adjusted for experimentally obtained room temperature behaviour for three basic orientations of the PST lamellar, e.g. 0°, 45° and 90°. For the numerical stress-strain response, the crystal plasticity model as proposed in section 2.3 is used. The microstructural descriptions of the multi-phase alloys with their anisotropy are defined by a unit cell as described in section 2.1 and 2.3.

To estimate the crystallographic strength and hardening parameters of the slip systems, a morphological description of all the slip systems as defined by Lebensohn et al. [9] is used as listed in Table 2. This description allows one to estimate crystallographic viscoplastic parameters with only a minimum set of experiments performed on 0°, 45° and 90° orientated lamellar PST-TiAl alloy. Details of the parameter estimation are given elsewhere [10]. In Table 2, the strength of the slip systems at a particular deformation mode is denoted as g_0, and Q_{so} is a strengthening factor for super dislocations.

Slip type	Lamellar deformation modes		
	Longitudinal	Mixed	Transverse
Ordinary	g_0^{long}	g_0^{mixed}	g_0^{trans}
Super	$g_0^{long}.Q_{SO}$	$g_0^{mixed}.Q_{SO}$	$g_0^{trans}.Q_{SO}$
Twin	g_0^{long}	g_0^{mixed}	g_0^{trans}

Table 2: Morphological classification of slip systems with respect to the lamellar deformation modes

According to the experimental evidence of slip system activity and stress analysis of Kishida et al. [11], we assume that for all slip systems the ordinary and twinning stresses are the same, super dislocation strength is higher. Now a series of numerical simulations has been performed for fitting the experimental stress-strain behaviour of 0°, 45° and 90° oriented lamellae. The experimental curves are taken from the work of Uhlenhut [12].

In Figure 3a the stress-strain behaviour obtained via simulation fitting is shown along with the experimental curves. Both yield and hardening behaviour have been captured very well with the proposed CPFEM model. Even the anisotropic yield for 0°, 45° and 90° lamellar orientation is satisfied very well, see Figure 3b.

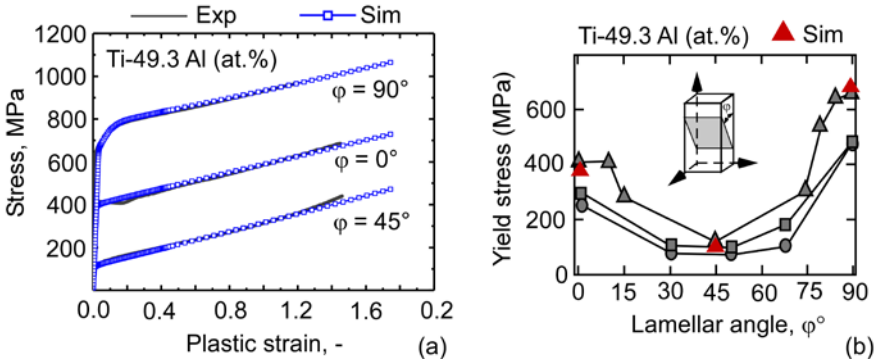

Figure 3: (a) Room temperature compression stress-strain curves for oriented PST crystal, (b) Yield anisotropy of PST-TiAl lamellar alloy

The crystal strengths, g_0 are obtained from these fitted curves, which are listed in Table 3. These parameters will be taken as the fundamental crystal plasticity parameters for TiAl lamellar structure and will be used to predict high temperature behaviour.

Slip type	Lamellar deformation modes		
	Longitudinal	Mixed	Transverse
Ordinary	75	235	260
Super	75	235	260
Twin	75	--	260

Table 3: Strength parameters for the crystal plasticity model.

3.2 Anisotropic yield at high temperature

To examine the temperature sensitivity of the proposed CPFEM model, the load-deformation behaviour is simulated for 27, 200, 400, 600, 800 and 1000°C. For the PST-TiAl, Inui et al. [13] have performed a series of experiments for high temperature behaviour with different oriented lamellar microstructure. He uses 31° lamellar orientation for 'soft deformation' of lamellae and 0° and 90° for 'hard deformation'. For numerical modelling we have used 45° lamellar orientation for 'soft deformation' as the model parameters for this lamellar arrangement has already been verified for room temperature. For hard deformation 0° and 90° lamellar orientation is considered as before.

In Figure 4, the simulated results for yield anisotropy depending on temperature and lamellar orientation have been plotted together with the experimental results from Inui et al. [12]. A very good prediction of yield anisotropy with respect to the lamellar orientation and temperature has been obtained. An overall reduction of yield stress with the increase of temperature has been seen for both experimental and numerical results. At low temperatures, the yield stress decreases quickly with the increase in temperature. At intermediate temperature range, the decrease is gradual for all orientations. At high temperature range, the yield stress decreases rapidly with increases in temperature.

For 0° oriented lamellae, an anomaly has been identified at 800°C. At this temperature range an increase in yield stress is observed, which was however not trivial for 45° and 90° orientation. This anomalous behaviour of high yield stress is associated with the lamellar boundaries of PST TiAl, which impose additional obstacles during dislocation movements crossing the lamellar boundaries [13].

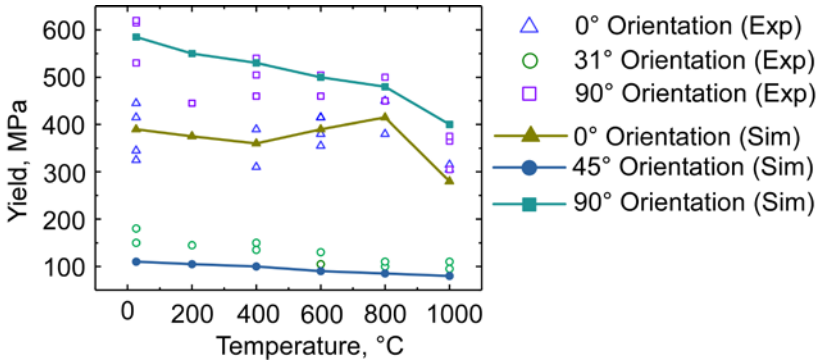

Figure 4: (a) Temperature dependency of yield behaviour for oriented lamellar grains, (b) Temperature dependency of the CRSS ratio of ordinary and super dislocation (Qso) as predicted from numerical analysis

3.3 Activity of slips at room and high temperature

The CPFEM model also allows us to study the activation of different slip modes, which are important for deformation behaviour in individual phases at different temperatures and differently oriented lamellae configurations. Following, we have calculated the relative activity of the slips at room (27°C) and 800°C temperature, and for 0°, 45°, and 90° oriented lamellae. The activity of slips has been calculated at the onset of yield. The predictions are shown in Figure 5.

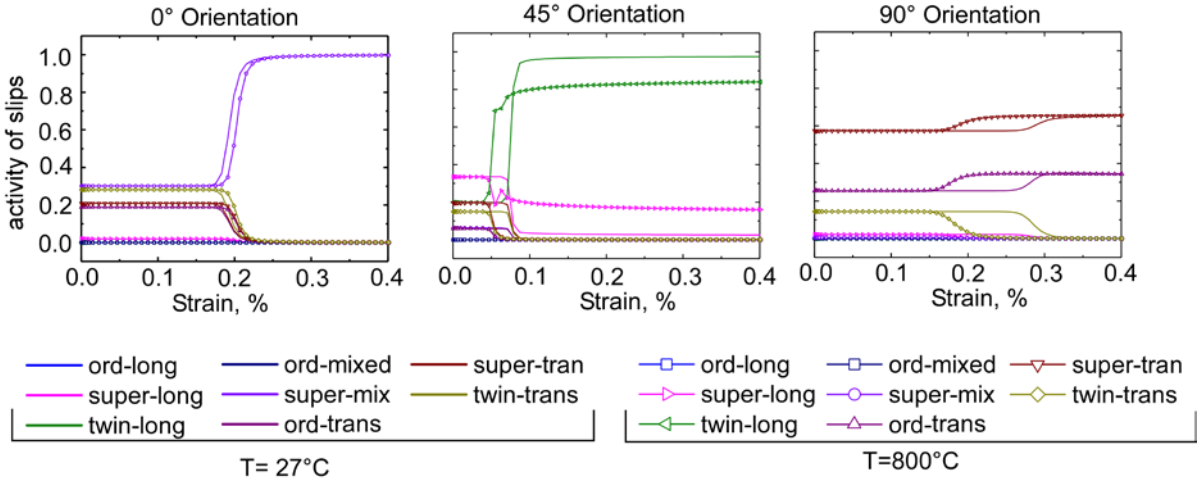

Figure 5: Activity of slips for 0°, 45° and 90° oriented lamellae at room temperature and 800°C

For 0° lamellar orientation, we observe that the super dislocations are dominant for plastic deformation at both room (27°C) and high temperature (800°C). For 45° lamellar orientation, the deformation occurs mainly due to twinning at room temperature. But at high temperature some super dislocations are also active in addition to the twinning. For the 90° lamellar orientation, both super and ordinary dislocations are dominant for slip deformation. For 45° and 90° lamellar orientation, at high temperature these slip modes are activated earlier compared to room temperature, which allows an early softening of the material. For 0° lamellar orientation, the super dislocation slips are activated later at 800°C than at room temperature, which is responsible for the anomalous behaviour of 0° oriented lamellae. The results seem consistent with the experimental observations of Kishida [11] for room temperature and Inui [13] for high temperature behaviour.

4 SUMMARY AND CONCLUSION

The crystal plasticity model proposed in this work incorporates the rate sensitivity of individual slips systems by a temperature dependent function proposed by Kothari and Anand [3]. In classical analysis of high temperature behaviour using crystal plasticity model the temperature sensitivity is obtained only by using a phenomenological parameter *m*, which was insensitive to slip rates and temperature sensitive. The main objective in this work was to show an alternative formulation of power law equation of crystal plasticity to predict the temperature sensitivity, which is more physics based.

This model has been validated using available data from the literature. We have validated the model for room temperature deformation behaviour capturing anisotropy due to oriented lamellar configurations. Further, high temperature yield anisotropy as well as temperature dependent yield behaviour has been predicted, which matches the experiments very well. The

model also explains the high temperature deformation behaviour with respect to the activity of slips systems for different oriented lamellar configuration.

Further, we have determined slip strength parameters for PST-TiAl alloy from the experimental fitting of room temperature deformation behaviour. Due to temperature sensitive rate equation in the crystal plasticity model, the strength parameters become temperature sensitive. Using this temperature sensitive strength parameter set the model is able to predict the high temperature behaviour of PST-TiAl as determined experimentally in [13].

The results presented in this work clearly state that this new formulation of CPFEM can be successfully used to predict room and high temperature deformation behaviour of fully lamellar PST-TiAl alloy. This model also shows huge potentials to understand the microstructure property correlations of the intermetallic systems. In future, further analysis will be conducted to validate this model for a wide range of TiAl alloy microstructure subjected to different temperatures.

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