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# Crystal plasticity modelling and experiments for deriving microstructure-property relationships in $\gamma$ -TiAl based alloys

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**Abstract.** Single-crystals of  $\gamma$ -TiAl cannot be grown for the compositions present inside the two-phase  $\gamma/\alpha_2$ -microstructures that show good mechanical properties. Therefore the single crystal constitutive behaviour of  $\gamma$ -TiAl was studied by nanoindentation experiments in single phase regions of these microstructures. The experiments were extensively characterized by a combined experimental approach to clarify the orientation dependent mechanical response during nanoindentation. They further were analyzed by a three-dimensional crystal plasticity finite element model that incorporated the deformation behaviour of  $\gamma$ -TiAl. The spatially resolved activation of competing deformation mechanisms during indentation was used to assess their relative strengths. On the length-scale of multi-grain aggregates two kinds of microstructures were investigated. The lamellar microstructure was analyzed in terms of kinematic constraints perpendicular to densely spaced lamellar boundaries which lead to pronounced plastic anisotropy. Secondly, the mechanical behaviour of massively transformed microstructures was modelled by assuming a lower degree of kinematic constraints. This resulted in less plastic anisotropy on a single grain scale and lower compatibility stresses in a 64-grain aggregate. On the macroscopic length scale, the results could possibly explain the pre-yielding of lamellar microstructures.

## 1. Introduction

Gamma-TiAl based alloys are currently investigated for application in turbine aero-engines. Due to their low density of about  $4\text{g/cm}^3$  they exhibit excellent specific mechanical properties [1].

In this paper two approaches are presented to analyze the micromechanics of  $\gamma$ -TiAl based alloys on different length scales. First the single phase behavior of tetragonal,  $L1_0$ -ordered  $\gamma$ -TiAl was studied by a combined analysis employing nanoindentation experiments and crystal plasticity finite element modeling (CPFEM). Second, on a larger length scale, the two-phase micromechanics of a lamellar and a refined microstructure were simulated by a homogenized CPFEM-model that takes into account the combined effect from single crystal plasticity and the interface-dominated flow behavior.

## 2. Analysis of the single phase properties by nanoindentation, EBSD, AFM and CPFEM

The inelastic deformation behavior of  $\gamma$ -TiAl is highly anisotropic [2]. Bulk single crystals cannot be produced for the near-stoichiometric compositions that are present in two-phase microstructures with balanced properties, e.g. [3]. Therefore an alternative approach was developed to analyze the

intrinsic properties of the constitutive phases. Nanoindentation experiments were performed in single phase regions of a two-phase microstructure. For the discrimination of the three order variants in  $\gamma$ -TiAl a newly developed indexing scheme for electron backscatter diffraction (EBSD) patterns was applied [4]. It was used to measure the crystallographic direction of the indentation axis. The pile-up formation around the indent was measured by atomic force microscopy (AFM). Finally, three-dimensional CPFEM simulation of the indentation process was employed to assess the deformation contributions from each deformation system.

Nanoindentation of TiAl alloys has previously been studied [5,6]. For the analysis of plastic anisotropy, axis-symmetric indenter shapes are well suited because they do not interfere with the plastic anisotropy of the crystal under consideration [6]. Figure 1 gives a view of the combined results from a topographic measurement and orientation mapping for several indentations. The Berkovich indenter geometry inhibited formation of pile-up in the directions of the edges.

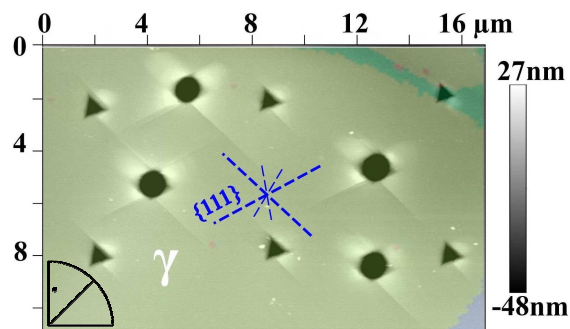


Figure 1) Nanoindents in  $\gamma$ -grains of nearly lamellar Ti-46Al-8Nb (at.-%); AFM topographic map (greyscale) combined with an EBSD orientation map (001 inverse polefigure colouring). The  $\{111\}$ -traces coincide with the observed surface steps. Cono-spherical (tip radius  $< 1 \mu\text{m}$ ) and Berkovich indentations were performed with maximum loads of 6 mN and 3 mN, respectively. The indentation axes were oriented along  $[1\ 10\ 6]$ . Remaining indent depths were about 250 nm for the 6 mN load.

### 2.1. Crystal plasticity modelling of the indentation deformation

An existing elasto-viscoplastic crystal plasticity formulation [7] based on the works of Kalidindi et al. [8] was changed to use specific strength and hardening characteristics for deformation systems of different types. Additionally, a coarse implementation of the four twin deformation modes in TiAl was carried out by the installation of uni-directional slip systems. Reorientation through twinning was neglected. The constitutive law was coupled with a finite element solver as a material subroutine. Four glide systems by ordinary dislocations,  $b=1/2 \langle 110 \rangle$ , eight by superdislocations,  $b=\langle 101 \rangle$ , and four true twinning modes,  $b=1/6 \langle 11\bar{2} \rangle$  were taken into account on the  $\{111\}$  planes of the  $\gamma$ -phase.

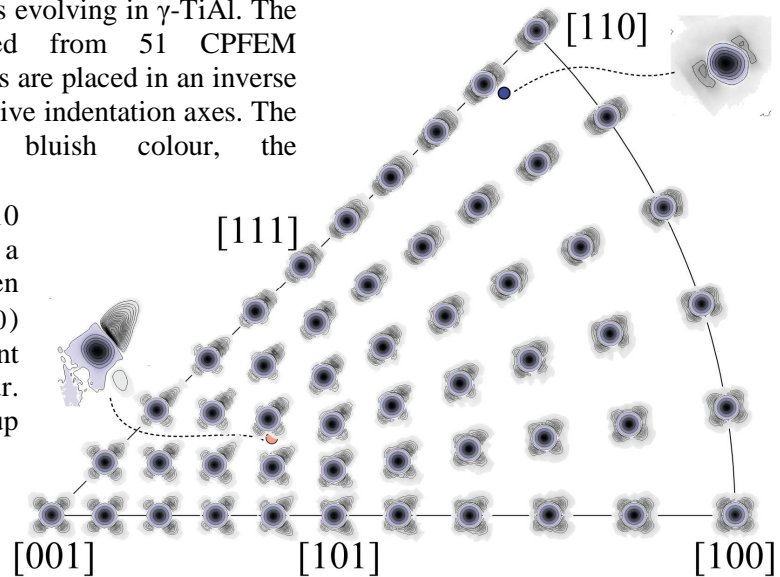
A three-dimensional finite element model of indentation was generated to simulate the nonlinear deformation during indentation of an axis-symmetric rigid body. The formation of hillocks was analyzed after unloading. The formation of characteristic pile-up patterns during the indentation could be related to the existence of distinct lobes of slip activity below the surface. The topography of the pile-up shape was a characteristic feature of the indented crystallographic direction as has been previously reported for indentation into high-symmetry orientations of copper [9].

Simulations were performed for indentation axes throughout the crystallographic unit triangle of  $\gamma$ -TiAl. To this end, the unit triangle was discretized at an approximate resolution of  $9^\circ$  ( $\Delta=9^\circ$ , cf. [10]) by a method after Helming et al. [10]. The simulated pile-up characteristics were found to be in good agreement with experimentally measured pile-up topographies, figure 2.

The measured pile-up patterns were analyzed and compared with the simulation results for different sets of constitutive parameters for several orientations. It was found that mostly ordinary and, to a minor extent, twinning deformation is operating during the indentation of single phase  $\gamma$ -TiAl. These two modes could explain the observed pile-up patterns throughout orientation space. The adjusted values for the critical resolved shear stress (CRSS) for ordinary dislocation glide and twinning were 150 MPa and for superdislocation glide a CRSS of 300 MPa was assumed which lead to almost complete suppression of this mode. Load-displacement curves showed good agreement with the experimental data for loading and unloading.

Figure 2) Predicted pile-up patterns evolving in  $\gamma$ -TiAl. The topographic data was obtained from 51 CPFEM simulations. The individual patterns are placed in an inverse polefigure projection of the respective indentation axes. The impressions are shown in bluish colour, the upheaval in greyscale.

Topographies in the 001–110–010 triangle can be obtained by a mirroring operation of the given topographies through the  $(\bar{1}10)$  plane. The number of dominant hillocks ranges from one to four. Two experimental pile-up topographies are also shown.



### 3. A homogenized model for two-phase $\gamma/\alpha_2$ microstructures

#### 3.1. Anisotropic yielding of lamellar bundles

The second length scale on which the micromechanics were studied was on the order of grain sizes. The yielding behaviour of lamellar poly-synthetically twinned (PST) samples that contain only one lamellar orientation, shows a pronounced dependency of the angle between the loading axis and the lamellar interfaces [11-14]. The micro-mechanics are dominated by the high density of parallel  $\alpha_2/\gamma$  and  $\gamma/\gamma$  interfaces. A homogenized CPFEM model was developed that reflects the kinematic constraints resulting from the interfaces, figure 3.

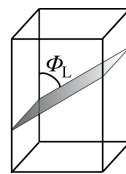
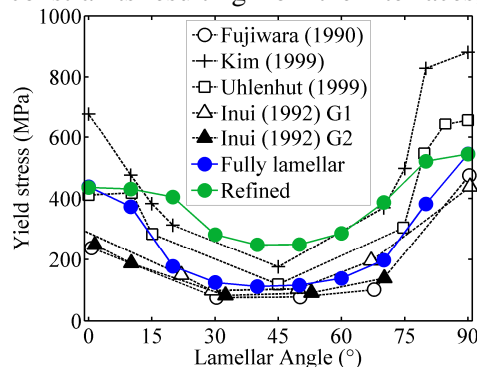


Figure 3) Anisotropic yielding of a simulated PST crystal in compression compared to literature data [11-14]. The assumed yielding for a refined microstructure is shown in comparison to the yield points from the fully lamellar model. The definition of the lamellar angle,  $\Phi$ , is shown for a vertical deformation axis.

#### 3.2. Polycrystal mechanics

To simulate the tensile response of real microstructures, a 64-grain aggregate was constructed with periodic boundary conditions. The parameters for fully lamellar (FL) microstructures were taken to be identical to the PST parameters. The parameters for refined (RF) microstructures were changed to reflect less plastic anisotropy. Both parameter sets were used for simulated tensile deformation of the 64-grain model with random grain orientations. The volume averaged response of the grain aggregates is shown in figure 4-a. The simulated curves were generally lying below the data from tensile tests on polycrystalline microstructures. That could be explained by different compositions of the PST crystals (binary) and the FL and refined microstructures that were additionally alloyed with 8 at.-% Nb or Ta and show a smaller lamellar spacing which is known to increase the overall strength. More important, however, is the observation that the simulated fully lamellar aggregate shows a flow curve in excellent agreement with the pre-yielding behaviour of the experimental data. The extended pre-yielding of the

FL microstructure is absent in the refined microstructure. Therefore the strong plastic anisotropy might explain the pre-yielding observed in fully lamellar microstructures [15-17].

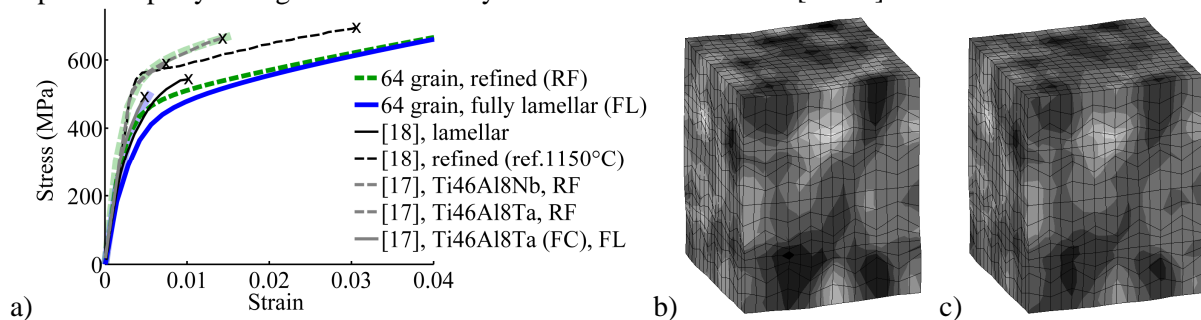


Figure 4) (a) Flow curves of simulated 64-grain clusters with FL (—) and refined (---) microstructures compared to literature data [17,18]; the bold, semi-transparent curves are the scaled results from the respective simulations and match the experimental curves from [17] almost perfectly; (b) Distribution of axial stress for the FL and (c) refined microstructure simulations, greyscale from 0 MPa (white) to 1600 MPa (black).

#### 4. Conclusions

The presented nanoindentation analysis combines experimental and computational methods to form a coherent picture of the single phase mechanics. Easy activation of ordinary dislocation glide in the  $\gamma$ -TiAl phase was found to be an intrinsic property, i.e. not mainly related to the interfaces.

The analysis of a 64-grain cluster with two different sets of constitutive parameters revealed the strong plastic anisotropy in lamellar microstructures as the probable source of the experimentally observed pre-yielding behavior.

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