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Defect density-based modeling of work hardening and recovery in fully lamellar TiAl alloys

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Micro Abstract
The dense arrangement of different microstructural interfaces in fully lamellar TiAl alloys necessitates microstructure informed modelling in order to predict the macroscopic mechanical behavior. Microtwinning within the lamellae leads to further interface related strengthening. The presented crystal plasticity model incorporates the evolution of dislocation density and afore mentioned twins during plastic deformation and accounts for thermally activated recovery of said defects.

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Introduction

Due to their beneficial combination of good thermomechanical properties with a low density, fully lamellar titanium aluminides (TiAl) become increasingly important as structural materials for high-temperature lightweight applications such as turbo chargers in combustion engines or turbine blades in aircraft engines [5]. The extraordinary thermomechanical properties of fully lamellar TiAl alloys are closely related to the specifics of their complex microstructure [2].

On the meso scale, fully lamellar microstructures consist of grain-shaped colonies that are subdivided into numerous thin lamellae which result from the strict orientation relation between the α_2 and the γ phase, i.e., the two main phases that occur in TiAl alloys. In addition to colony and lamella boundaries a third type of microstructural interface is present in the γ lamellae, subdividing domains of different crystal orientation. Besides these three types of microstructural boundaries, additional obstacles for dislocation motion and twin propagation arise in the form of micro twins that evolve in the γ lamellae during plastic deformation. This dense arrangement of different microstructural interfaces in fully lamellar TiAl alloys necessitates microstructure informed modelling in order to predict the macroscopic mechanical behavior. Therefore, we set up a microstructure sensitive thermomechanically coupled crystal plasticity model of fully lamellar TiAl which incorporates the three simulataneously acting Hall-Petch effects, the typical yield stress temperature anomaly and that accounts for defect density evolution as well as the correlated work hardening [4, 15].

In this contribution we now focus on the defect density evolution with deformation and thermal recovery and the correlated work hardening.

1 Work hardening

While most of the reported crystal plasticity models for fully lamellar TiAl used linear [3, 6–9, 17, 18] or hyper secans [11, 13, 14] hardening laws, we describe work hardening in terms of evolving defects, i.e. as function of dislocation densities and twinned volume fractions. In the presented model, dislocation densities and twinned volume fractions evolve with the plastic shear rates on respective slip and twinning systems as they are predicted by crystal plasticity. The work hardening due to evolving dislocation densities is described by classical Taylor hardening while the strengthening effect of evolving twins on the non-coplanar slip and twinning systems is modeled via a Hall-Petch type strengthening law (cf. [10]).

Since so-called polysynthetically twinned crystals are specimens that only contain lamellae of one specific orientation and thus basically represent a single lamellar colony, they are the best source for basic investigation of the micromechanics in fully lamellar TiAl. Thus, the defect density evolution and the correlated work hardening is calibrated against the experiments with differently oriented polysynthetically twinned crystals reported in [16]. The simulation results of the calibrated crystal plasticity model meet the initial yield of the differently oriented polysynthetcially twinned crystals and reproduce their hardening behavior reasonably well as shown in [15].

Due to its physics based formulation of work hardening, this crystal plasticity model enables investigation of the evolution of relative activity of deformation systems in the lamellae of polysynthetically twinned crystals which is not easily done via experiments. The few fragmented experimental results that exist on the relative activity in polysynthetically twinned crystals are, however, met well by the simulation results confirming the models ability to correctly predict the defect density evolution.

By applying this defect density based crystal plasticity model of a polysynthetically twinned crystal to a polycolony microstructure, it was furthermore possible to determine the Hall-Petch coefficient for colony boundary strengthening and its dependence on the lamella thicckness and domain size [15] which so far was not possible by experiments. With all three Hall-Petch effects and the defect density based hardening incorporated, this model ultimately allows microstructure sensitive prediction of the yield stress and post yield behavior of fully lamellar TiAl.

2 Recovery

Recovery, i.e. annihilation of dislocations, is modeled here via an Arhenius type law similar to [1, 12]. The model is calibrated against static recovery experiments with differently oriented polysynthetically twinned crystals, carried out at the Metal Physics department of the Institute of Materials Research at the Helmholtz-Zentrum Geesthacht, Germany. The recovery simulations showed that – unlike most other thermomechanical effects in fully lamellar TiAl – the functional dependence of recovery rate on the current dislocation density on a system is isotropic.

With this claibrated recovery model it is possible to do first predictive simulations of the recovery behavior in both polysynthetically twinned crystals and polycolony microstructures.

Conclusions

Introducing the evolution of defect densities and the correlated work hardening into a crystal plasticity model of fully lamellar TiAl greatly improves its predictive abilities as compared to reported models. In particular the evolution of micro twins and their pronounced strengthening effect on all non-coplanar systems is crucial for precisely reproducing the hardening behavior of fully lamellar TiAl. While this hardening model was already successfully applied to identify the colony boundary strengthening Hall-Petch coefficient [15] – which could not consistently be determined experimentally – it has the potential to support various other experimental investigations of the micromechanics in fully lamellar TiAl.

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