Publishing House
AKAPIT

COMPUTER METHODS IN MATERIALS SCIENCE
Informatyka w Technologii Materiałów

Vol. 17, 2017, No. 1

FINITE ELEMENT MODELLING OF TITANIUM ALUMINIDES

IRINA SIZOVA*, ALEXANDER SVIRIDOV, MARTIN GÜNTHER, MARKUS BAMBACH

[1] *Chair of Mechanical Design and Manufacturing, Brandenburg University of Technology Cottbus - Senftenberg, Konrad - Wachsmann - Allee 17, Cottbus D-03046, Germany*
**Corresponding author: sizova@b-tu.de*

Abstract

Hot forging is an important process for shaping and property control of lightweight titanium aluminide parts. Dynamic recrystallization and phase transformations play an essential role for the resulting grain size and accordingly the mechanical properties. Due to the fact that titanium aluminides require forging under isothermal conditions, reliable process modeling is needed to predict the microstructure evolution, to optimize the process time and to avoid excessive die loads. In the present study an isothermal forging process of a compressor blade made of TNB-V4 (Ti–44.5Al–6.25Nb–0.8Mo–0.1B, at. %) is modeled using the Finite Element (FE) – Software Q-Form. A microstructure model describing the microstructure evolution during forging is presented. To calibrate the model, the high-temperature deformation behavior was investigated using isothermal compression tests. The tests were carried out at temperatures from 1150°C to 1300°C, applying strain rates ranging from 0.001 s^{-1} to 0.5 s^{-1}, up to a true strain of 0.9. The experimentally determined flow stress data were described with model equations determined form the course of the strain hardening rate in Kocks-Mecking plots. An isothermal forging process of a compressor blade was carried out and used to validate the results from the FE simulations.

Key words: titanium aluminide alloy, hot forming, flow stress, dynamic recrystallization, modelling

1. INTRODUCTION

Intermetallic titanium aluminide (TiAl) alloys are important high temperature materials which are developed for lightweight design in aerospace and automotive applications. These alloys offer a favourable combination of low density, high strength and oxidation/corrosion resistance (Clemens & Kestler, 2000; Clemens & Smarsly, 2011). However, conventional forging is not appropriate for these alloys due to their low workability, even at elevated temperatures. Accordingly, an important task in processing of TiAl-based alloys consists in the investigation of the materials behavior, to overcome the problems associated with the limited workability of these alloys and to design an economic manufacturing process. For this reason, the experimental determination and modeling of the mechanical response in compression testing is of great practical importance. In recent years there have been many investigations on the hot deformation behavior (Semiatin et al., 1992; Schmoelzer et al., 2013) as well as on the constitutive modeling of TiAl-based alloys, since these models are needed for accurate Finite Element (FE) simulations of isothermal forging processes. The flow behavior of TiAl-based alloys has been studied intensively and a number of constitutive relationships and processing maps have been proposed in a literature. For instance, Cheng et al. (2014) investigated TiAl-alloys with a nominal composition of Ti–42Al–8Nb–0.2W–0.1Y (at %) and applied the model proposed by Laasraoui and Jonas (1991). Werner et al. (2014) and Godor et al. (2015) applied two phenomenological constitutive models, the Sellars–McTegart model and the Hensel-Spittel model, for the description of the hot deformation behavior of different TiAl-alloys. Werner et al. (2014) considered the flow behaviour of *β*-

 ISSN 1641-8581

solidifying TNM alloy with nominal composition Ti-43.5Al-4Nb-1Mo-0.1B. Godor et al. (2015) researched two *γ*-TiAl alloys with nominal compositions Ti–41Al–3Mo–0.5Si–0.1B and Ti–45Al–3Mo–0.5Si–0.1B. Schwaighofer et al. (2014) studied a modified TNM alloy, with a nominal composition of Ti–43Al–4Nb–1Mo–0.1B which contains a small amount of C and Si (C+Si less than 1 at. %). The authors also applied the Sellars and McTegart model and established processing maps with the demonstration of stable and unstable deformation regions. However, present descriptions of the flow behavior of TiAl-alloys are based on empirical models, which were derived originally for steels and do not consider the presence of the multiphase microstructure.

Some studies on forging process of TiAl-based alloys have also been reported in the literature. Millett et al. (1999) investigated a *γ*-TiAl-based alloy with nominal composition Ti-48Al-2Mn-2Nb. The forging experiments were carried out on as cast material and on material that was treated at different temperatures and strain rates. In order to analyze the flow stress data the authors used the model developed by Blackwell et al. (1998). An increase in the degree of flow softening with increasing temperature and decreasing strain rate has been reported. Semiatin et al. (1999) reported on isothermal forging of a near *γ* titanium aluminide Ti–46.6Al–2.7Nb–0.3Ta–0.2O and found similar results. The investigations suggested that the flow softening was also a result of adiabatic heating. Tetsui et al. (2005) reported about hot forging and subsequent machining of a Ti-42Al-5Mn alloy and represented that the presence of the *β*-phase improves the hot-workability of TiAl alloys. Moreover, some researches carried out FE simulations of forging processes of TiAl alloys. Brooks et al. (1998) considered the possibility of forging and FE simulation of titanium aluminide aerofoil. The authors studied TiAl-alloys with a composition of Ti-47.9Al-2.06Nb-1.93Cr-1.07B. The constitutive algorithm has been used in two finite element codes (ABAQUS and FORGE 3) to model the forging of a turbine blade.

However, the transition between incipient yield over the peak stress to the steady-state is often not well represented in available models. The purpose of the present study was investigation of the hot deformation behaviour of a high Nb containing TNB-V4 (Ti–44.5Al–6.25Nb–0.8Mo–0.1B, at. %) alloy using isothermal high temperature compression tests. On grounds of these data a constitutive model has been developed and applied to the simulation of isothermal forging of a compressor blade. This model enables the prediction of recrystallized grain sizes in the hot forging process. The emphasis was put also on an evaluation of microstructure evolution during forging.

The process simulations were conducted following the course of a real hot forging process. The findings of the simulation are confirmed through the observation and comparison of the recrystallized grains size in the real forging process of the compressor blade from TNB-V4 alloy.

2. MATERIALS AND HOT COMPRESSION TESTS

The material used to forge the compressor blade is a titanium aluminide alloy commercially known as TNB-V4 with a nominal composition of Ti–44.5Al–6.25Nb–0.8Mo–0.1B (in at %). Isothermal compression tests were performed at temperatures of 1150–1300°C and at strain rates of 0.001–0.5 s^{-1} using a Gleeble 3500 thermomechanical simulator. The alloy was prepared by VAR melting and heat-treated by hot isostatic pressing at 1260 °C for 4 h with a pressure of 200 bars. The dimensions of the cylindrical test specimen are 15 mm in height and 10 mm in diameter. Compression tests were carried out in vacuum of 10^{-4} mbar. Specimens were heated to testing temperature with a rate of 10 K/s, soaked for 5 min, and then upset under constant strain rate conditions to a strain of 0.9. Each specimen was quenched immediately after upsetting. To determine the effect of forging on the microstructure, the compression samples were sectioned axially and prepared by means of standard metallographic techniques. The sample surfaces were treated by vibrational polishing. The sections were also analyzed using scanning electron microscopy. Figure 1 shows the flow curves at different temperatures and strain rates obtained from compression tests and corresponding microstructure for selected combinations of deformation parameters.

Since the results of forging experiments of the compressor blade are not available during the phase of process design, additional physical simulations were carried out on a dilatometer for the purpose of validating the simulation results. Cylindrical samples for the physical simulation were machined from the heat-treated material with 5 mm diameter and 10 mm length. The samples were subjected to hot compression testing using Bähr Dil 805D deformation dilatometer. The testing conditions were extracted from the thermo-mechanical history of a validation point in the blade obtained from the forging simulation. The experiments were performed under vacuum using inductive heating and deformation through molybdenum platens. After the physical simulation, the samples were quenched in helium gas in order to conserve the high temperature microstructure, and then analyzed using scanning electron microscopy.

3. FLOW STRESS BEHAVIOUR AND KOCKS-MECKING PLOTS

The flow stress is sensitive to the deformation temperature and the strain rate. The typical flow stress of TNB-V4 alloy display a single peak at the initial deformation stage, and then the flow stress decreases rapidly towards a steady state stress. The flow stress behavior at different temperatures obtained from tests is shown in figure 2a.

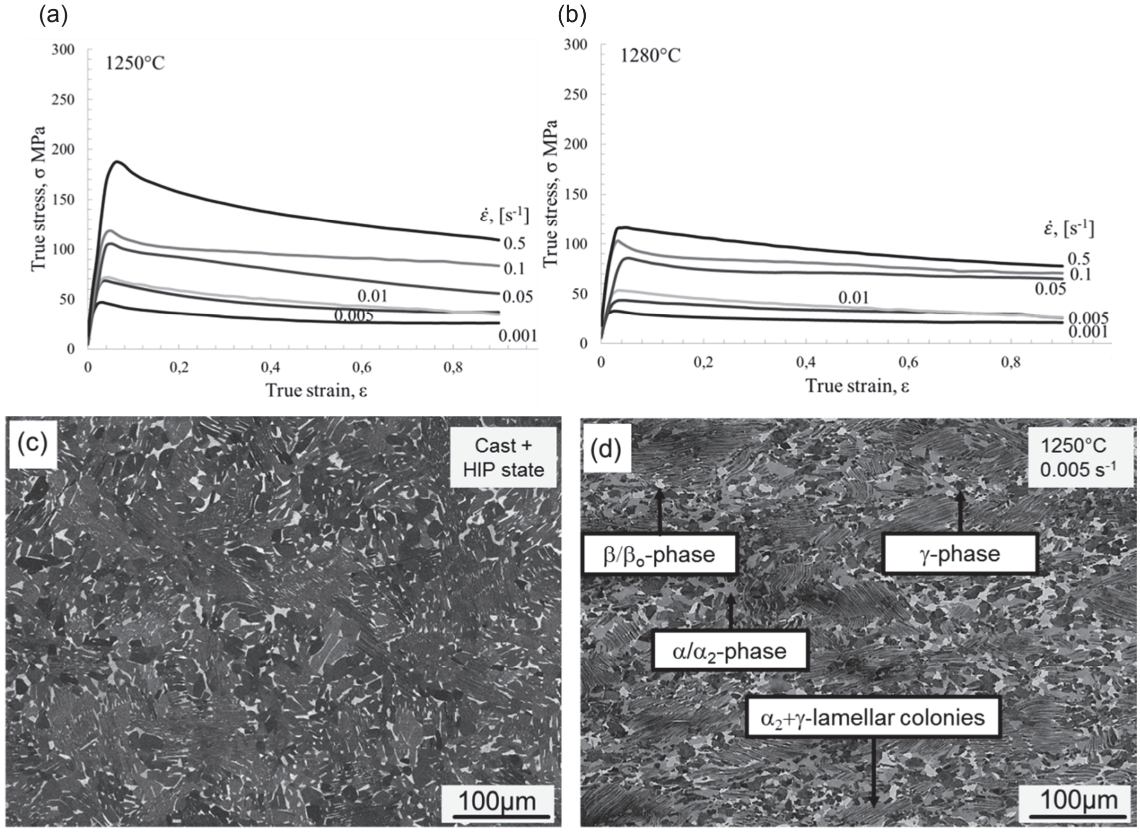


Fig. 1. *Flow curves (a) at 1250°C, (b) at 1280°C and different strain rates and determined microstructure (c) before deformation cast +HIP state, (d) compressed to a strain of 0.6*

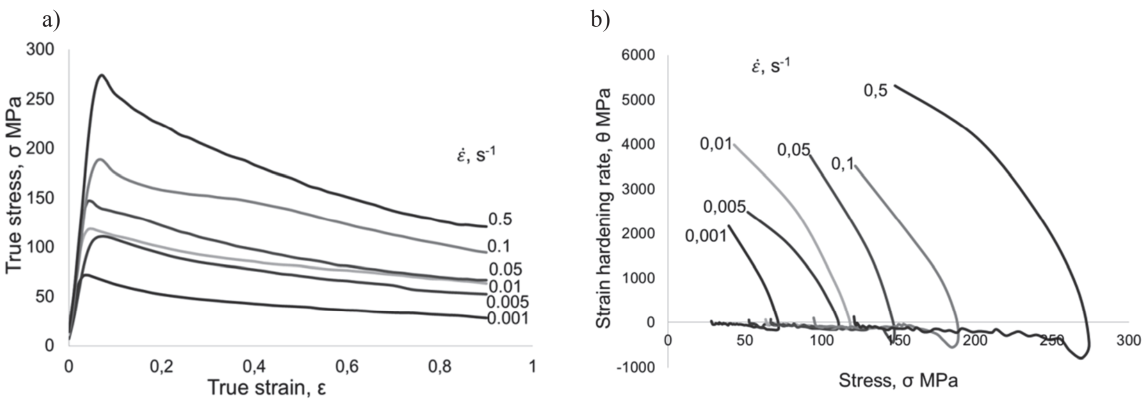


Fig. 2. *(a) The flow stress curves and (b) Kocks–Mecking plots at temperature 1200 °C and various strain rates for the TNB-V4 alloy*

The flow behaviour is analyzed by means of Kocks-Mecking plots. The TNB-V4 alloy demonstrates an untypical non-linear course of strain hardening rate θ (i.e., no stage-III hardening), no a plateau (stage IV hardening) and no inflection point (figure 2b). This work-hardening behavior is, in large part, a consequence of the complex multiphase microstructure of the TNB-V4-alloy, and differs greatly from the behaviour observed in single phase austenitic steel. Semiatin et al. (1998) reported also about the existence of other factors that may influence the hot deformation behavior of TiAl-alloys, such as occurrence of shear localization, dynamic recrystallization and wedge cracking.

Table 1. *Model equations for TNB-V4 alloy.*

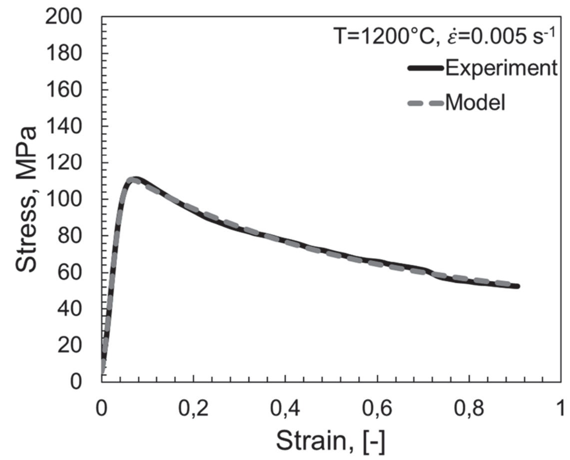
Zener Hollomon Parameter	$Z = \dot{\varepsilon} \cdot \exp\left(\frac{Q_w}{RT}\right)$	(1)
Strain hardening	$\sigma(\varepsilon) = \sigma_p \left[\frac{\varepsilon}{\varepsilon_p} \exp\left(1 - \frac{\varepsilon}{\varepsilon_p}\right)\right]^C$	(2)
Critical strain	$\varepsilon_{cr} = \alpha\varepsilon_p$	(3)
Peak strain	$\varepsilon_p = a_1 \cdot d_0^{a_2} \cdot Z^{a_3}$	(4)
Steady state stress	$\varepsilon_{ss} = e_1 \cdot \varepsilon_m + e_2 \cdot d_0^{e_3} \cdot Z^{e_4}$	(5)
Peak stress	$\sinh(f_3 \cdot \sigma_p) = f_1 \cdot Z^{f_2}$	(6)
Steady state stress	$\sinh(h_3 \cdot \sigma_p) = h_1 \cdot Z^{h_2}$	(7)
DRX grain size, separate for each phase	$d_{DRX}(\gamma) = b_{1\gamma} \cdot Z^{b_{2\gamma}}$ $d_{DRX}(\beta) = b_{1\beta} \cdot Z^{b_{2\beta}}$	(8) (9)
DRX kinetics, separate for each phase	$X(\gamma) = 1 - \exp\left[k_\gamma \cdot \left(\frac{\varepsilon - \varepsilon_{cr}}{\varepsilon_{ss} - \varepsilon_{cr}}\right)^{q_\gamma}\right], \quad \varepsilon \geq \varepsilon_{cr}$ $X(\beta) = 1 - \exp\left[k_\beta \cdot \left(\frac{\varepsilon - \varepsilon_{cr}}{\varepsilon_{ss} - \varepsilon_{cr}}\right)^{q_\beta}\right], \quad \varepsilon \geq \varepsilon_{cr}$	(10) (11)
Flow stress	$\sigma_Y = \begin{cases} \sigma_0 & \text{if } \varepsilon < \varepsilon_{cr} \\ \sum_{i=0}^{n-1}(X_i - X_{i+1})\sigma_i + X_n\sigma_n & \text{if } \varepsilon \geq \varepsilon_{cr} \end{cases}$	(12)

4. MATERIAL MODEL

The constitutive equations relating the flow stress with temperature, strain rate and strain are calibrated from the data of the hot compression tests conducted in a wide range of temperatures and strain rates. A number of flow curves exhibit a peak stress and subsequent flow softening, which may be caused by different microstructure changes such as dynamic recrystallization, adiabatic heating, grain growth as well as occurrences of flow localization, kinking and rotation of lamellas from hard into soft orientations (Schwaighofer et al., 2014; Semiatin et al., 1990). Kim and Hong (1999) also reported about the strong influence of the primary structure of the material on the hot forming behaviour. The microstructure of TNB-V4 alloys consist of a duplex microstructure with globular γ-grains and lamellar α2+γ – colonies. Moreover, forgeable TiAl alloys such as TNB-V4 have a significant amount of β/β0-grains that affect the workability. The β/β0-phase acts as a lubricant within the microstructure and supports the rotation or buckling and breakdown of hard lamellar α2+γ –colonies (Schwaighofer et al., 2014). All these phenomena may be decisive for the design of a sound forging process of titanium aluminide alloys.

Based on the experimental results and the Kocks-Mecking plots a phenomenological flow stress model for hot deformation of present alloy was established. The empirical equation proposed by Cingara and McQueen (1992) was used for the flow curve up to the peak (equation 2), where C is a constant of the material which is weakly dependent on temperature and strain rate and determines the curvature of the flow curve up to the peak. This model is able to show also a right concave down course of the strain hardening rate in the Kocks-Mecking plot, as observed experimentally. The other models, which were derived in terms of dislocation theory, would not be applicable to TNB alloy since they cannot reproduce the right curvature of the Kocks-Mecking plots. An overview of various dislocation-based models, the model equations and parameters were presented in previous work of the authors (Bambach et al., 2016).

The effects of strain rate and temperature on flow stress and microstructure can be integrated into the model using the Zener Hollomon parameter, cf. (equation 1), where $\dot{\varepsilon}$ is the strain rate, Q_w is the a)



b)

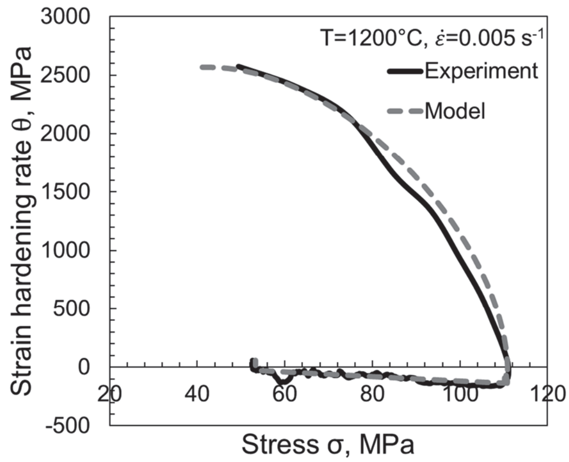


Fig. 3. *Model prediction vs. experimental data: (a) flow curve of TNB-V4; (b) Kocks-Mecking plot of TNB-V4.*

apparent activation energy for hot deformation, R is the universal gas constant and T is the deformation temperature. Conventional equations describing the relationship between characteristic points as well as the processes of dynamic recrystallization (equations 10, 11), cf. (Laasraoui & Jonas, 1991; Beynon & Sellars, 1992) and the dynamically recrystallized grains size (equations 8, 9) for TNB-V4 alloy are presented in table 1. The evolution of flow stress is determined by a linear mixture rule (equation 12). Details of the model and the process of parameter determination were described in recent research of the authors (Bambach et al., 2016). Due to the fact that the microstructure consists of multiple phases, the recrystallized grain sizes of the phases undergoing recrystallization were considered separately. Recrystallization occurs only in the β/β_0 - and γ- phase, the α-phase forms first during hot forming. The proposed models well predicts the course of flow stresses for the present alloy during hot deformation (figure 3) and was hence used in FE - simulation of isothermal forging.

5. SIMULATION STUDY OF FORGING PROCESS

The software used in this study is the FE program Q-Form. Figure 4 shows 3D FE model for the compressor blade forging. The process is carried out in a single stroke from a preformed billet. The upper and lower dies were modelled as rigid bodies. The temperature of the billet was 1260°C which was determined as optimal deformation temperature for compressor blade forging of the TNB-V4 alloy from the compression test data. The forging velocity was 0.17 mm/s. The billet was meshed with 226060 tetrahedral elements. The friction between dies and billets along the contact surface was assumed to follow a Levanov friction factor of 0.1. The simulation includes the pre-heating of the billet and closing the gap with the upper die.

6. PRODUCTION AND VALIDATION

This section focuses on the microstructural assessment of forged part based on the result of the simulation. The compressor blade was forged with a pre-heating temperature of 1260 °C and forging rate of 0.17 mm/s (forging time about 3 minutes) according to the simulation results. These parameters guarantee for required microstructure transformation and reduce the occurring forging loads.

Since during the real forging experiments the work piece cannot be quenched, and since the model needs to be validated during the design of the model based forging process, the examination of the microstructure and model validation was conducted on the dilatometer with deformation parameters determined from simulation of the compressor blade. The testing conditions included deformation with various strain rates in agreement with data history obtained from the simulation process (figure 5b). Figure 6 shows the results of comparison of the predicted grain size determined from the compression test in comparison with results from the simulation. The microstructure of TNB-V4 as consists of the fine recrystallized fractions of β/β_0 -(white) and the γ-phase (dark gray) as well as the α-phase (light gray), which forms first during hot forming. The model shows a good agreement between measured and calculated grain sizes.

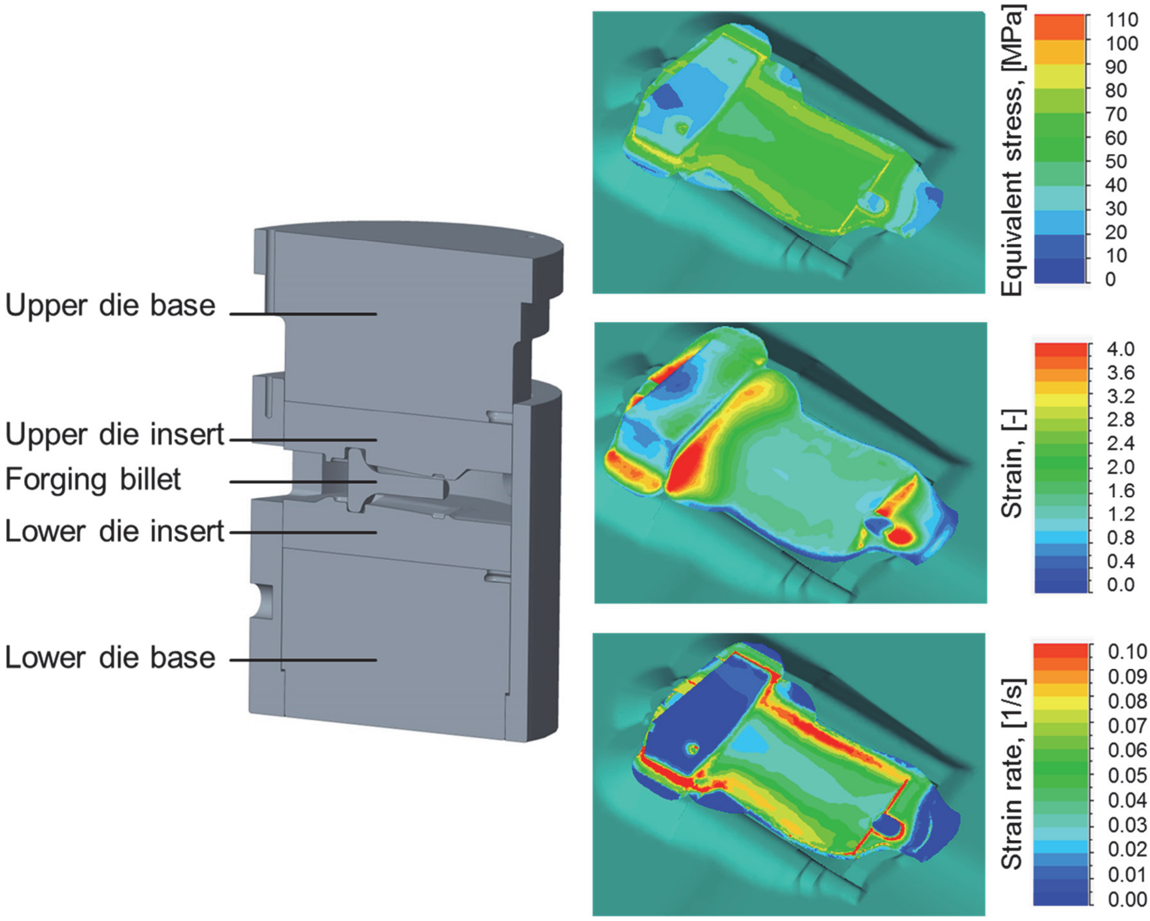


Fig. 4. *FE model of the forging process of the compressor blade from TNB-V4 alloy.*

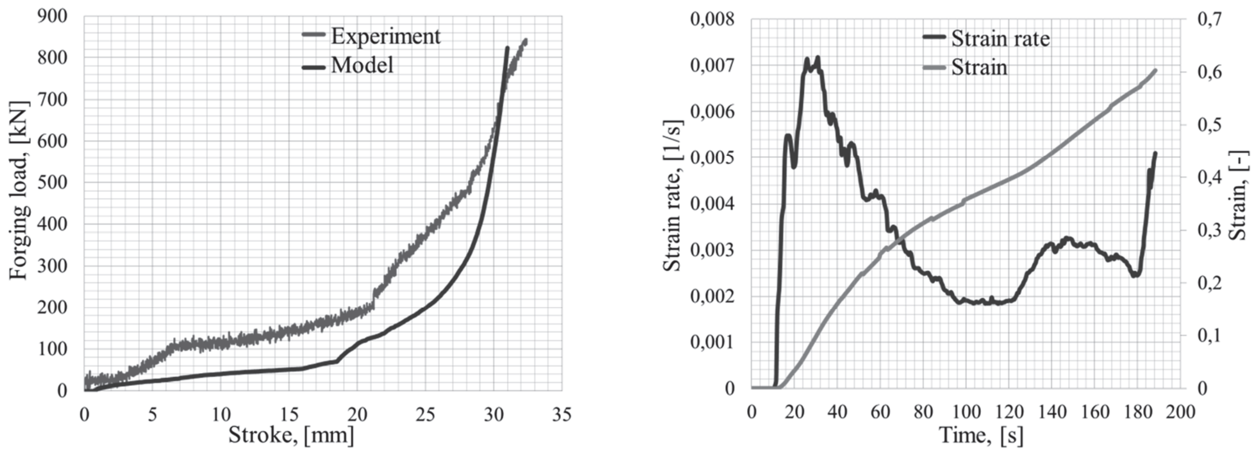


Fig. 5. *(a) Comparison of forging loads and (b) testing conditions for physical simulation in agreement with data history from simulation*

Point	Calculated grain size, μm	Measured grain size, μm
γ-phase	12.71	10.37
β/β_o-phase	12.86	10.24

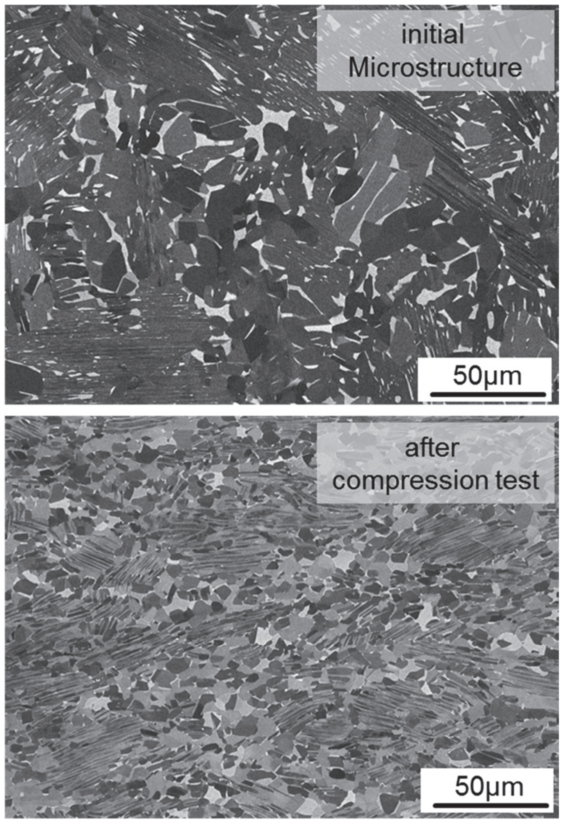


Fig. 6. *Comparison of predicted grain sizes with experimental determined grain sizes*

7. CONCLUSION

The forging process of the TNB-V4 alloy was successfully simulated using the commercial finite element program Q-Form. The results of the simulation may be further used to study the optimal press speed during forging, the loading of the die set and to ensure the required geometry of the final products and the desired microstructure. The following conclusions can be drawn from the present study:

- The proposed model well predicts the flow stresses for the TNB-V4 alloy during hot deformation and predicts the forging force quite accurately
- It also predicts the recrystallized grains size of the recrystallizing phases.
- The forging was carried out successfully without forming defects with the designed process, which shows the capability of the model for process design.

ACKNOWLEDGEMENTS

The authors are grateful to the colleagues from the Chair of Physical Metallurgy and Materials Technology of BTU Cottbus-Senftenberg for the preparation of the metallographic images used in this study.

REFERENCES

Bambach, M., Sizova, I., Bolz S., Weiß, S., 2016, Devising Strain Hardening Models Using Kocks–Mecking Plots—A Comparison of Model Development for Titanium Aluminides and Case Hardening Steel, *Metals*, 6(9), 204.

Beynon, J.H., Sellars, C.M., 1992, Modelling microstructure and its effects during multipass hot rolling, *ISIJ,* 32(3), 359-367.

Blackwell, P.L., Brooks, J.W., Bate, P.S., 1998, Development of microstructure in isothermally forged Nimonic alloy AP1, *Mat. Sci. and Tech*, 14, 1181-1188.

Brooks, J.W., Dean, T.A., Hu, Z.M., Wey, E., 1998, Three-dimensional finite element modelling of a titanium aluminide aerofoil forging, *J. of Mater. Proc. Tech.*, 80-81, 149-155.

Cheng, L., Xue, X., Tang, B., Kou, H., Li, J., 2014, Flow characteristics and constitutive modeling for elevated temperature deformation of a high Nb containing TiAl alloy, *Intermetallics*, 49, 23-28.

Cingara, A., McQueen, H.J., 1992, New formula for calculating flow curves from high temperature constitutive data for 300 austenitic steels, *J. Mater. Proc. Tech.*, 36, 31-42.

Clemens, H., Kestler, H., 2000, Processing and applications of intermetallic γ-TiAl based alloys, *Adv. Eng. Mater.,* 2, 551–570.

Clemens, H., Smarsly, W., 2011, Light-weight Intermetallic Titanium Aluminides – Status of Research and Development, *Adv. Mater. Research*, 78, 551-556.

Godor, F., Werner, R., Lindemann, J., Clemens, H., Mayer, S., 2015, Characterization of the high temperature deformation behavior of two intermetallic TiAl–Mo alloys, *Mat. Sc. Eng. A*, 648, 208-216.

Kim, H.Y., Hong, S.H., 1999, Effect of microstructure on the high-temperature deformation behavior of Ti-48Al-2W intermetallic compounds, *Mater. Sci. and Eng. A*, 271, 382-389.

Laasraoui, A., Jonas, J.J., 1991, Prediction of steel flow stresses at high temperatures and strain rates, *Metall. Mat. Trans. A*, 22(7), 1545-1558.

Millett, J.C.F., Brooks, J.W., Jones, I.P., 1999, Assessment and modelling of isothermal forging of intermetallic compounds Part 1 – TiAl, *Mat. Sci. and Tech.*, 15, 697-704.

Schmoelzer, T., Liss, K.-D., Kirchlechner, C., Mayer, S., Stark, A., Peel, M., Clemens, H., 2013, An in-situ high-energy X-ray diffraction study on the hot-deformation behavior of a β-phase containing TiAl alloy, *Intermetallics*, 39, 25-33.

Schwaighofer, E., Clemens, H., Lindemann, J., Stark, A., Mayer, S., 2014, Hot-working behavior of an advanced intermetallic multi-phase γ-TiAl based alloy, *Mater. Sci. and Eng. A*, 614, 297-310.

Semiatin, S.L., Frey, N., El-Soudani, S.M., Bryant, J.D., 1992, Flow Softening and Microstructure Evolution during Hot Working of Wrought Near-Gamma Titanium Aluminides, *Metalurgical Trans. A*, 23, 1719-1735.

Semiatin, S.L., Frey, N., Thompson, C.R., Bryant, J.D., 1990, Plastic flow behaviour of Ti-48A1-2.5Nb-0.3Ta at hot-working temperatures, *Script. Met. et Mater.*, 24, 1403-1408.

Semiatin, S.L., Seetharaman, V., Ghosh, A.K., 1999, Plastic flow, microstructure evolution, and defect formation during primary hot working of titanium and titanium aluminide alloys with lamellar colony microstructures, *Phil. Trans. R. Soc. Lond. A*, 357, 1487-1512.

Semiatin, S.L., Seetharaman, V., Weiss, I., 1998, Hot workability of titanium and titanium aluminide alloys—an overview, *Mater. Sci. and Eng. A*, 243, 1-24.

Tetsui, T., Shindo, K., Kaji, S., Kobayashi, S., Takeyama, M., 2005, Fabrication of TiAl components by means of hot forging and machining, *Intermetallics*, 13, 971-978.

Werner, R., Lindemann, J., Clemens, H., Mayer, S., 2014, Constitutive Analysis of the Flow Curve Behavior of an Intermetallic β-solidifying γ-TiAl-based Alloy and Microstructural Characterization of the Deformed State, *BHM Berg- und Hüttenmännische Monatshefte*, 159 (7), 286-288.

MODELOWANIE METODĄ ELEMENTÓW SKOŃCZONYCH GLINKÓW TYTANU

Streszczenie

Plastyczna przeróbka na gorąco jest ważnym procesem pozwalającym nadawać kształt i kontrolować własności wyrobów z glinków tytanu. Dynamiczna rekrystalizacja i przemiany fazowe odgrywają kluczową rolę w kształtowaniu końcowej wielkości ziarna i, w konsekwencji, własności mechanicznych wyrobu. Ponieważ glinki tytanu wymagają kucia w warunkach izotermicznych, potrzebny jest dokładny model rozwoju mikrostruktury aby umożliwić optymalizację czasu trwania procesu i aby uniknąć przeciążenia matryc. W niniejszej pracy proces kucia łopatki kompresora został zamodelowany metodą elementów skończonych (MES) z wykorzystaniem programu Q-Form. Badanym materiałem był stop TNB-V4 (Ti–44.5Al–6.25Nb–0.8Mo–0.1B, at. %). W pracy przedstawiono zastosowany model rozwoju mikrostruktury. Model został skalibrowany na podstawie wyników prób ściskania na gorąco w warunkach izotermicznych. Badania przeprowadzono w temperaturach w zakresie 1150°C - 1300°C i dla prędkości odkształcenia w zakresie 0.001 s^{-1} d 0.5 s^{-1}. Całkowite odkształcenie w tych próbach wynosiło 0.9. Wyznaczone doświadczalnie naprężenie uplastyczniające zostało opisane za pomocą prędkości umocnienia zgodnie z krzywymi Kocksa-Meckinga. Fizyczny proces kucia łopatki kompresora został wykorzystany do walidacji modelu MES.

Received: November 25, 2016
Received in a revised form: December 21, 2016
Accepted: January 2, 2017