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Numerical prediction of the stress-strain response of a lamellar γ TiAl polycrystal using a two-scale modelling approach

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Abstract

An advanced model incorporating a two-scale structural description with integrated constitutive formulations of crystal plasticity was adopted to describe the mechanical behaviour of a γ TiAl polycrystal with grains of staggered (γ/α_2)-phase lamellae. The numerical model assembles a polycrystalline compound of 64 lamellar grains generated from periodic unit cells (PUC) taking relevant phase configurations. The representative parameter set for the crystal plasticity are estimated by modelling the lamellar deformation and fitting the compression and tension test results in two steps: firstly, the fundamental parameters were identified for a poly-synthetically twinned single crystal (PST) under compression, and secondly, these PST parameters were adjusted to the γ TiAl polycrystal consisting of fully lamellar grains. Numerical results show that the compression-tension anomaly in the stress-strain curves can be successfully described by a ‘high-grade’ PUC model including six domain variants of the γ -phase occurring in the lamellae. Using a PUC model with simplified mapping of lamellar microstructure, the prediction quality remains unsatisfactory with respect to the observed compression and tension anomaly and

the crystal parameters are found to be inconsistent. Differently aligned lamellar grains in polycrystalline cubic model are predicted, which showed that the global stress-strain curves are weakly affected by different local alignments (or textures) of the grains, whereas, the single grain analyses show strong variations in local stress-strain curves. The simulated nature of local variations in grain scale stress-strain behaviour accords with the independent results from instrumented indentation testing of the same lamellar polycrystal.

Keywords:

A. Finite element method, micromechanics.

B. Intermetallics, titanium aluminide alloy.

D. Crystal plasticity, mechanical properties.

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1. Introduction

Lightweight intermetallic two-phase titanium aluminides (γ TiAl) represent a viable engineering material for numerous structural engineering applications in high operating temperature environments, such as engine valves or blades in turbine engines. Among the various microstructures, fine-grained lamellar γ TiAl is attractive for engineering applications due to its relatively high trans-lamellar fracture toughness, high specific strength and good resistance to creep.

The microstructural deformation mechanisms of such γ TiAl polycrystals are influenced mainly by several internal characteristics of the lamellar grains (or colonies), for example: orientation, spacing and size of lamellae. During the last few decades, numerous investigations (in particular, SEM and TEM analyses) have been performed for characterising the mechanics of this material, for instance: anisotropy of yield strength, elongation to failure, fracture toughness, influence of colony sizes, and lamellar orientations [1–6]. Such local property variations and their responses to the global stress-strain relations have also been experimentally investigated [7–9].

Numerical methods have been developed for understanding the deformation and fracture behaviour on micro- and macro scale using crystal plasticity or continuum damage models [10–14]. In particular, the crystal plasticity based constitutive modelling approaches serve as a valuable tool for characterising the anisotropic deformation of two-phase γ TiAl alloys in different aspects, for example, combining the modelling of local stress-strain behaviour with nanoindentation testing across the lamellae to explore grain scale plasticity [15] or finding simplification limits of grain wise homogenisation to predict overall plasticity [16].

In advance numerical modelling that includes particular micromechanics of polycrystals, often the restrictions and limitations of modelling approach as well as the relevance of estimated parameters to the physical mechanism are not properly discussed. As an extension to recent progresses in the modelling of γ -based TiAl deformation behaviour, the following issues will be addressed in this work:

(1) *Systematic estimations of relevant crystal parameters of the two-phase lamellar γ TiAl.* The macroscopic behaviour of polycrystal deformation is the collective response from the hierarchical anisotropic microstructure deformation. Therefore, the crystallographic parameters of the two-phase ($\alpha_2+\gamma$) lamellar structure (grain) have to be estimated and validated under different lamellar configurations and loading. Estimating the locally defined crystallographic parameters directly from fitting the global polycrystal behaviour leads to parameter sets ignoring sufficient physical relation, as the sensitivity of global response with respect to important micromechanisms of lamellar deformation is not well pronounced. In the present work the estimation of crystal parameters for the deformation of a lamellar based γ TiAl has been qualified stepwise under single crystal (single grain) and polycrystal with lamellar ($\alpha_2+\gamma$) phases.

(2) *Microstructure simplification in the modelling.* Modelling of lamellar deformation requires proper descriptions of the specific lamellar microstructure and its implementation in the numerical modelling. At micro-scale many interactions occur in oriented lamellar domains maintaining twin-matrix correlations. If a model is not consistent with such physical micromechanisms due to model simplification, it will obviously lose its validity for predictive analysis of the material behaviour. Although in published numerical works the crystallographic model parameters have been determined by fitting experimental results [11,13,16,17], the consistency of these parameters with respect to the model

simplifications and underlying assumptions is still an issue, which needs to be further discussed.

(3) *Compression-tension anomaly in the deformation behaviour.* A model should have the ability of describing and justifying the observed deviations in the stress-strain (σ - ε) curves for compression and tension loading (e.g. compression-tension anomaly) with an equal set of crystal parameters. In the present work the consistency of the presented modelling approach as well as the validity of the crystal plasticity parameters has been justified for the observed compression-tension anomaly of the considered lamellar γ TiAl polycrystal.

(4) *Validation of local and global plasticity.* The two-scale modelling approach (including microstructural aspects) allows the estimation of both local (i.e. grain wise or mesoscopic) and global (macroscopic) deformation response. A quantitative validation for the modelling of local plasticity for randomly oriented grains is still open in the literature. In this work the simulated grain-scale stress-strain responses are validated comparing the mesoscale results (local σ - ε curves) from an indentation method.

(5) *Effects of lamellar orientations on macroscopic response.* Using numerical simulations the σ - ε curves have been predicted for a single crystal (more precisely called PST¹ single crystal) as well as for a polycrystal consisting of different lamellar alignments (respective texture) of the lamellar grains. The anisotropic deformation behaviour of a PST single crystal has been previously demonstrated in compression experiments [18]. However, the mechanical behaviour of a lamellar polycrystal with respect to the lamellar grain orientations in extruded samples has not yet been systematically investigated.

¹ In such crystals, the major consistent γ -phase is composed of numerous thin twin-related lamellae; these crystals are called polysynthetically twinned (PST) crystals from an analogy with the phenomenon of polysynthetic twinning in mineral crystals.

2. Experimental analysis

2.1 Material and microstructure

The γ TiAl alloy used in this investigation has the compositions (in at.%) Ti-47Al-3.7(Nb,Cr,Mn,Si)-0.5B (developed at GKSS²), abbreviated here as γ TAB. To obtain a fine-grained fully ($\alpha_2+\gamma$)-phase lamellar polycrystal, certain heat treatments are applied as described by the following steps: preheating at 800°C for 30 min, then furnace cooling, followed by annealing at 1360°C (approximately 20°C above the α -transus temperature) for 30 min, then rapid oil cooling. Stress release is ensured by further heating at 800°C for 6 h and then subsequent air cooling. This treatment provides a mean colony size of about 100 μm .

Examination of the polished microstructure via SEM indicates a transverse isotropy of the colonies in which the lamellar alignments of the lamellar grains are nearly randomly distributed, whereas in the extrusion direction, the lamellar grains show only slight tilting within a range of about $\pm 20^\circ$. The lamellar grains consist of the intermetallic phases, γ (TiAl) and α_2 (Ti₃Al), with the minor α_2 -phase maintaining a volume content of 5–10% for an Al content of 45–48 at%.

2.2 Compression and tension testing

Several round-bar compression specimens of appropriate slenderness (2.5 mm diameter and 4.56 mm height) were spark eroded from an $\text{Ø}22$ mm extruded rod. The lateral surface of the round bar was refined by centre-less grinding, providing high precision in the final shapes with low surface roughness. For the tensile tests, flat bar tension specimens with a square cross-section (2x2 mm²) were spark eroded from a neighbour piece of the $\text{Ø}22$ mm rod. The rough spark-eroded surface was refined by fine-diamond

² GKSS Research Centre, since Nov. 2010 under the new name Helmholtz-Zentrum Geesthacht or HZG.

grinding and finally lapped. The compression and tension specimens were tested on a universal spindle-driven testing machine.

For both tests, loading with plastic strain rate of approximately $1 \times 10^{-4} \text{ s}^{-1}$ was applied. **Fig. 1a** shows the σ - ε curves for both tests over the total compression strain range, while **Fig. 1b** shows an appropriate resolution of the tensile tests. The initial linear slope of all σ - ε curves provides a mean value for the elastic modulus of $E_0 = 175 \text{ GPa}$.

Due to the low tensile ductility of the γTiAl alloy, the σ - ε curves for tension display early termination by unstable translamellar fracture at approximately 1.5% of total strain. The tension tests exhibit an obvious range of scatter. The activation of anisotropic deformation in different weak colonies against tensile yielding seems to be an interpretation for this behaviour. Local micro-cracking along lamellar interfaces could also be involved, but from the SEM images taken along a longitudinal cross section of fractured tensile specimens no micro-cracking could be observed. Micro-cracking typically evolves only along the fracture plane at failure. Surface preparation may also be involved in the scattered tensile behaviour, but no such indications could be found.

In contrast, the compression tests ($\varnothing 2.5 \text{ mm}$) show no discernible scatter in the σ - ε curves; the direct measured force-displacement curves of 17 tests are almost overlapping. As large strains are obtained, possible microcracking under compression seems to be fully suppressed. At larger plastic deformation slight differences emerged due to different deformation types of the round specimens, which became primarily S-curved and, less often, barrel-shaped. Due to such disturbed deformation the compression specimens failed macroscopically by slant cracking. To confirm the σ - ε behaviour in the small-sized compression tests, the σ - ε curve from a larger compression specimen with 4 mm diameter

is included (see **Fig. 1b**). This additional σ - ε curve coincides completely with those of the smaller specimens ($\varnothing 2.5$ mm).

From the comparison of averaged σ - ε curves a compression-tension asymmetry (or anomaly) is identified as a significant property for the γ TAB alloy. This aspect will be treated in the modelling part.

2.3 Indentation testing

The instrumented indentation testing employs a spherical indenter tip with $R = 0.2$ mm and provides σ - ε curves, each belonging to a group of some grains activated beneath the indentation. These σ - ε curves represent the mesoscale deformation of the grains. This local testing technique is used to validate the grain deformation response of a lamellar γ TiAl polycrystal predicted from the presented numerical two-scale approach. The σ - ε curves from the indentation testing were determined by an inverse analysis using the Artificial Neuronal Network Analysis (ANNA) [19-21]. The experiments and the data evaluation procedures for the γ TAB alloy are elsewhere presented in detail [22]. Here, the results will be used to confirm the trends from the modelling part.

3. Deformation mechanisms of the (α_2 + γ) lamellar system

In the lamellar γ TiAl alloy, the crystallographic structure of the γ -phase is tetragonal ($L1_0$) and the α_2 -phase is hexagonal ($D0_{19}$). The orientation relationship between the α_2 - and γ -lamellae is fixed, i.e. their $(0001)\alpha_2$ versus $\{111\}_\gamma$ planes and the closely packed directions, $\langle 11\bar{2}0 \rangle_{\alpha_2}$ versus $\langle 1\bar{1}0 \rangle_\gamma$, are parallel. Six distinct orientation variants within the γ -phase fulfil this relationship: 120° staggered domains within the matrix and twin lamellae, and 180° flip for the matrix and twin relations along the $\{111\}_\gamma$ plane,

respectively [23]. This means, each γ -lamella consists of three orientation domains: m_1 , m_2 , m_3 in the matrix, and t_1 , t_2 , t_3 in the twin lamella. In addition, one γ -lamella belongs completely to either the matrix or the twin variants. Room-temperature deformation occurs by crystallographic slip and mechanical twinning.

In the α_2 -phases possible active slip modes are the prismatic $\langle 01\bar{1}1 \rangle$, basal $\langle 11\bar{2}0 \rangle$, and pyramidal slip systems $\langle \bar{1}\bar{1}26 \rangle$ with a yield stress ratio of nearly 1:3:9. For the γ -phases, slip occurs on the habit $\{111\}$ -planes by ordinary dislocations $1/2[1\bar{1}0]$, superdislocations $\langle 0\bar{1}1 \rangle$, and for higher temperature also the superdislocation $1/2[11\bar{2}]$. The partial dislocations are responsible for the $1/6[11\bar{2}]$ twinning [24].

In γ -lamellae with six oriented domains the deformation predominantly occurs due to the contribution of ordinary and twinning. The contribution of $\langle 0\bar{1}1 \rangle$ superdislocations to the total deformation system depends on the γ -domain orientation with respect to the loading axis. Investigation on PST single crystals showed that among the six domain variants the 0° (parallel to the load axis) oriented domains deform due to the contribution of symmetrical double slip of superdislocations along $[011](111)$ and $[101](111)$ [24]. Inui et al. [25] concluded that the superdislocations occurred in some favourable oriented domains within the γ -phase lamellae after preceding some applied strain (about 2 %). That means, in an unsuitable oriented γ -domain a local kinematic condition arises to force the activation of superdislocations. The other possible superdislocation with $b = 1/2[11\bar{2}]$ forms a sessile type of non-planer configuration at room temperature restriction and is, therefore, not activated in the numerical model.

In most cases the deformation in the domains are promoted by the glide of ordinary dislocation and mechanical twinning, where the CRSS of both should be lower than that of the superdislocations ensuring an easier activation of these slip systems in the model.

The CRSS of the α_2 -phase have been estimated for a bulk α_2 single crystals [23,26,27]. Due to the less volume content of the α_2 -phase in the lamellar unit (grain) and less contribution to the overall deformation, this parameter set has been kept fixed in the numerical investigation.

For the γ -phase domains the determination of CRSS of each slip system by experimental means is highly complicated due to the morphology of the lamellar structure. So far, experiments have only been performed on bulk γ -single crystals with an aluminium concentration of 54–56% (at.%) [28,29]. Such individual CRSS parameters will not be appropriate for describing the slip activity of staggered lamellae, because the lengths of mean free path of dislocation vary due to the thickness of the lamellae or the size of γ -domains [6,8], which influence the effective CRSS of the γ -domain slip systems.

Therefore, γ -phase parameters for the elementary lamellar structure were estimated from experiments of at two-phase binary PST single crystal (with the composition Ti-49.3Al in at.%) [18] combined with the numerical approach for fitting the true lamellar deformation behaviour. These parameters of a PST single crystal have to be further adjusted to the lamellar structure of the present γ -based TiAl polycrystal with slightly different chemical composition (Ti-47Al-3.7(Nb,Cr,Mn,Si)-0.5B in at%). Due to the different alloy constituents and thermo-mechanical processing the lamellar thickness or the γ -domain sizes in this polycrystal are not identical to the tested PST single crystal.

To estimate the free parameters of the available slip systems, the total 16 individual γ -phase slips are grouped according to the deformation modes of the lamellar system. The

deformation modes are classified as longitudinal, mixed and transverse with respect to the lamellar plane [30]. In **Fig. 2** the three deformation modes are shown. This classification of the deformation modes, denoted as ‘morphological deformation modes’, each with a particular group of slip systems. Lebensohn et al. [31] showed that the crystallographic parameters following this classification of modes provide best prediction of the lamellar deformation behaviour.

With the morphological classification of the slip systems the number of free parameters is strongly reduced and can be estimated from appropriate experiments. Kishida et al. [24] showed that the slip activations are favoured or non-favoured according to the morphological deformation of the lamella. For example, with the 45° orientation of the lamellae against the loading axis, the slip systems for the longitudinal deformation modes can be estimated. Furthermore, for 0° orientation of the lamellae (parallel to load axis) the slip systems for the mixed deformation, and for the 90° orientation (perpendicular to load axis) the slip systems for the transversal deformation mode can be estimated. At least three experiments corresponding to three different PST single crystal orientations (i.e. 0°, 45° and 90°) are needed to estimate the full set of crystal parameters.

For the α_2 -phase, the crystallographic and morphological classifications can be directly correlated, where the basal slips have a longitudinal orientation, the prismatic slips have a mixed orientation, and the pyramidal slips have a transversal orientation. As the deformation of γ and α_2 lamella is interdependent, the interactions between the α_2 - and γ -slip systems play an important role for the co-deformation of γ and α_2 phases. For example, easy deformation occurs for the interaction between the prismatic α_2 -slip and the mixed γ -slip systems, while the basal (longitudinal) and pyramidal (transverse) slip systems promote hard deformation.

4. Numerical approach

4.1 Constitutive behaviour of lamellar microstructure and two-scale modelling

In this work a micromechanical two-scale FE model has been applied to capture the deformation behaviour of the lamellar microstructure. The model includes the crystal plasticity constitutive behaviour for the lamellar α_2/γ -phases, which is implemented in an ABAQUS user-defined material subroutine (UMAT) [32]. This UMAT was first established in [33] for homogeneous single phase and subsequently upgraded for analysing two-phase TiAl alloys, which was developed during a collaborative research work [30,34-36]. The model was later extended to investigate duplex-type microstructures [37].

The model considers the following rate-dependent viscoplastic formulation for the single crystal plasticity:

$$\frac{\dot{\gamma}^{(\alpha)}}{\dot{\gamma}_0} = \left[\frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right]^{m-1} \frac{\tau^{(\alpha)}}{g^{(\alpha)}}, \quad (1)$$

where $\dot{\gamma}^{(\alpha)}$ is the shear rate of the slip system α , $\dot{\gamma}_0$ is a reference shear rate, $g^{(\alpha)}$ is the current strength of the slip system α , $\tau^{(\alpha)}$ is the current *Schmid* stress in α , and m is the strain rate exponent. For large values of m the equation is almost rate independent. In this numerical modelling viscoplasticity is suppressed by setting $m = 10$.

The evolution of the slip strength, $g^{(\alpha)}$, is described by a linear hardening law, which allows a minimum number of model parameters to be identified:

$$g^{(\alpha)} = h_0^{(\alpha)} \sum_{\beta} q_{\alpha\beta} \dot{\gamma}^{(\beta)}, \quad (2)$$

where $h_0^{(\alpha)}$ 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 $1/6\langle 11\bar{2} \rangle$ as suggested by [38] and is activated by a set of parameters same as slip activation. Crystallographic reorientation due to twinning is ignored in the present model.

For the simulation two parameters are needed for each slip system: $g_0^{(a)}$, the critical resolved shear strength (CRSS), and $h_0^{(\alpha)}$, the hardening moduli. According to the morphological classification (section 3), the slip parameter g_0 for ordinary dislocation is defined for each deformation mode (**Fig. 2**): g_0^{long} (for longitudinal), g_0^{mixed} (for mixed), and g_0^{trans} (for transverse). The strength of $\langle 0\bar{1}1 \rangle$ superdislocation slips are characterised by a free ratio parameter, Q_{so} , related to the ordinary dislocations as follows, $g_0^{\text{super}} = Q_{so} \cdot g_0^{\text{ordinary}}$. The enhanced strength of superdislocations for the activation under a higher local kinematic condition can be assessed with $Q_{so} > 1$, but not exceeding a certain upper range, i.e. $Q_{so} < 3$ [30]. Twinning is assumed to have the same resistance as the ordinary dislocations, i.e. $g_0^{\text{twinning}} = g_0^{\text{ordinary}}$.

Thus, under morphological classification the total of 16 γ -phase slips fall under three slip types (ordinary, super and twin) each with respect to three deformation types (longitudinal, mixed and transverse), as listed in **Table 1**. This classification significantly reduces the free parameters to be estimated from the experimental and numerical fitting. The hardening parameters are also morphologically classified by h_0^{long} , h_0^{mixed} , and h_0^{trans} .

Both parameters will be numerically identified by fitting experimental data e.g. compression tests.

Table 1. Morphological classification of γ -phase slip systems.

Slip type	Longitudinal mode	Mixed mode	Transverse mode
Ordinary	g_0^{long}	g_0^{mixed}	g_0^{trans}
Super	$g_0^{\text{long}} \cdot Q_{\text{so}}$	$g_0^{\text{mixed}} \cdot Q_{\text{so}}$	$g_0^{\text{trans}} \cdot Q_{\text{so}}$
Twinning	g_0^{long}	g_0^{mixed}	g_0^{trans}

4.2 Two-scale modelling

In the two-scale approach, the lamellar microstructure is modelled using a three-dimensional periodic unit cell (PUC) composed of multi-phase ($\alpha_2 + \gamma$) lamellae staggering. Each lamellar phase (α_2 , γ_{matrix} , γ_{twin}) is idealized as a representative volume element (RVE). The multi-phase lamellar structure is obtained by setting the RVEs of different phases parallel to each other until a PUC is completed. By setting a set of PUCs parallel to each other a complete lamellar grain (colony) or a PST single crystal is obtained.

For the two-scale model a PUC (containing microscale lamellar description) is coupled with a continuum finite element (represents mesoscale effective properties of a lamellar system). The coupling is done by localizing the macroscopic deformation field and homogenizing the local stress response due to the applied deformation of the multi-phase PUC (known as FE^2 approach).

In the FE implementation the PUCs are generated as sub-structures within a continuum FE element. Each PUC represents an integration point and for numerical reasons each FE element consists of 8 PUC (respective 8 integration points).

Several assumptions have been made for the arrangements of the lamellar phases (RVEs) within the PUC to capture the essential characteristics of the lamellar co-deformation. The very simplified assumption of the lamellar microstructure may consist of a set of γ -twin, γ -matrix and α_2 lamellae, which are attached in parallel. An advanced model should incorporate additional description of 6 γ -domain arrangements in twin-matrix phases as well as the orientation relationship among the domains [23].

In reality, the lamellae can be thick or thin, thus the aspect ratio of the γ -domain size and lamellae thickness varies. Local stress strain situations in the γ -domains vary accordingly. To capture the micromechanical responses properly, several types of PUCs with different RVE arrangements are proposed. They take into account either simplified or complex deformation mechanisms of a lamellar grain. With respect to the lamellar microstructure they can be described with simplified or high-grade configurations of RVEs as subsequently described:

- (a) In a simplified PUC all lamellae are assumed to be quasi homogeneous, i.e. no domain variants of the γ -phases are present. Here, the PUC is assembled by three RVEs: one γ -matrix, one γ -twin, and one α_2 -lamella, denoted as PUC3 in **Fig. 3a**. Each lamella represents the average deformation for the γ -variants. To capture the matrix-twin co-deformation relaxed constraint boundary condition [34] along the lamellae (RVEs) has been implemented. The average volume % of the phases is maintained by the RVEs. The matrix-twin crystallographic relation are defined by assigning 0° crystallographic orientation to γ -matrix and 180° orientation for γ -twin.
- (b) In a high-grade PUC the lamellar structure is constructed with matrix and twin lamellae containing six distinct γ -domains and a single α_2 -lamella. The volume contents of the six domains are assumed to be the same. The lamellae are assumed to

be "thin", i.e. the width to thickness aspect ratio of the domain is large. For such microstructure each γ -domain can be interpreted as a thin lamella where each domain is subjected to an iso-strain boundary condition. With this assumption, the PUC is constructed with six thin elements, each of which represents a single γ -domain, denoted as PUC7 in **Fig. 3b**. Crystallographic orientation relationships are attributed to the six-domain RVEs. The α_2 lamella and the six γ -domains are treated as parallel lamellae; thickness is according to their volume content. Again relaxed constraint boundary condition is implemented.

- (c) In this high-grade PUC the lamellar γ -domains are assumed to be "thick" so that the thickness aspect ratio of the domain is small. For such microstructure each γ -domain is subjected to an iso-stress boundary condition. To capture such lamellar structure, 9 RVEs have been used: 6 for describing the six γ -domains and 3 for describing one α_2 -lamellae, denoted as PUC9 in **Fig. 3c**. Again, each set of domains (γ -matrix or γ -twin) are subjected to relaxed constraint boundary condition to ensure the matrix-twin co-deformation. Crystallographic orientation relationships are attributed to the six-domain RVEs.

These unit-cells are defined at a local co-ordinate system to assign arbitrary rotations with respect to the global loading axis. Periodic boundary condition has been applied to the PUC and crystal plasticity based constitutive behaviour is defined for each domain RVEs. A lamellar grain with a particular crystallographic orientation can be modelled using several periodically arranged PUCs. Finally, a polycrystalline compound is obtained by assembling many of randomly oriented lamellar colonies. Texture can be incorporated by distributing distinct grain orientations.

In **Fig. 4a** a lamellar polycrystal with 64 lamellar colonies (4x4x4) has been generated. In the corresponding FE cube, each idealised grain is refined by 8 regular cubic FE elements, as shown in **Fig. 4b**. No pre-defined constitutive behaviour is given to these FE elements; rather the constitutive behaviour is directly derived from the (micro-scale) PUC response at each incremental deformation. Each FE element consists further of 8 PUCs as shown in **Fig. 4c**. One PUC delivers the results at one Gauss point, of a FE element, **Fig. 4d**, thus 8 PUCs are required to couple local deformation in a quadratic FE element with 8 integration points.

For numerical accuracy one lamellar grain is constructed with 64 PUCs, thus the whole FE model (respective to the polycrystal compound) contains 4096 PUCs. The 64 PUCs in a lamellar grain have the same crystal orientation. The nodal points (and at integration points) of a FE element provide the internal reaction forces (and stresses respectively) of a grain obtained from the PUCs. Further details of the two-scale model can be found in [30,34-36].

5. Parameter estimation

5.1 Crystal plasticity parameters for the PST single crystal

For the α_2 -phase, the existing parameters for the CRSS and the hardening were taken from the literature [27,28,39] and are morphologically assigned as listed in **Table 2**. These parameters were not adjusted in this work.

Table 2. CRSS and hardening parameters for α_2 -phase taken from Ref. [27,28,39].

Slip type	Morphological mode	CRSS $g_0^{(\alpha)}$ MPa	Hardening $h_0^{(\alpha)}$ MPa
Basal	Longitudinal	330	96
Prismatic	Mixed	100	329
Pyramidal	Transverse	910	911

To estimate the crystal parameters of the γ -phase, the compression tests [18] on a binary PST single crystal (Ti-49.3Al in at%) in various orientations were simulated using the two-scale model [30,34-36]. According to [30,36] we found that each experimental curve for a PST single crystal, aligned under 0° , 45° and 90° orientation, can be fitted up to 15% global compression strain with any Q_{so} for superdislocation (defined in section 4.1) within the range of $1 < Q_{so} < 3$, combined with slightly varying parameters for CRSS (g_0) and hardening (h_0).

This means, the same experimental compression curve can be fitted using different values for Q_{so} , and no unique solution can be obtained for Q_{so} from a single σ - ε curve. In [36] it has been shown that for completely suppressed superdislocations (i.e. infinite Q_{so}) the experimental compression records of the PST single crystal could not be described in a consistent manner. Hence, in the numerical simulations the presence of superdislocations is necessary to realise the possible contributions from all intra-lamellar deformation modes.

A consistent Q_{so} parameter for the superdislocations can be derived from the deviation of σ - ε curves of the compression and tension tests (i.e. compression-tension anomaly), as the activation of superdislocations in the γ -domains is orientation dependent (with respect

to load direction) and they are not equally activated during compression and tension loading [24]. The unidirectional process of twin activity is also involved in the compression-tension anomaly, however, twinning contribution alone is not sufficient to capture complete compression-tension anomaly [30,36].

For a PST single crystal there are no tension test records available for distinct orientation directions due to the early failure after onset of plastic strains. Hence, compression-tension anomaly for the determination of the Q_{so} parameter is not feasible from PST single crystals. Considering a reasonable Q_{so} within the range of $1 < Q_{so} < 3$ the experimentally determined σ - ε curves of the PST single crystal in [18] can be closely described for the main lamellar alignments of 0° , 45° and 90° . The parameter sets for $Q_{so} = 1.0$ and 2.0 are listed in **Table 3** [30].

In **Table 3** numerically obtained Hall-Petch (HP) parameters $k^{(\alpha)}$ for three deformation modes are also included, which can be compared with known experimental Hall-Petch parameters to validate the numerically determined crystal parameters $g_0^{(\alpha)}$ (CRSS) as described following. The $g_0^{(\alpha)}$ can be approximated from the fit of experimental data using the empirical Hall-Petch law for particular lamellar microstructure [40]:

$$g_0^{(\alpha)} = \tau_F + \frac{k^{(\alpha)}}{\sqrt{d^{(\alpha)}}}, \quad (3)$$

where τ_F is the lattice friction stress related to the *Peierls-Nabarro* strength and solute hardening, $d^{(\alpha)}$ is the relevant microstructure length scale for the slip system α , and $k^{(\alpha)}$ is an empirical constant indicating the effectiveness of the microstructural glide barriers. The microstructural length $d^{(\alpha)}$ represents the free path of dislocation movement, which for an unconstrained PST single crystal can simply be defined as follows: for the two hard modes (0° and 90° orientation) it is the thickness of the lamellae and for the soft mode

(45° orientation) it is the diameter of the domain. For the present PST single crystal the average lamellae thickness is about 2 μm and average domain width is about 10 μm [36], which are taken as the approximate values of $d^{(\alpha)}$ for respective lamellar orientation.

Table 3. Parameter set for binary PST single crystal Ti-49.3Al.

Morphological mode	Type of mode	Lamellar orientation	Q_{so}	CRSS $g_0^{(\alpha)}$ MPa	Hardening $h_0^{(\alpha)}$ MPa	$k^{(\alpha)}$ MPa $\sqrt{\text{m}}$
Longitudinal	Soft	45°	1.0	55	400	0.047
Mixed	Hard	0	1.0	150	320	0.155
Transverse	Hard	90°	1.0	185	135	0.205
Longitudinal	Soft	45°	2.0	45	310	0.016
Mixed	Hard	0	2.0	85	350	0.064
Transverse	Hard	90°	2.0	150	180	0.155

In the literature HP parameters were experimentally determined for γ -based lamellar PST single crystals for different lamellae orientation. Umakoshi and Nakano [41] obtained τ_{F} in the range of 70–400 MPa within the limits of soft and hard lamellar orientation, while Dimiduk et al. [40] and Kishida et al. [42] reported this value to be in the range of 30–50 MPa. For $k^{(\alpha)}$ the estimated values in [41] ranges within 0.27–0.5 and in [40,42] within 0.06–0.15 MPa $\sqrt{\text{m}}$. According to eq. (3) the HP parameter $k^{(\alpha)}$ for the PST single crystal in this work are determined backwards from the numerically determined values for $g_0^{(\alpha)}$ using the average values: $\tau_{\text{F}} = 40$ MPa, 2 μm lamellar thickness, and 10 μm domain size. It can be seen that the values of $k^{(\alpha)}$ in **Table 3**, estimated from the present

numerical results, are in good accordance with the independent experimentally based estimations of Kishida et al. [42] for PST single crystals.

5.2 Parameters for the polycrystal alloy

As the alloy compositions and production histories of PST single crystal and fully lamellar polycrystal are different, the microstructural parameters, e.g., lamellar spacing, domain size as well as the strength properties of the phases are different in PST and in polycrystal. However, in both the alloys the two-phase (α_2 and γ) crystallographic structure, the sequential arrangements of lamellae and their deformation modes are the same.

Due to the fundamental similarities of lamellar structure in PST-single grain and in polycrystal grains, it can be assumed that the crystallographic parameter set ($g_0^{(\alpha)}$, $h_0^{(\alpha)}$) of the PST single crystal can be adjusted by a single scaling factor for each deformation mode to obtain the crystallographic parameter set of the polycrystal. The scaling factors can be interpreted as model parameters that describe the change in slip strength and slip hardening of a lamellar microstructure due to different lamellar sizes, neighbouring grain constraints and variation of physical alloy properties.

To estimate the polycrystal parameters from the knowledge of PST parameters, simulations are carried out on a polycrystal cube consisting of 64 regular lamellar grains, **Fig. 4**. In the polycrystal cube, the real extrusion texture was best adopted using a longitudinal alignment of lamellar grains with a random tilting variation of $\pm 20^\circ$ with respect to the loading axis and a full random alignment across to the extrusion direction, as informed by experimental SEM images. The PUC7 model is preferred for this analysis as the lamellae are "thin" (about 0.8 μm) within a lamellar grain of 100 μm mean size.

The new parameter set for the polycrystal alloy (γ TAB) has been iteratively estimated by best fitting the compression and mean tension σ - ε curve, as shown in **Fig. 1**. Both σ - ε curves are fitted simultaneously by stepwise adjustment the scaling factors of the starting parameter set of the PST single crystal ($g_0^{(\alpha)}$ and $h_0^{(\alpha)}$ in **Table 3**) combined with the parameter Q_{so} until good overall agreement has been achieved.

The best approximation of the polycrystal compression-tension anomaly has been obtained with $Q_{so} = 1.8$ and the respective parameters $g_0^{(\alpha)}$ and $h_0^{(\alpha)}$ are listed in **Table 4**. It should be mentioned that the parameter set of the polycrystal (**Table 4**) is related to the set of the PST single crystal (**Table 3**) by constant factors, which is 1.63 for $g_0^{(\alpha)}$ and 2.75 for $h_0^{(\alpha)}$. The enhancement reflects both the different alloy history (composition, forging, heat treatment) and the lamellar grain constraints inside the polycrystal compound.

An arbitrary fitting choice (trial and error or use of any optimization program) without pre-knowledge of PST parameters seems impractical due to a large number of possible combinations of parameters that have to be handled intuitively leaving with uncertainty to obtain parameters with mechanical/physical significance. In the present approach the parameters determined for a PST single crystal are based on clear defined background and from close cooperating of experimental and modelling estimation that ensures some physical relevance of the model parameters to simulate the microstructural deformation behaviour of lamellar γ TiAl.

Table 4. Estimated crystallographic parameter set for TiAl polycrystal (γ TAB alloy).

Morphological mode	Q_{so}	CRSS $g_0^{(\alpha)}$ MPa	Hardening $h_0^{(\alpha)}$ MPa
Longitudinal	1.8	90	1100
Mixed	1.8	244	880
Transverse	1.8	302	371

Fig. 5 shows the influence of the parameter Q_{so} (enhanced superdislocation strength) on the σ - ε compression curve for the polycrystal within the range, $1.5 \leq Q_{so} \leq 3.0$. The parameters $g_0^{(\alpha)}$ and $h_0^{(\alpha)}$ were kept fixed to verify the tentative influence of Q_{so} . The superimposed experimental σ - ε curve (dashed line in **Fig. 5**) shows good agreement with the simulated curve for $Q_{so} = 1.8$. Due to the linear hardening law, the simulated σ - ε curves follow a straight line after elastic to plastic transition, whereas the experimental σ - ε curves exhibit a slight continuous curvature at larger strains, likely due to non-uniform S-type or barrelling deformation of the compressive samples.

The margin of the experimental compression-tension anomaly is shown in **Fig. 6** together with the corresponding simulations up to 2% strain. The σ - ε anomaly for compression and tension curves show good agreements between the simulation and experiment except that the simulation under tension slightly underestimates the initial plastic strain evolution.

For this anomaly calculation the tension curve resulted from the same parameters obtained for the fitting approximation of the compression σ - ε curve up to 17 % strain. In this case, the short tension σ - ε curve up to only 2 % strain range has not been well approximated with this parameter set. However, the margin of this deviation can be

reasonably reduced by better fitting the initial part of the strain range for both σ - ε curves (e.g. up to 2% strain range instead the whole compression curve).

The tensile curves from **Fig. 6** shows slight mismatch at the initial yield region for experiments and simulation. The reason lies mainly on the use of simplified linear hardening law in the crystal plasticity model. The linear hardening law provide almost a sharp deviation/transition from elastic slope for both compression and tensile curve at the initial yield region. This behaviour can be improved using some other non-linear hardening assumptions, for example, using Bassani-Wu model. However, non-linear hardening models generally impose additional unknown parameters, which are for the case of TiAl alloys not accessible using available experimental data. As a compromise, the simplest linear hardening law is used, which has been proven to be sufficient in predicting the anisotropic deformation of the lamellar alloy/structure.

In addition, the experimental tensile curves (Fig. 1b) show a stochastic behaviour, which might be due to additional damage (or microcracking) contribution. For the present calculation the tensile curve is purely elastic-plastic without any assumptions for damage accumulation. Regarding all possible contributions from the real behaviour, the prediction of the tensile behaviour seems reasonable.

For the elastic behaviour of the α_2 - and γ -phases, the anisotropic elastic properties are taken from the literature [43]; however, the elastic anisotropy is not the focus of the present work.

5.3 Remarks on the parameter estimation

The estimated parameters are in general dependent on idealization of the microstructure in modelling and kinematic assumptions for the boundary condition. Care should be taken for the model simplification as strong simplified model may inadequately describe the

most important micromechanisms of the lamellar deformation. Some important aspects with respect to the modelling assumptions and appropriate choice of PUCs are given below.

- (1) The macroscopic load-deformation response depends on the activation of numerous crystallographic deformation modes in the models PUC3, PUC7 or PUC9. Due to the spatial alignment of lamellar grains in the polycrystalline cube (**Fig. 4**), each single grain has ‘soft’ and ‘hard’ neighbours that exhibit significant mechanical constraint effects in the stress and strain states. Consequently, the local deformation of each grain activates the internal six γ -variants in the PUC7 or PUC9 model in a different manner. In **Fig. 7** the model sensitivity on the prediction of compression and tension σ - ε curves is shown. Here, for the same parameter set the predicted σ - ε curve from the PUC3 model is much stiffer compared to those of PUC7 and PUC9 models. Due to the absence of domain interactions in PUC3, the compression-tension anomaly in this model is much less pronounced. The results indicate that the models with more simplified assumptions, for example, a 2D representation of the lamellar systems, which further neglect the relevant mechanisms in third direction or a 3D model without including lamellae effects, may not be an appropriate choice for the prediction of lamellar deformation behaviour.
- (2) As the PUC3 does not adequately contain the true micromechanisms of lamellae deformation due to the absent of γ -domains, the crystallographic parameters deduced from this models may lack sufficient physical relevance. In the literature [**11,16**] certain homogenisation approaches using effective lamellar properties in FE models have been proposed for the prediction of deformation behaviour of lamellar γ TiAl

polycrystals. However, micromechanical basis of such "homogenized" FE elements seems weakly founded as the effective deformation of lamellar phases resulted from co-deformed matrix-twin lamellae cannot be contained in this element in contrast to the presented PUC models. Such homogeneous models may lack relevant mechanisms to establish proper correlations among and within the lamellar grains.

- (3) Two main crystallographic parameters, g_0 and h_0 , for the lamellar system have been estimated from the knowledge of particular slip activity in different lamellar deformation modes for 0° , 45° and 90° orientation of a PST single crystal. Such estimated crystallographic parameters are physically relevant to the principal lamellar deformation. Numerically determined parameters are also verified in conjunction with the Hall-Petch relation of the PST crystal. To obtain the crystallographic parameters for any lamellar polycrystal of γ TiAl alloy the basic parameter sets from the PST single crystal need to be adjusted by scaling the PST parameters by a constant factor.
- (4) It should be noted that any combination of sufficient numbers of crystallographic free parameters for the TiAl phases can be numerically estimated by a direct fitting of only one experimental σ - ε curve of a polycrystal [13] without pre-knowledge of lamellar deformation modes. In this case, physical significance of the parameters cannot be well established to understand the alloy deformation. In our view, the crystallographic parameter fitting with respect to the deformation of PST single crystal is a necessary step to obtain a physical meaningful fundamental set of crystallographic parameters that incorporate basic micromechanisms of lamellar deformation.

6. Polycrystal behaviour

6.1 Local stress-strain response

To obtain the internal σ - ε behaviour within a polycrystal, σ - ε curves are determined for all lamellar grains in the polycrystal cube (**Fig. 4**). The individual stress and strain components for the α_2 - and γ -phases in the PUC7 model are averaged by their volumetric content. The grain wise σ - ε curve is determined using the *von Mises* yield criterion and taking the averaged components of all PUCs in a lamellar grain as follows:

$$\sigma_e = \frac{1}{\sqrt{2}} \sqrt{(\sigma_{11} - \sigma_{22})^2 + (\sigma_{22} - \sigma_{33})^2 + (\sigma_{33} - \sigma_{11})^2 + 6(\sigma_{12}^2 + \sigma_{23}^2 + \sigma_{31}^2)} \quad (4a)$$

$$\varepsilon_e = \frac{\sqrt{2}}{3} \sqrt{(\varepsilon_{11} - \varepsilon_{22})^2 + (\varepsilon_{22} - \varepsilon_{33})^2 + (\varepsilon_{33} - \varepsilon_{11})^2 + 6(\varepsilon_{12}^2 + \varepsilon_{23}^2 + \varepsilon_{31}^2)} \quad (4b)$$

Fig. 8a shows the σ - ε curves for the 64 lamellar grains for the polycrystal cube. The variation of the σ - ε curves within the polycrystal is rather large. This variation band is, however, smaller compared to the band consisting of the upper and lower limits of the σ - ε curves obtained from PST single crystal calculations (indicated as dotted curves and labelled as 1 and 3), which were obtained using the same parameter set as of the polycrystal parameters.

A direct experimental validation of the grain-wise σ - ε curves from the simulation results seems not accessible. The variation of these grain-wise σ - ε curves shown above can be qualified indirectly by the instrumented indentation method, which has been applied by the authors [22] and stated briefly in section 2.3. The force-indentation record from a spherical indenter reflects an integral response of several differently oriented grains (100 μm mean size) underneath the indenter tip ($R = 200 \mu\text{m}$). Thus, the σ - ε curves derived from the force-indentation data are similar to a group of some grain-wise σ - ε curves estimated from the polycrystal simulations in **Fig. 8a**.

The σ - ε curves were calculated for 17 indentation imprints and are shown in **Fig. 8b**. All σ - ε curves exhibit a characteristic curvature due to the analytical formulation:

$$\sigma = k_0 + \frac{\gamma}{\beta} \left(1 - e^{-\beta \varepsilon_{pl}} \right), \quad (5)$$

with the yield strength, k_0 , and hardening parameters, γ and β . Due to the analytical expression of eq. (5), for which the extrapolated yield stress (k_0) needs to be calculated at $\varepsilon_{pl} = 0$, the initial elastic-plastic gradient in the σ - ε curves is not well captured. The formulation also introduces some nonlinear hardening in the σ - ε curves, which is somewhat different to the linear hardening formulation as used in the crystal plasticity implementation.

Although, the individual curves from the indentation are not directly comparable with the grain-wise σ - ε curves from the polycrystal simulation, the mean σ - ε curve and the standard deviation, SD , derived from the scattered σ - ε curves obtained from the both methods coincide very well. In **Fig. 9** the mean σ - ε curves and the standard deviation from σ - ε curves estimated from the both approaches, i.e. indentation (with 17 imprints) and simulation of the polycrystal (with 64 grains), are compared. The results of the average curves as well as of the SD data from simulation and indentation results show a very nice agreement within the determined uncertainty. This good result could only be achieved by comparing both approaches on the same scale, which is related to the mesoscale grain behaviour, where the local microstructural response is averaged over a lamellar grain.

Some minor differences in this comparison can be pointed out, for example, the variation band of the σ - ε curves from the indentation is smaller than that of the polycrystal simulations. However, this difference is obvious as the indentation records contain the averaging of several grains underneath the imprint area, while for the polycrystal estimation the σ - ε curves represent each individual grain response.

6.2. Texture arrangements and compression-tension anomaly

The global mechanical response (σ - ε curve) depends on the arrangement (or texture) of lamellar grains in a polycrystal. So far, the background of the polycrystal behaviour due to differently oriented lamellar grains has not been demonstrated by numerical methods. It is only known that the macroscopic response of a PST single crystal due to different lamellar alignments is quite significant, as has been experimentally validated in [18].

In the following, the effects of lamellar alignments in a polycrystal are described. For this purpose different arrangements of oriented lamellar grains have been defined by the cases **A** to **F**, as depicted in **Fig. 10**. In all cases the lamellar grains are subjected to discrete random rotation (i.e. $0^\circ \leq \varphi_y \leq 360^\circ$) around the loading axis (y-axis). Further details of the alignment cases **A** to **F** are as follows.

In **case A** all 64 lamellar grains are fully randomly oriented. This case is taken as a reference for a texture-free microstructure. Cases **B**, **C**, **D** have idealised alignments with uniform rotation of the lamellar grains around x-axis, i.e. case **B** with $\varphi_x = 0^\circ$, case **C** with $\varphi_x = 20^\circ$, and case **D** with $\varphi_x = 45^\circ$ (all with $\varphi_z = 0^\circ$). The arrangement in case **E** is adapted for describing a real extrusion microstructure (known from SEM images) in which the lamellar grains are randomly tilted within the range of $-20^\circ \leq \varphi_x \leq +20^\circ$ around x-axis (but $\varphi_z = 0^\circ$). Previously, case **E** was used for the determination of the crystal parameters for the true polycrystal alloy. Case **F** is obtained by a slight modification of case **E** with a perfect 90° rotation around the x-axis showing a significantly different alignment compared to the others. This alignment is equivalent to a fully transverse loading, i.e. perpendicular to the extrusion direction.

The macroscopic σ - ε curves for the cases **A** to **F** are shown in **Fig. 11**. The margins of the PST single crystal with its lower ($\varphi_x = 45^\circ$) and upper ($\varphi_x = 90^\circ$) σ - ε curves are indicated by dashed lines with curve signed by a,b, and c. The results show that only the σ - ε curve for case **D** ($\varphi_x = 45^\circ$ uniform) deviates at most from the others. From the PST single crystal analysis it is known that a perfect alignment under $\varphi_x = 45^\circ$ ($\varphi_y = \varphi_z = 0^\circ$) provides the lowest σ - ε curve. However, for a polycrystal with the full random distribution around the load-axis ($0^\circ \leq \varphi_y \leq 360^\circ$) the strength increases considerably even for a uniform alignment at $\varphi_x = 45^\circ$.

The σ - ε curves of all other cases show a relatively small variation band. A particular observation is that the σ - ε curve of the PST single crystal with $\varphi_x = 0^\circ$ (curve signed by a) follows roughly the mean polycrystal behaviour.

In the initial strain region (i.e. $\leq 2\%$) the σ - ε curve of the reference case **A** (with full 3D random alignment) is softer than the other cases, (except for case **D** with a uniform alignment $\varphi_x = 45^\circ$). Case **F** shows pronounced hardening with increasing deformation, although the initial behaviour is quite similar to the reference case **A**.

In contrast to the highly anisotropic σ - ε behaviour of the PST single crystal, the spectrum of the anisotropic σ - ε behaviour in a polycrystal found to be weakly pronounced with respect to any texture, if at least one orientation angle is nearly randomly distributed. This weak anisotropy in lamellar polycrystal is due to the presence of sufficient internal constraints between the lamellar grains, which minimize the alignment (texture) effect on the polycrystal σ - ε behaviour. However, in the initial strain region the relative deviation among the σ - ε curves is larger than for the overall scale. For example, at about 0.2 % offset strain the range of strength variation is from 450 MPa for case **D** and 750 MPa for case **B**.

The compression-tension asymmetries with respect to lamellae alignments in a polycrystal are also studied. The margin of the σ - ε anomaly depends considerably on the alignments of the grains, as shown in **Fig. 12** for the cases of **A** to **F**. Herein, case **B** (with a uniform arrangement $\varphi_x = 0^\circ$) provides the largest effect of the σ - ε anomaly because the contribution of superdislocations in tension are significantly reduced for $\varphi_x = 0^\circ$ due to different activations of the morphological deformation modes with pronounced transversal contributions of ordinary slips and twinning [30,36]. Also, the PST single crystal exhibits a similar large σ - ε anomaly for the alignment with $\varphi_x = 0^\circ$ (and $\varphi_y = \varphi_z = 0^\circ$).

In particular for case **D** ($\varphi_x = 45^\circ$ uniform) the σ - ε anomaly is hardly pronounced. In this case superdislocations are (almost) not contributed and only twinning alone is responsible for the σ - ε anomaly. These results also support that not only twinning but also some contributions from superdislocations were required for a larger σ - ε anomaly in lamellar TiAl alloy.

7. Summary and conclusions

With respect to our objectives conclusions on particular issues are summarized as follows.

1. *Estimation of polycrystal parameters.* The estimation of crystallographic parameters for a γ TiAl polycrystal is based on two key steps: (i) the lamellar deformation is described by three morphological deformation modes (longitudinal, mixed and transversal), each with its own crystallographic classification of slip directions and slip activations (ordinary, super, and twinning), and (ii) for each morphological deformation mode it is assumed that the crystallographic classification remains fixed in lamellar grains but possess only different strength due to different alloy

compositions. The presented approach demonstrates how the fundamental crystallographic parameter sets can be estimated based on the microstructural deformation mechanisms of a lamellar system. Any adjustment of the crystal parameters for a polycrystal of different alloy compositions and lamellar morphologies (e.g. thickness of lamellae, strength of the phases, etc.) can be done by up-scaling the validated parameter sets for a PST single crystal. To estimate a full set of parameter at least three experiments (at 0° , 45° , and 90° lamellar orientations) of PST single crystal are required. Estimating the crystal parameters directly by fitting the macroscopic σ - ε curve of a polycrystal would not provide a physically consistent parameter set, as the global behaviour can be fitted with any combination of crystallographic parameters without capturing the local micromechanics of lamellar deformation.

2. *Microstructural idealization in PUC.* Among the presented PUC models, the high-grade PUC with six γ -domain variants (here, PUC7 or PUC9) provide the most consistent results for lamellar microstructure and satisfy specific compression-tension anomaly. Due to the lack of γ -domain interactions in PUC3 the estimated crystal parameters obtained from this simplified model may not contain enough physical (mechanical) relevance. Internal constraint interactions within the lamellar domains should be incorporated. Therefore, any modelling of lamellar alloys without considering physical coexistence of α_2 - and γ -phases as well the γ -domain variants are not sufficient for predicting material relevant crystal parameters.
3. *Prediction of compression-tension anomaly.* Compression-tension anomaly has been captured only by a higher-grade PUC with appropriate domain representation. This anomaly has been simulated using a single set of crystallographic parameters. A simplified model like PUC3 is not sensitive to the anomalous compression-tension

behaviour due to the absence of distinct γ -domain representation considering important internal deformation constraints within the randomly oriented grains in a polycrystal. From the results of simplified PUC3 model we presume that the micromechanisms of lamellar staggered grains (colonies) cannot be represented by a single FE element under homogenized description of slips.

4. *Local response of lamellar grains.* The numerically obtained local variation of the grain wise σ - ε curves has been confirmed by the stress-strain behaviour from indentation testing. Although completely different and independent approaches were applied, the mean σ - ε curves obtained from both the data sets are consistent. Some differences occurred mainly due to the hardening formulations (linear in FE model on the single crystal scale versus exponential in the indentation on the macroscopic scale). The variation band for the indentation analysis is smaller, which is due to both the low number of imprints and the averaging of several lamellar grains beneath the spherical imprints.
5. *Polycrystal behaviour under grain orientation.* The PUC7 model with six variations in the γ -phase domains allows the prediction of local and global σ - ε responses for different arrangements of lamellar grains, including textures in the polycrystal. The σ - ε responses for the texture-free case (i.e. with fully spatial random distribution of lamellar grains) as well as for the cases with uniformly aligned arrangements show a common trend within a small (overall) variation. In contrast, a PST single crystal with free boundaries exhibits stronger anisotropic behaviour. Weak anisotropy in the overall deformation behaviour in the polycrystal model is due to the strong interactions among the lamellar grains in the polycrystal, in which significant three-dimensional constraints of local deformation occurs evolving multi-axial stress states. On each lamellar grain,

the possible crystallographic slips in the γ -domains can always be activated with enough crystallographic slip deformation to subside a significant anisotropic response. The compression-tension anomaly of the polycrystal is significantly pronounced only for particular arrangements, whereas the fully random case exhibits a moderate margin.

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Figure Captions

Fig. 1. Experimental test data with tension and compression σ - ε curves. (a) Overall strain range, (b) tension strain range (magnification of (a)).

Fig. 2. Morphological modes for the classification of the slip systems in a PST single crystal. (a) Longitudinal, (b) mixed, (c) transverse mode.

Fig. 3. Periodic unit cells representing different intra-lamellar conditions. (a) PUC3 with homogeneous lamellae (i.e. without domains along the lamellae), (b) PUC7 with small domain aspect ratio representing thin lamellae, (c) PUC9 with large domain aspect ratio representing thick lamellae.

Fig. 4. Polycrystal modelling. (a) Polycrystalline cube with 64 randomly oriented brick-type lamellar grains, (b) finite element cube with 8 finite elements per grain, (c) basic finite element consisting of several PUC, (d) embedded PUC with individual crystal orientations.

Fig. 5. Stress-strain curves for compression from simulations with different Q_{so} parameter for superdislocation strength enhancement and comparison with an experimental compression test. The crystallographic parameter set is fixed for all variations of Q_{so} . The ratio $Q_{so} = 1.8$ provides a good relation for both compression and tension responses.

Fig. 6. Evolution of tension-compression anomaly within the tension strain range. Simulation results are superimposed with the experimental stress-strain curve.

Fig. 7. Stress-strain curves from three PUC models for compression and tension behaviour using the estimated crystal parameter set. For PUC3, the compression-tension anomaly results mainly from the unidirectionality of twinning but not additionally from superdislocation contribution as given for PUC7 and PUC9.

Fig. 8. Variations of local σ - ε curves for the polycrystalline γ TAB. (a) From the two-scale simulations of the polycrystalline cube and the PST single crystal for the three main orientations ($\varphi_x = 0^\circ, 45^\circ, 90^\circ$); the dashed σ - ε curve is the mean curve of all grain wise curves, (b) from spherical indentation testing and the inversion to σ - ε curves by Artificial Neuronal Network analysis. (For the definition of lamellae rotations see Fig. 10).

Fig. 9. Comparison of mean σ - ε curves from compression test, indentation, and polycrystal simulation. Behaviour of standard deviation, SD , from indentation and simulation are included.

Fig. 10. Different cases of A–F for assumed lamellar grain alignments within in the polycrystalline cube of 64 grains (colonies). Definition of alignment and rotations are also shown.

Fig. 11. Simulated σ - ε curves of the polycrystal for the different texture arrangements A–F (Fig. 10) and superposition of the stress-strain curves for the PST single crystal in the three main orientations ($\varphi_x = 0^\circ, 45^\circ, 90^\circ$).

Fig. 12. Simulated σ - ε curves representing the polycrystalline behaviour under compression and tension loading for the assumed arrangements A to F (Fig. 10) with their tension-compression anomalies.