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Advanced Material Models of Titanium Alloys Ti-6Al-4V ELI and Ti-13Nb-13Zr for Severe Plastic Deformation *-Explanation of the Data Sets-*

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Accurate modeling of material behavior is essential for realistic FEM simulations. This article presents advanced material models for the titanium alloys Ti-6Al-4V ELI and Ti-13Nb-13Zr. These models take into account temperature (20°C < T < 800°C), degree of deformation (0.5 < φ < 1.5), and strain rate (0.1 1/s < $\dot{\varphi}$ < 100 1/s). The models also consider the effects of strain hardening, strain rate sensitivity, and thermal softening, based on El-Magd's et al. constitutive material model. The models are validated by forge-like cylinder compression tests. They are intended for severe plastic deformation and forming processes of titanium alloys with high strains and strain rates at elevated temperatures.

Keywords: Ti-6Al-4V ELI, Ti-13Nb-13Zr, titanium alloys, material model, severe plastic deformation

Introduction

Accurate modeling of material behavior is crucial for realistic FEM simulations, particularly when designing forming processes with high strains and strain rates. This is especially important for severe plastic deformation processes, which can produce fine-grained titanium alloys. Such materials are of great interest for medical technology applications, as they enable biomechanically optimized implants. The authors aim to comprehend the multiphysical relationships among process parameters, material behavior, and microstructure evolution during severe plastic deformation under high strains, high strain rates, and elevated temperature. This comprehension will enable the production of nanostructured semi-finished products for medical implants. This explanation deals with the material models and data sets established for the research.

Material and Methods

The chemical compositions of Ti-6Al-4V ELI (Ti-64 ELI) and Ti-13Nb-13Zr (TNZ) titanium alloys are listed in Table 1. Ti-64 ELI is a first-generation medical titanium alloy that is commonly used and meets the quality standards of ASTM F136. It is available on the market in diameters of 10 mm round bars. TNZ is a second-generation medical titanium alloy that is standardized as medical implant material according to the ASTM F1713 standard. The material can be obtained from sources outside the EU, but it is important to note that there are significant variations in quality between different batches and manufacturers [8]. Therefore, to ensure consistency, the TNZ material used in this study is melted into 50 mm diameter ingots at *GfE Metalle und Materialien GmbH* in Nuremberg, Germany.

Table 1: Chemical composition of the titanium alloys in wt%, manufacturer data

		elements									
		Ti	Nb	Zr	Al	V	Fe	C	H	N	O
alloy	Ti-64 ELI	balance	-	-	6,01	3,97	0,17	0,02	-	0,01	0,12
	TNZ	balance	13,21	12,89	-	-	0,022	0,014	0,003	0,003	0,065

These ingots are then reduced to a diameter of 10 mm at *GFM GmbH* in Austria using radial forging with intermediate annealing to prevent adiabatic shear band formation due to strong work hardening.

The material behavior is determined through tensile tests conducted in accordance with DIN EN ISO 6892-1 [3] using the *Zwick/Roell AllroundLine* universal tensile testing machine. Strains are recorded using a video extensometer, and at least three specimens are tested. It is important to note that the elongation at break may be underestimated due to off-centre specimen breakage, and therefore is measured manually. To analyze the compression stress state and to achieve a higher degree of deformation, cylinder compression tests are conducted following DIN 50106 [4]. The tests utilize a chamber furnace and a press equipped with heatable tools, force and temperature measurement (fig. 1A). The specimen are cylinders with a diameter of 15 mm and a height of 15 mm (fig. 1B). They are compressed by the press die (fig. 1C). Deformation localisation and shear band cause damage at high strain rate and/or low temperatures (fig. 1D).

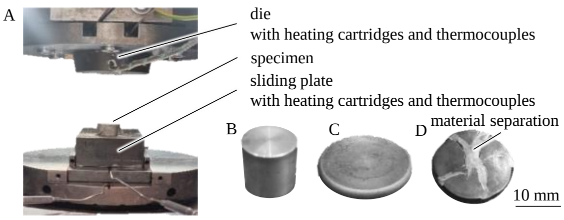

Figure 1: The test setup for forging-like cylinder compression tests (A), cylinder specimen (B), forged specimen (C), and separation by shear bands (C).

The parameters for the forging-adapted process are as follows:

- temperature (20°C < T < 800°C)
- degree of deformation (0.5 < φ < 1.5)
- strain rate (0.1 1/s < $\dot{\varphi}$ < 100 1/s)

In addition, the coefficient of friction can be can determined with this setup (fig. 2). The sample is compressed with a defined force until plastic deformation occurs. This is followed by the sliding process, in which the sliding plate is moved under the load of the compressed material sample at a defined speed. The required friction force is measured. The coefficient of friction μ between the material sample and the material of the sliding plate can then be determined from the compression and friction force. [9]

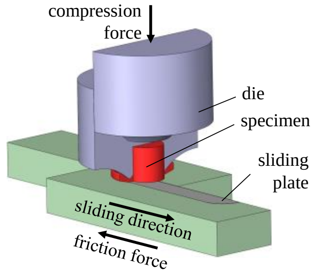

Figure 2: Sliding compression test. [9]

The coefficient of friction depends on the contact normal stress / compression force, the temperature and the sliding speed. This test is only determined for two conditions for TNZ, which is the subject of the main investigations: dry and with MoS_2 lubrication, force of 30 kN, temperature of 300°C and 10 mm/s sliding speed.

Constitutive modelling for material flow curves

El-Magd et al. conducted comprehensive research to describe the material behavior at high strains and strain rates at different temperatures, focusing on constitutive modeling for material flow curves. The materials were analyzed by performing split Hopkinson bar tests to determine their flow behavior at high strain rates and elevated temperatures. [1]

The data suggests that titanium alloys, such as Ti-64 ELI, experience dynamic stress relaxation when undergoing plastic deformation at high temperatures. El-Magd's constitutive material model and Swift's solidification function can be used to describe the flow curves with the material parameters shown in table 2 as follows [2]:

$$\sigma = \frac{\sigma_0}{\left[1 + \left(\frac{\sigma_0}{\sigma^*}\right)^{v} * e^{\frac{T}{T^*}} * \frac{\dot{\varepsilon}^*}{\dot{\varepsilon}} * \varepsilon\right]^{\frac{1}{\vartheta}}}$$

The yield stress is a function of stress, strain rate and temperature [2]:

$$\sigma_0 = (\sigma_h * \dot{\varepsilon}^m * \varepsilon^n + \eta * \dot{\varepsilon}) * \Psi(T)$$

With the experimentally determined temperature function [2]:

$$\Psi(T) = \left[e^{-\frac{T}{T_1}} + A^* * e^{-\left(\frac{T}{T_2}\right)^{\mu}}\right]$$

In order to transfer the material model into a simulation program, the strain ε is converted into

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the degree of deformation φ using the following equation [5]:

$$\varphi = \ln(\varepsilon + 1)$$

Implementation of the data in FEM

The simulation is set up using experimental, literature, and constitutive data. Table 3 shows the material properties.

The data sets shown in the figures 3 and 4 represent the flow curves of Ti-64 ELI and TNZ for the temperatures (20°C, 200°C, 400°C, 800°C) and strain rates (0.1 1/s, 1 1/s, 10 1/s, 100 1/s) and plastic strain (0.5 to 1.5).

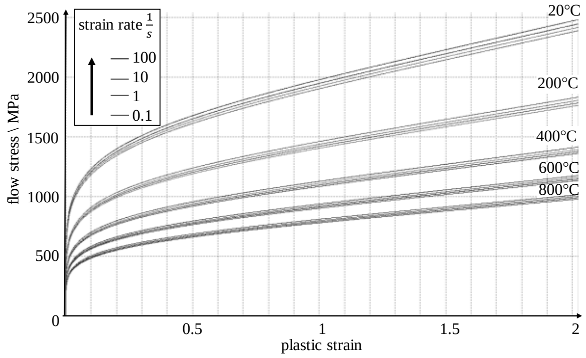

Figure 3: Flow curves of Ti-64 ELI depending on strain rate and temperature.

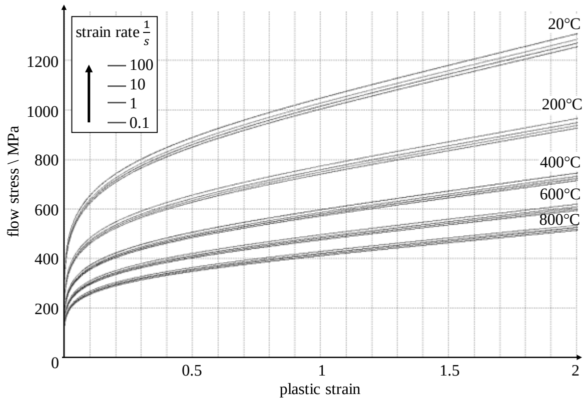

Figure 4: Flow curve of TNZ depending on strain rate and temperature.

Table 3: Material properties of the titanium alloy Ti-6Al-4V ELI and Ti-13Nb-13Zr samples

			alloy: Ti-64 ELI	alloy: TNZ
properties	density	kg/m^3	4430	5294
	Poisson's ratio [10]	-	0.34	0.34
	yield strength	$R_{p0.2}$ \ MPa	1083	-
	tensile strength	R_m \ MPa	1119	632
	elongation at break	A \ %	12	24
	young's modulus	E \ GPa	114	58
	thermal conductivity [2]	W/m K	7.1	7.1
	specific heat capacity [2]	J/kg K	560	560
	thermal expansion coefficient [10]	1/K	9.2 x10^{-6}	9.2 x10^{-6}
	β - transus temperature	T_β \ °C	985 ± 15	720 ± 15

Figure 5 depicts the data from the sliding compression tests, resulting in a friction coefficient of μ = 0.12 under the given tribological load spectrum.

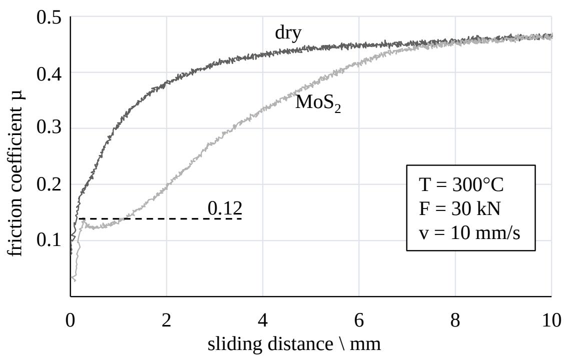

Figure 5: Sliding compression test of TNZ, dry and with MoS_2 lubricant.

Validation and conclusion

The material models for Ti-64 ELI and TNZ are validated both thermally and geometrically. The forming process is observed using a thermal camera (see fig. 6A) and compared with the simulated temperatures using simufact forming (see fig. 6B). The forged specimen is then measured using a 3D scan (GOM ATOS 5) and compared with the simulated geometry.

Table 2: Material parameters for the modelling of flow curves based on [2]

		parameter of the constitutive model										
		σ^* MPa	σ_h MPa	m -	n -	η MPa s	T^* K	A -	T_1 K	T_2 K	$\dot{\varepsilon}^*$ $1/s$	ϑ -
alloy	Ti-64 ELI	1	1119	0.005	0.17	0.0599	111	0.52	346	128	$2.07 * 10^{-27}$	3.7
	TNZ	1	632	0.005	0.17	0.0599	111	0.52	346	128	$2.07 * 10^{-27}$	3.7

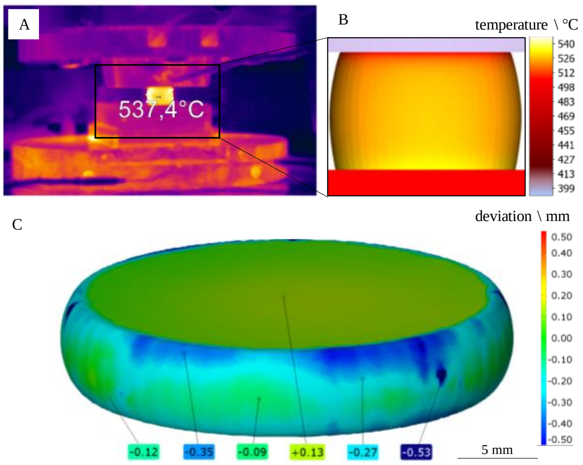

Figure 6: Thermal observation (A) and simulation (B) were performed on forged Ti-64 ELI and TNZ samples, which were also subjected to 3D scanning (C)

Both, the thermal and geometric validation show only minor deviations, indicating that the material model is suitable for simulating severe plastic deformation or forging-like processes with high strains and strain rates at elevated temperatures.

Authorship note and acknowledgments

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References

[1] El-Magd, E.; Treppmann, C.; Korthäuer, M. (2005): Experimentelle und numerische Untersuchung zum thermomechanischen Stoffverhalten, Seite 192ff. In: Tönshoff, H. K.; Hollmann, C.: Hochgeschwindigkeitsspanen metallischer Werkstoffe. Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim

[2] El-Magd, E.; Abouridouane, M. (2006): Characterization, modelling and simulation of deformation and fracture behaviour of the light-weight wrought alloys under high strain rate loading, In: International Journal of Impact Engineering, DOI: 10.1016/2005.03.008.

[3] DIN EN ISO 6892-1:2020-06; Metallic materials - Tensile testing - Part 1: Method of test at room temperature, 2019

[4] DIN 50106:2016-11; Testing of metallic materials - Compression test at room temperature, 2016

[5] Simufact Engineering GmbH: Info-Sheet Fließkurven. Hamburg, 2021.

[6] Klinge, L.; Kluy, L.; Spiegel, C.; Siemers, C.; Groche, P.; Coraça-Huber, D. (2023): Nanostructured Ti-13Nb-13Zr alloy for implant application - material scientific, technological, and biological aspects. In: Frontiers in Bioengineering and Biotechnology, 11, Frontiers, ISSN 2296-4185, DOI: 10.3389/fbioe.2023.1255947

[7] Kraus, S. O.; Kluy, L.; Groche, P. (2023): Production of fine-grained Ti-6Al-4V ELI for medical implants using equal-channel-angular-swaging. In: Production at the leading edge of technology, Congress of the German Academic Association for Production Technology (WGP), Springer, ISBN 978-3-031-47394-4, DOI: 10.1007/978-3-031-47394-4_60

[8] Klinge, L.; Siemers, C.; Kluy, L.; Groche, P. (2022): Nanostructured Ti-13Nb-13Zr for dental implant applications produced by severe plastic deformation. In: Journal of Materials Research, Springer, e-ISSN 1092-8928, DOI: 10.1557/s43578-022-00587-1

[9] Sliding compression test, Institute for Production engineering and Forming Machines (2024), Website

[10] ASM Matweb (2024), Website