



**22. Workshop  
Composite Forschung in der Mechanik  
3. Forum Metallplastizität  
01. und 02. Dezember 2009  
Paderborn, Liborianum**

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o. Prof. em. Dr. rer. nat. K. P. Herrmann,  
LTM, Universität Paderborn

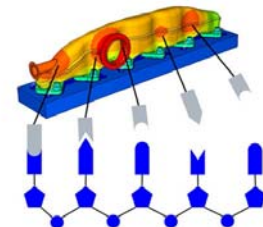
Prof. Dr.-Ing. T. Böhlke  
o. Prof. Dr.-Ing. E. Schnack,  
ITM, Universität Karlsruhe (TH)

Prof. Dr.-Ing. O. Wunsch  
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Prof. Dr. rer. nat. B. Nestler  
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DFG Sonderforschungsbereich  
Transregio 30



GRADUATE SCHOOL 1483

Process Chains in Production:  
Interaction, Modelling and Assessment of Process Zones



## 22. Workshop

### Zielsetzung der Veranstaltung

Das makroskopische Materialverhalten von Werkstoffen resultiert von deren Mikrostruktur und thermomechanischen Eigenschaften. Für die Entwicklung neuer Werkstoffe müssen spezielle Mikrostrukturen realisiert werden, die sensitiv von der thermomechanischen Prozessführung beim Herstellungsprozess abhängen. Beispielhaft seien funktional gradierte Werkstoffe und hochfeste Stähle genannt.

Ziel des Workshops ist, aktuelle Fragestellungen der Werkstoffmechanik unter Berücksichtigung der Mehrskaligkeit und thermomechanischer Kopplungen zu diskutieren. Dabei stehen sowohl methodisch grundlegende Fragestellungen der Modellierung im Vordergrund als auch aktuelle Entwicklungen in der Prozess- und Werkstofftechnologie. Weiterhin werden aktuelle Entwicklungen bei Simulationsmethoden zur Beschreibung, Bewertung und Optimierung von Bauteilzuständen in verketteten Fertigungsprozessen thematisiert.

Ermöglicht durch die freundliche Unterstützung  
des DFG-Sonderforschungsbereichs  
Transregio 30



## 22. Workshop Composite Forschung / 3. Forum Metallplastizität

*A joint workshop of the DFG Graduiertenkolleg 1483  
and the DFG Sonderforschungsbereich Transregio 30*

### Program

**Tuesday, December 01, 2009**

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**9.00            Opening**

#### **Polycrystalline Materials**

(Chairman: Mahnken)

09:10-09:50 **S. Berbenni**: Internal length scale effects on the overall behavior of polycrystals

09:50-10:20 **S. Wilmanns, R. Mahnken**: Numerical implementation of a micromechanical multi variant model for textured polycrystalline shape memory alloys

#### **Process simulation of functional graded materials**

(Chairman: Wunsch)

10:20-10:50 **A. Güzel, A. Jäger, N. B. Khalifa, A. E. Tekkaya**: Simulation der Abschreckempfindlichkeit von Aluminiumlegierung 6082

10:50-11:15 Coffee break

11:15-11:45 **T. Kayser, F. Parvizian, B. Svendsen**: Experimental and theoretical investigation of the microstructural evolution in aluminium alloys during extrusion

11:45-12:15 **A. Schneidt, R. Mahnken**: Modellierung der martensitischen und der bainitischen Umwandlung

**12:15-14:00    Lunch**

(Chairman: Berbenni)

14:00-14:40 **F. D. Fischer, J. Svoboda, D. Vollath**: Formation of hollow nanospheres from metallic solid nanospheres

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**Tuesday, December 01, 2009**

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**Process chains in sheet metal manufacturing**

(Chairman: Böhlke)

14:40-15:10 **S. Schendel, R. Möning, O. Kraft:** Deformation behavior of small steel samples with dimensions in the micro- and submicron range

15:10-15:35 **P. Bienger, D. Helm:** Microstructure evolution during rolling and annealing of high-strength-steels

15:35-16:00 **A. Vondrous, M. Selzer, B. Nestler, M. Jainta:** Performance optimized phase-field simulations of grain structures under the effect of mechanical forces

16:00-16:20 Coffee break

(Chairman: Svendsen)

16:20-16:45 **T. van Phan, K. Jöchen, A. Melcher:** Development of material models for the microstructure evolution during deep drawing

16:45-17:00 **M. Baiker, D. Helm:** Modelling and simulation of deep drawing

17:00-17:25 **M. Senn, N. Link:** Monitoring and control of process behavior

17:25-17:55 **K. Jöchen, T. Böhlke:** Prediction of elastic and inelastic material properties of cubic crystal aggregates by semi-analytical homogenisation

18:30 Dinner in the Liborianum

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**Wednesday, December 02, 2009**

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**Combinations of different manufacturing processes for solid components**

(Chairman: Schulze)

- 8:45-9:15 **H. Meier, R. Pabst, V. Schulze**: Process chains in production
- 9:15-9:40 **D. Stancheva, M. Schwenk, J. Hoffmeister, V. Schulze**: Simulation of heat treatment processes
- 9:40-10:05 **J. Osterried, F. Zanger, V. Schulze**: Chip formation simulations in hard machining
- 10:05-10:30 **C. Qin, B. Nestler**: A multiphase-field simulation for carbon diffusion in austenite
- 10:30-10:45 Coffee break

**Strain Localization and Heterogenous Materials**

(Chairman: Fischer)

- 10:45-11:15 **V. Palnau**: Anwendung eines netzfreien Diskreditierungsverfahrens auf die Scherbandanalyse
- 11:15-11:45 **K. Weinberg, D. Anders**: Simulation von Entmischungsvorgängen in zweiphasigen Legierungen
- 11:45-12:15 **F. Fritzen, T. Böhlke**: Nonuniform Transformation field Analysis of Materials with anisotropic microstructure
- 12:15 Closure



## **ABSTRACTS**

## MODELLING AND SIMULATION OF DEEP DRAWING

*M. Baiker, D. Helm*

**Fraunhofer Institute for Mechanics of Materials IWM**

### **Abstract**

Regarding the process chain of sheet metal manufacturing, the last processing step is often performed by deep drawing. The design of an optimal deep drawing process is very complex. For example, spring back compensation requires an optimized shape of the tool. Additionally, the blank holder forces or beads must be appropriate in order to avoid damage and wrinkling. Simulation is an established tool to avoid long adjusting times of the deep drawing tools. Therefore an overall goal of the project is the development of advanced material models to improve the simulation. The results of the simulation allow making reliable predictions of adequate process parameters as blank holder forces appearing in the process. As the deep drawing process is settled at the end of the process chain, the microstructure of the sheets exhibits anisotropic behaviour due to the previous process steps. Moreover, deep drawing involves large strains and several strain path changes. Therefore, the anisotropy develops during the deep drawing process [2] and also the Bauschinger effect is an important issue. Adequate material models should take this behaviour into account.

Different experiments are carried out to investigate the behaviour of the material. Tension tests as well as tension-compression tests on thin sheets are performed to measure the stress-strain curves and to determine the r-values. Draw bending tests of sheet strips are used to investigate the spring back behaviour. Some of the experimental results are used to fit the parameters of the material model.

In a first approach an established phenomenological plasticity model [1] is used to describe the material behaviour. The model includes a combination of isotropic and kinematic hardening. For the kinematic hardening multiple Armstrong-Frederick-terms are used. For first investigations, the model is applied to DC04, which is a typical deep drawing steel. The comparison of simulation results and experimental data will be presented as well as the influence of the friction parameter will be studied.

### **Literature**

- [1] Krasovskyy, A., "Verbesserte Vorhersage der Rückfederung bei der Blechumformung durch weiterentwickelte Werkstoffmodelle", Karlsruhe, 2005.
- [2] Walde, T., "Modellierung der Textur- und Anisotropieentwicklung beim Walzen – Kopplung der Finite Elemente Methode mit mikrostrukturbasierten Modellen", Karlsruhe, 2004.



## INTERNAL LENGTH SCALE EFFECTS ON THE OVERALL BEHAVIOR OF POLYCRYSTALS

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### Abstract

A breakthrough in the general hypothesis of spatially homogeneous intragranular fields accepted in mean field approaches based on the classic Eshelby's inclusion problem (Mori-Tanaka, Self-consistent schemes etc) is proposed. Instead of considering uniform intra-granular plastic strains as usually prescribed in mean field approaches, intragranular slip patterns are modeled in single slip configurations both by distributions of coaxial circular glide loops [1] and by distributions of flat ellipsoids (also called oblate spheroids) [2]. Both types of modeling assume slip configurations constrained by spherical grain boundaries, and, mechanical interactions between slip bands are taken into account (for mechanical fields and elastic energy). Here, distributions are restricted to be periodic considering constant slip line spacing, but, other types of distributions can be studied without any further difficulties. It is then found that intra-granular mechanical fields strongly depend on the grain size and the slip line spacing. In addition, in the case of glide loops, the modeling is able to capture different behaviors between near grain boundary regions and grain interiors. In particular, a grain boundary layer with strong gradients of internal stresses (and lattice rotations) is found. These results are confirmed quantitatively by EBSD measurements carried out with orientation imaging mapping (OIM) on deformed Ni polycrystals and on specific grains undergoing single slip. Furthermore, as a result of the computation of the elastic energy, an average back-stress over the grain (in the case of loops) or over slip bands (in the case of oblate spheroids) can be derived so that it is possible to define new interaction laws for polycrystal's behavior which are naturally dependent on grain size and slip line spacing [2,3]. Hence, using a "diluted" model in terms of concentration of plastic grains, the macroscopic deformation of a fcc polycrystal (e.g. Ni or Cu) at very low plastic strains has been computed either in rate-independent or rate-dependent plasticity. Contrary to conventional mean-field approaches, which are unable to capture internal length scale effects, a grain-size effect on the initial strain hardening stage is reported for both types of configurations.

### References

- [1] S. Berbenni, M. Berveiller, T. Richeton. Intra-granular plastic slip heterogeneities: discrete vs. mean field approaches. *International Journal of Solids and Structures* 45, 4147-4172, 2008.
- [2] C. Collard, V. Favier, S. Berbenni, M. Berveiller. Role of discrete intra-granular slip bands on the strain-hardening of polycrystals. *International Journal of Plasticity*, in press, 2009
- [3] T. Richeton, S. Berbenni, M. Berveiller. Grain-size dependent accommodation due to intragranular distributions of dislocation loops. *Acta Materialia* 57, 1347–1356, 2009

## MICROSTRUCTURE EVOLUTION DURING ROLLING AND ANNEALING OF HIGH-STRENGTH STEELS

*P. Bienger, D. Helm*

Fraunhofer Institute for Mechanics of Materials IWM

### Abstract

After casting, the process chain of products made of sheet metals consists of different forming techniques like hot rolling, cold rolling, deep drawing and final heat treatment operations like annealing. To design and optimize the whole manufacturing process as well as the final product properties, adequate material models and appropriate numerical simulation techniques are required. The project in the Graduiertenkolleg 1483 focuses on the production of sheet metals as semi-finished products. For simplicity, only a part of the process chain will be regarded in the presentation: i.e. the cold rolling process of a hot rolled strip and the annealing procedure. For fundamental studies, a ferritic mild steel DC04, which is a typical steel grade for automotive applications, is analyzed. Therefore, specimens after hot and cold rolling and final annealing are extracted from a real manufacturing process. These samples are intensively investigated in order to study the texture evolution and other material properties.

The texture evolution of a polycrystalline material during cold rolling is modelled in the framework of crystal plasticity in combination with different homogenization concepts. The description of the texture development is hardly possible with classical models, like the Taylor model. Therefore, advanced texture models like the viscoplastic self-consistent model (VPSC, [1]) or the grain interaction model (GIA, [2]) are applied. Computations of these different models are compared with experimentally determined EBSD data to give information about the models' accuracy.

After cold rolling, the strip is annealed in order to obtain a recrystallized grain structure with intended properties like strength and ductility. In contrast to texture evolution during plastic deformation, static recrystallization is very complex due to nucleation and growth processes. Consequently, modelling recrystallization is much more complex (cf. [3]). Therefore, the first experimental recrystallization texture results are analyzed and appropriate modelling strategies are discussed.

### Literatur

- [1] Lebensohn, R. A. ; Tome C. N.: "A self-consistent anisotropic approach for the simulation of plastic deformation and texture development of polycrystals : application to zirconium alloys , Acta metallurgica et materialia, 41 (1993), 2611-2624
- [2] Eisenlohr, P.; Tjahjanto, D.; Hochrainer, T.; Roters, F., Raabe, D.: "Comparison of texture evolution predicted by various grain cluster homogenization schemes", J Mater. Sc., 100 (2009) 500-509.
- [3] Sebald, R. : "Modellierung der Rekristallisationstextur: Wechselwirkung zwischen Keimbildung und Keimwachstum", Aachen (2001)

## FORMATION OF HOLLOW NANOSPHERES FROM METALLIC SOLID NANOSPHERES

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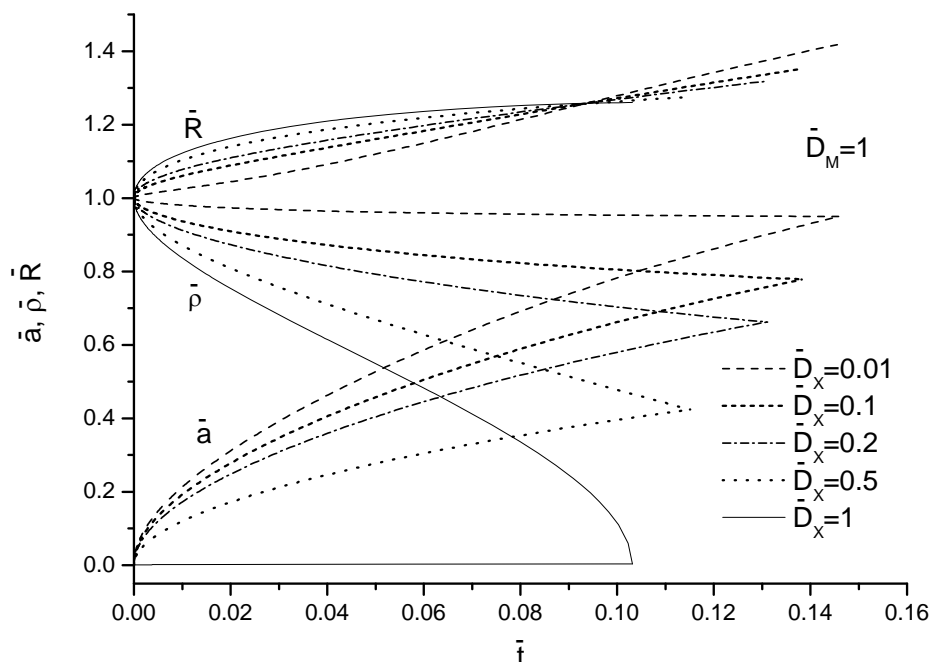
<sup>2</sup>Institute of Physics of Materials, Acad. Sci. Brno, Czech Republic.

<sup>3</sup>NanoConsulting, Stutensee, Germany.

### Abstract

The thermodynamical extremum principle [1], [2] has been successfully applied to understand the high temperature instability of hollow nanospheres [3]. This concept can also be applied to derive a kinetic model for formation of a binary-phase hollow nanosphere from a solid nanosphere, as observed by Nakamura et al. [4]. The formation of the hollow nanosphere is due to reaction of the metallic nanosphere with the non-metallic component in the surrounding atmosphere. The metallic component moves due to self-diffusion to the interface between the inner sphere and the outer ceramic shell, leaving a hollow in the core. From there the metallic component diffuses through this shell. The formation of the hollow occurs, however, under the condition that the diffusion coefficient of the metallic component in the binary phase is higher than that of the non-metallic component. Figure 1 shows diagrams for the dimension-free quantities  $\bar{a}$  (hole radius),  $\bar{\rho}$  (interface radius) and  $\bar{R}$  (outer radius) of the hollow nanosphere as function of the ratio  $\bar{D}_x$  of the diffusion coefficient of the non-metallic component and the metallic component in the outer ceramic shell.

The experimentally observed times to formation of the binary-phase hollow nanosphere agree with those predicted by the model, if the diffusion coefficient of the metallic component in the metallic phase is increased drastically. This can be explained by existence of a significant hydrostatic tensile stress in the metallic nanosphere occurring after the formation of a binary-phase layer on the nanosphere surface. Therefore, a detailed stress analysis of the hollow nanosphere is presented. The results support the idea of a hydrostatic tension stress state in the inner metallic core of severals GPa. Furthermore, this fact is confirmed by the experimental observation that pores appear at the interface between the metallic core and the outer ceramic shell.



**Figure 1: Simulation of kinetics of hollow nanosphere formation for different values of  $\bar{D}_x$ .**

### References

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2. K. Hackl, and F.D. Fischer, On the relation between the principle of maximum dissipation and inelastic evolution given by dissipation potentials, *Proceedings of the Royal Society A*, 464:117-132, 2008.
3. J. Svoboda, F.D. Fischer, and D. Vollath, Modeling of formation of binary-phase hollow nanospheres from metallic solid nanospheres, *Acta Materialia*, 57:1912-1919, 2009.
4. R. Nakamura, D. Tokozakura, J.-G. Lee, H. Mori, and H. Nakajima, Shrinking of hollow  $Cu_2O$  and NiO nanoparticles at high temperatures, *Acta Materialia*, 56:5276-5284, 2008.

# NONUNIFORM TRANSFORMATION FIELD ANALYSIS OF MATERIALS WITH ANISOTROPIC MICROSTRUCTURE

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## Abstract

Most materials applied in engineering practice show specific microstructures at different scales. These microstructures influence the effective material response under loading and are, hence, subject of many experimental and numerical investigations. While the linear elastic properties of materials can efficiently be estimated by either numerical (e.g. [1]) or (semi-) analytical (e.g. [2]) methods, the prediction of physically non-linear effects is a challenging undergoing. Michel and Suquet [3] developed a computational method for the estimation of the physically non-linear behaviour of isotropic two-dimensional materials by introducing so called non-uniform inelastic modes. The methodology has been adapted to the Finite Element Method (FEM) in [4] and applied to materials with three-dimensional quasi-isotropic microstructures with great success.

In this paper we apply the method to materials with anisotropic, three-dimensional microstructure. The evolving anisotropy of the material is examined in terms of subsequent yield surfaces. These are compared to the ones of (quasi-) isotropic micro heterogeneous materials. The homogenized material model is employed in structural problems and the effects of the microtopological anisotropy on the overall behaviour of structures is discussed.

## Literature

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- [4] Fritzen, F., and Böhlke, T., "Homogenization of the physically nonlinear properties of three-dimensional metal matrix composites using the Nonuniform Transformation Field Analysis", *Proceedings of the 17<sup>th</sup> International Conference on Composite Materials*, Edinburgh, Scotland, 2009.

## SIMULATION DER ABSCHRECKEMPFLINDLICHKEIT DER ALUMINIUMLEGIERUNG 6082

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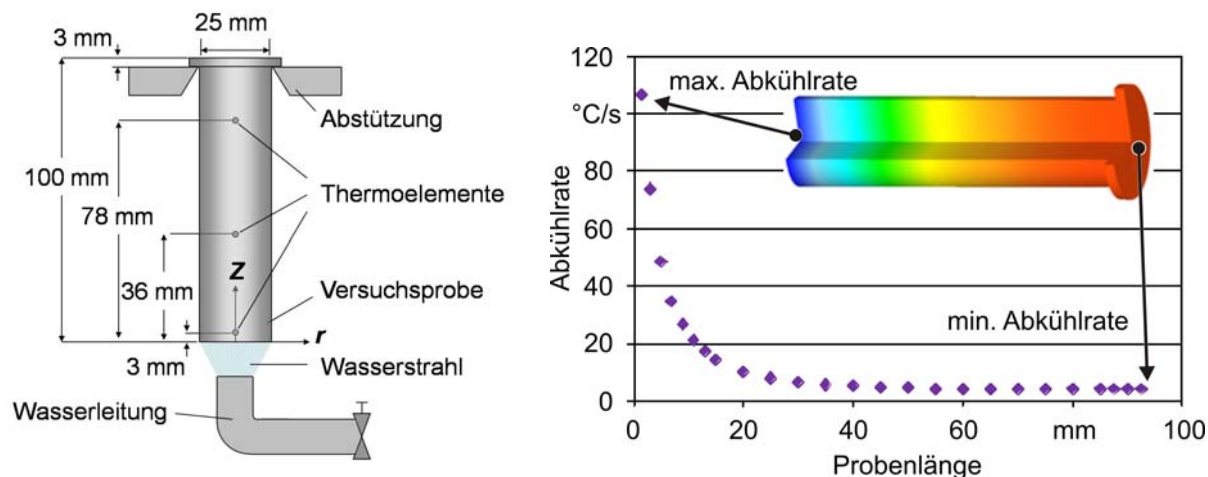
\* entsprechender Autor

**Schlagwörter:** Aluminium, Jominy Test, Finite Element Analyse.

### Abstract

Energieengpässe und daraus folgende umweltbedingte Belange führen zu einem erhöhten Bedarf an Leichtbaustrukturen, besonders in der Automobilindustrie. Stranggepresste Produkte aus aushärtbaren Aluminiumlegierungen des Typs Al-Mg-Si sind hier, auch unter den eingesetzten Leichtbaukonstruktionsprofilen in Fahrzeugen, weitverbreitet. Diese Materialien erreichen ihre geforderten mechanischen Eigenschaften infolge einer Wärmebehandlung nach halbfertiger Herstellung. Unter diesen Gesichtspunkten werden die mechanischen Eigenschaften für diese Aluminiumlegierungen durch eine feinkörnige Mikrostruktur und dem Ausscheiden von Mg<sub>2</sub>Si aus dem Gitteraufbau ermöglicht. Das Ausscheidungshärten spielt neben dem Lösungsglühen, Vergüten und dem Härten eine wichtige Rolle in der Wärmebehandlung [1]. Nach dem Prozess des Warmumformens, des Abschreckens und des Härtens des Metalls, ist die Folge ein feines übersättigtes Korngefüge, welches einen direkten Einfluss auf die letztendlichen mechanischen Eigenschaften wie Härte und Festigkeit besitzt.

Mit der Absicht die Aushärtbarkeit eines Materials zu ermitteln wird die experimentelle Methode des „Jominy Stirnabschreckversuchs“ herangezogen (Abbildung 1). Der Test basiert auf dem Erwärmen eines standardisierten Vollzylinders bis Lösungsglüh-temperatur. Anschließend wird die Probe senkrecht über einen konstanten Wasserstrahl positioniert und nur an der Stirnfläche abgeschreckt. Das Ergebnis ist von der Stirnseite aus fortschreitende Abkühlung in Längsrichtung der Probe. Nachdem die Probe vollständig vergütet wurde, wird diese, zur Ermittlung der maximal erzielbaren Härteeigenschaften des Materials, ausgelagert.



**Abbildung 1: (Links) Jominy-Probe. (Rechts) Simulation der Abkühlrate.**

Im Anschluss werden Härtemessungen an der Oberfläche über die gesamte Probenlänge vorgenommen [2]. Diese Methode wurde ursprünglich für Eisenlegierungen entwickelt. Seitdem wurden bis heute nur wenige Einsatzmöglichkeiten dieser Methode für Nicht-Eisenlegierungen wie Aluminium genutzt.

Die Absicht der derzeitigen Forschung ist die Ermittlung der Beziehung zwischen dem Abkühlverhalten und dem Härteverlauf der Aluminiumlegierung 6082. Es wurde eine Methode zur numerischen Beurteilung der letztendlichen Härteverteilungen von wärmebehandelten Aluminiumlegierungen entwickelt und in konventionale Finite-Elemente Programme implementiert. Zudem wurden Jominy Stirnabschreckversuche herangezogen um die Abschreckempfindlichkeit der Aluminiumlegierung EN AW-6082 zu bestimmen. Die Härteverteilung in der Legierung konnte nach den Versuchen auf den Abkühlverlauf zurückgeführt werden. Die daraus her leitbare Beziehung wurde zwecks der industriellen Anwendungsmöglichkeiten mittels lokaler Wärmebehandlung für Crashenergie absorbierende Bauteile erforscht. Numerische Vorhersagen wurden mit experimentellen Messungen validiert. Zudem wurden die Effektivität der abgeleiteten Methode und mögliche Verbesserungen diskutiert.

## Literatur

- [1] Totten G. E., Mackenzie D. S., "Handbook of Aluminum", CRC Press, New York, 2003.
- [2] Dolan G.P., Flynn R.J., Tanner D.A., Robinson J.S., Quench factor analysis of aluminum alloys using the Jominy end quench technique, Mater. Sci. Eng. 21 (6) (2005), pp. 687–691.

# PREDICTION OF ELASTIC AND INELASTIC MATERIAL PROPERTIES OF CUBIC CRYSTAL AGGREGATES BY SEMI-ANALYTICAL HOMOGENIZATION

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## Abstract

The macroscopic material behavior of crystalline materials is significantly influenced by the constitutive behavior of the grains but also by the texture induced by the manufacturing process. Therefore it is required to incorporate microstructural information into the evaluation schemes in order to accurately predict the macroscopic material response of crystalline aggregates.

In this contribution, the prediction of the self-consistent homogenization method [1,2] with regard to the effective material response of face-centered cubic crystal aggregates is analyzed and compared to results obtained by full field simulations.

The main focus is on the examination of the effect of the grain morphology and the crystallographic texture on the macroscopic elastic and inelastic material behavior of the microheterogeneous material. Both kinds of texture can be introduced in the self-consistent method and in the finite element full field simulations, which are based on Voronoi tessellations to generate the microstructure [3]. By using uniform and non-uniform orientation distribution functions and also isotropic and anisotropic Voronoi tessellations, we are able to clearly separate or combine the impact of the different types of texture. For the elastic as well as for the inelastic behavior of rolled sheets it is shown that the effect of crystallographic texture plays a major role compared to the one of the morphological texture. The influence of the latter is though observable.

## Literatur

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## EXPERIMENTAL AND THEORETICAL INVESTIGATION OF THE MICROSTRUCTURE OF ALUMINUM ALLOYS DURING EXTRUSION

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### Abstract

The purpose of this work is the investigation of the material behavior of aluminum alloys during extrusion and cooling. In particular, the alloys of the 6000 series (Al-Mg-Si) and 7000 series (Al-Zn-Mg) are relevant here, which are commonly used in automotive and aircraft industries. Under the high temperature conditions during extrusion, the material behavior of these alloys is controlled mainly by dynamic recovery during the forming process and static recrystallization during cooling. To simulate the material behavior and microstructural evolution during the process a thermoelastic viscoplastic material model is used. This model depends on the microstructural variables grain misorientation and subgrain size. Both parameters can be directly accessed by use of the Electron Backscatter Diffraction (EBSD) method. Beside the commercial Orientation Imaging Microscopy (OIM) software an additional program is developed to produce microstructure images based on EBSD data and to perform statistical investigations.

In this work a block of Al6060 is partly extruded and afterwards cut over the length to determine the material flow into the die. Several points are measured with the EBSD method along the material flow path in the center of the specimen. The graphical and statistical analysis of the EBSD data shows in detail the microstructural evolution and the development of textures in the profile which has also been simulated with the commercial FE solver ABAQUS.

## PROCESS CHAINS IN PRODUCTION / PROZESSKETTEN IN DER FERTIGUNG

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### **Abstract**

The increase of product quality at reduced production times and minimized costs can nowadays not only be realized by optimizing single manufacturing processes but by the holistic examination of the process chain. Research Area B examines the process chain of an solid component, represented by a shift collar which is used in automotive gearings. Project part B1 is aimed to optimize process management of the process steps during soft and hard broaching.

The shift collars geometry is at first simplified from the original tooth structure and demonstrated by an off-site broaching process. Afterwards the verifications will be created on a realistic geometry with the intended inner broaching process on the rotary symmetric shift collar. The necessary process parameters will be determined experimentally and through a parameter variation a wide data base is created to develop a simulation model. The component's conditions are being analyzed after the broaching process concerning residual stresses and dimensional change (distortion) and are applied with cutting forces and tool changes (i.e. wear) to the simulation model.

## CHIP FORMATION SIMULATIONS IN HARD MACHINING

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### **Abstract**

Broaching of hardened steels is one of the sub-processes of the process-chain examined in Graduate School 1483. This topic aims at predicting the surface layer conditions, like residual stresses and distortion, after hard machining within the process chain. A hard machining strategy with minimal machining effort will be developed consequential for best possible surface layer and component conditions.

Therefore the broaching of hardened materials is mapped to simulation, based on the component characteristics resulting from preceding heat treatment. In doing so, the component's machining history is taken into account when simulating broaching within the process chain.

Based on a global view of the component at heat treatment, it is crucial to transfer quantities specifying component state to a local mesh for chip forming simulations. Input data from heat treatment simulation have to be implemented to describe the actual component condition before hard machining. This condition has then to be set as an accurately defined initial state for the hard machining simulation. Defining the initial state is of great importance for simulations within the process chain, as the sub-processes are linked by inheriting the respective component conditions like residual stress behaviour. Therefore appropriate techniques have to be provided.

For the development of the machining strategy, simulations with varied process parameters can be triggered consequently. At the end of the hard machining simulation process the present output quantities have to be translated into a global mesh of the three-dimensional component.

# ANWENDUNG EINES NETZFREIEN DISKRETISIERUNGS- VERFAHRENS AUF DIE SCHERBANDANALYSE

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## Kurzfassung

Die Eignung netzfreier Methoden für die numerische Analyse materieller Instabilitäten wird geprüft. Hierzu wird ein auf der *Moving Least Squares Approximation* [1] basierendes Diskretisierungsverfahren implementiert.

Die Grundlage für die numerischen Studien endlicher elasto-plastischer Deformationen bildet das Energiekriterium für stabile Deformationsprozesse [2], [3]. In Verbindung mit einem zeitunabhängigen, inkrementell nichtlinearen Materialmodell wird der stabile Deformationspfad beim Auftreten einer Bifurkation automatisch ermittelt. Als ein geeignetes Materialmodell wird die  $J_2$  corner theory [4] verwendet.

Es wird gezeigt, dass das implementierte Verfahren mit netzunabhängigen Ansatzfunktionen zum Zeitpunkt des Elliptizitätsverlustes einer homogenen Deformation die theoretisch vorhergesagte Ausbildung von Scherbändern gut approximiert. Sowohl der Zeitpunkt der ersten Bifurkation als auch die Orientierung der dann entstehenden Lokalisierungsänderungen des diskreten Systems stehen in guter Übereinstimmung mit den theoretischen Vorhersagen für das Kontinuum. Für die räumliche Diskretisierung des Grundgebietes können dabei nahezu beliebige, insbesondere unstrukturierte Stützstellenverteilungen genutzt werden.

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## A MULTIPHASE-FIELD SIMULATION FOR CARBON DIFFUSION IN AUSTENITE "PROCESS CHAINS IN PRODUCTION"

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### **Abstract**

In production, the hardening by carbonization from the free surface of a component is an important manufacturing process. Carbon diffuses from the free surface into the austenitized body of the workpiece. The diffusion is simulated using the multicomponent multiphase field method [1]. The model is capable to consider both, the diffusion in the bulk grain regions as well as an enhanced diffusion along the grain boundaries. To set up the simulations, material constants and free energies of the system have to be defined. The necessary thermodynamical values for the sub-regular solution of the free energy density formulation are derived applying the thermodynamical database Calphad. Two and three dimensional simulations of the diffusion in the polycrystalline austenite are presented. The final carbon concentration field delivers the required data for pre-processing the subsequent computation of the phase transformation from austenite to martensite during cooling.

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## DEFORMATION BEHAVIOR OF SMALL STEEL SAMPLES WITH DIMENSIONS IN THE MICRO- AND SUBMICRON RANGE

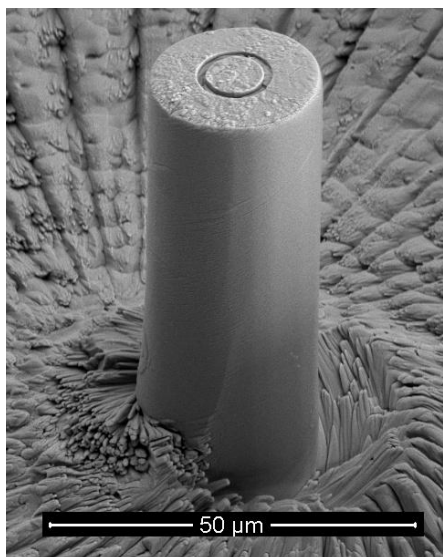
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### Abstract

Deep drawing steels are important materials in many fields. For example they are commonly used in the automotive industry. Often the process chain for manufacturing consists of a combination of individual processes which can have a significant influence on the mechanical and microstructural properties of the final product. Examples for such process steps are rolling, heat treatment or deep drawing processes. For an optimization of the process chain with respect to product properties, cost and time, a better understanding of the effects of individual processes on the final product is required. This can be obtained by a computational simulation of the process chain which is attempted within Graduiertenkolleg 1483. In Graduiertenkolleg 1483, a sample process chain has been divided into six Ph.D. projects. In the talk an overview of the six projects will be given and the interrelation between them will be addressed.

Besides introducing into Graduiertenkolleg 1483, this talk concentrates on one of the Ph.D. projects that deals with the experimental determination of input parameters for the computational simulations. As a simple material for starting the process simulations, a non-alloyed deep drawing steel (DC04) was selected which will be introduced in the talk. Samples were hot and cold rolled as well as heat treated. Using Electron backscattered diffraction (EBSD), the different microstructures and textures after these processes will be presented. The macroscopic and microscopic mechanical behavior was examined by tensile tests and microcompression tests. For the microcompression tests pillars were micro-machined and compressed with a flat punch (Fig. 1). In the talk the procedure of the microcompression test will be explained and results on DC04 will be presented.



**Fig. 1: Pillar cut in DC04 steel with EDM and finished with FIB**

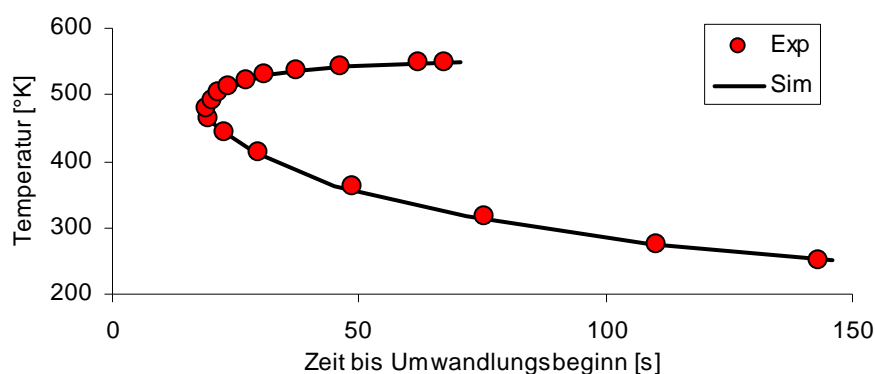
## MODELLIERUNG DER MARTENSITISCHEN UND DER BAINITISCHEN UMWANDLUNG

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### Abstract

Bei dem Hybridumformprozess in [1] zur Einstellung gradierter Strukturen werden Kalt- und Warmumformung kombiniert. Dabei ist die gleichzeitige Umformung erwärmter und nicht erwärmter Bereiche eine verfahrensspezifische Besonderheit im Prozess. Durch die Einstellung eines vordefinierten Temperaturprofils werden Werkstücke mit gradierten und somit flexiblen Werkstoffeigenschaften erreicht. Aufgrund der simultan auftretenden kalten und erwärmten Bereiche während des Hybridumformprozesses herrschen in dem Bauteil verschiedene Gefügestände vor. Es treten sowohl weiche perlitische und ferritische als auch harte martensitische und bainitische Gefügestände auf. Der Schwerpunkt unserer Arbeit liegt auf der Austenit-Bainit und Austenit-Martensit Umwandlung. Zur Simulation der bainitischen Umwandlung wird ein Materialmodell, basierend auf der Veröffentlichung von Garrett et al. [2], theoretisch erweitert und numerisch implementiert. Dabei wird eine experimentell bestätigte Unsymmetrie bezüglich einer Referenztemperatur in dem ZTU- Diagramm für den unteren und den oberen Bainit berücksichtigt (Abb. 1). Außerdem wird ein makroskopisch plastisches Materialmodell unter Berücksichtigung der Umwandlungsplastizität (TRIP) und großer Deformationen präsentiert. Die numerische Implementierung erfolgt für eine UMAT/Abaqus-Subroutine.



**Abb. 1 Isothermes ZTU-Diagramm für 51CrV4: Vergleich von Experiment und Simulation der Inkubationszeit (Zeit bis Umwandlungsbeginn)**

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## MONITORING AND CONTROL OF PROCESS BEHAVIOUR

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### **Abstract**

Dynamic processes, which are components of a production process chain, are subject to noise in the process constraints and process states. Consequently, these deviations from the ideal behaviour have to be compensated by adjusting the process parameters by a closed loop control in order to reach a final goal state with desired material properties. The state variables needed for this purpose are usually not directly accessible during process execution. It is therefore necessary to extract the state information from observable quantities via observers. If multiple processes are linked in a process chain, the initial state of an individual process is the final state of its predecessor. The information about the preceding final state is important for the process parameter settings of the subsequent state. The transfer of the information about the final state is linking the process controls downstream the chain.

For an overall process chain optimisation also upstream linking is needed. One single process of the chain will have different efforts to reach a specific final state depending on the initial state and process noise. The subsequent process will have an average cost associated with each of its initial states, making some of them more favourable than others. It is proposed to forward this information upstream in the form of a cost function depending on the final state of the preceding process. The receiving process can then adjust its parameters to find the common optimum. This recursive process linking yields a global optimum control strategy.

The pre-requisite for efficient control is nevertheless detailed information about the state evolution of the process. The extraction of such information follows the concepts of observer technologies based on process models. The crucial point is the formation of the models, where statistical learning is used to form models from experimental or simulation data [1]. The alternative employment of generic models for process modelling [4] will be investigated in future work. The basic idea of process observation and control is applied to deep drawing simulation for anisotropic sheet metal behaviour [2]. An approach to predict material properties and friction coefficients according to observable process quantities has been presented in [3].

The process states are usually characterised by fields of physical quantities, which are subject to discretization for numerical purposes, resulting in high-dimensional vector quantities. This high dimensionality is problematic with statistical learning, when only a limited number of samples are available. Therefore dimension reduction methods are applied to reduce the dimensionality of the process space, thus completing the system of process monitoring and control.



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## **SIMULATION OF HEAT TREATMENT PROCESSES**

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### **Abstract**

The leading motivation within this research project is the simulation of the heat treatment process as a part of a process chain. In this context it is important to consider the state of the component after the previous processing step, being described by distortion, residual stress, strain hardening and microstructure. Subsequently, the evolution of the listed quantities has to be analysed during the heat treatment in order to get input data for the next manufacturing operation. The process chain comprises two different heat treatments: case hardening and dual frequency induction surface hardening. For the former one in the first step just the residual stresses were mapped onto the component. The work steps of case hardening, namely heating, carbonisation and quenching, were simulated with ABAQUS/Standard. Therefore user-defined subroutines including phase transformation, transformation heat and transformation induced plastic strains were applied. In the latter case the initial investigation was focused on the effects of temperature gradients, caused by the induction heating, on the component characteristics during quenching. Furthermore other aspects, which shall be integrated in the simulation, will be pointed out.

## DEVELOPMENT OF MATERIAL MODELS FOR MICROSTRUCTURE EVOLUTION DURING DEEP DRAWING

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### **Abstract**

In the presentation, the identification, validation and application of a two-scale approach for the description of metal forming operations is discussed. In the first step, finite element simulations of uniaxial compression tests of micropillars performed with single crystals made of steel type DC04 are used to identify the material parameters of a geometrically nonlinear crystal plasticity model.

In a second step, the model is validated based on a full-field finite element simulation based on two-dimensional EBSD data. The discretization of the EBSD data is discussed in detail.

In the third step, a deep-drawing simulation is performed applying the Taylor model at the integration point level. The single crystal orientations used in the two-scale simulation are extracted from EBSD data by a specific algorithm reducing the EBSD data to a set of weighted crystal orientations of prescribed size. The numerical results are compared to experiments.

## PERFORMANCE OPTIMIZED PHASE-FIELD SIMULATIONS OF GRAIN STRUCTURES UNDER THE EFFECT OF MECHANICAL FORCES

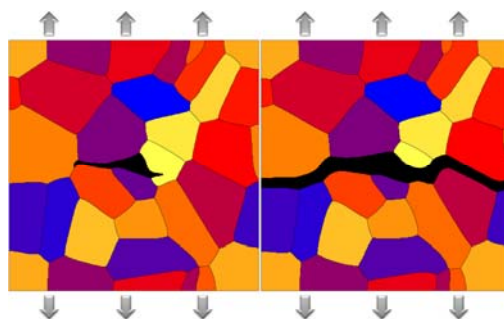
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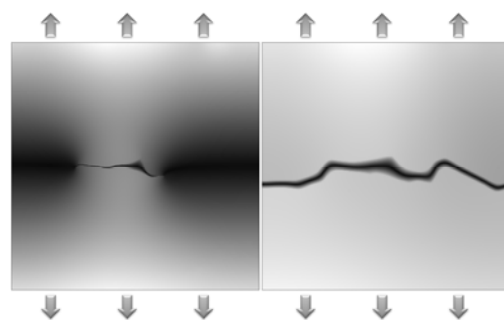
### Abstract

An extension of the phase-field model for polycrystalline materials is presented that incorporates the effect of mechanical forces on the microstructure. We discuss the coupled set of dynamical equations and the numerical solving method. We show applications to grain structure evolution under the influence of elastic stresses and investigate the formation of micro cracks (Figs. 1 and 2). A new approach to describe plastic deformations is introduced by using a simplified plasticity model in the phase-field formulation.

Simulations of complex polycrystalline microstructures based on a phase field model are computational intensive and must be optimized to increase efficiency of the numerical solving algorithm. As in many optimization processes, parallelization is a modern, widely used technique in the field of computational engineering that enables for employing high performance computing facilities. Other optimization strategies depend on the specific simulation setup. We present the parallelization of the phase-field model and further performance optimization methods such as dynamical domain decomposition and the introduction of locally reduced order parameters.



**Figure 1: Crack (black) propagation in a Voronoi generated microstructure with applied tensile stress.**



**Figure 2: Illustration of the norm of the deformation field showing areas with high displacement (white)**

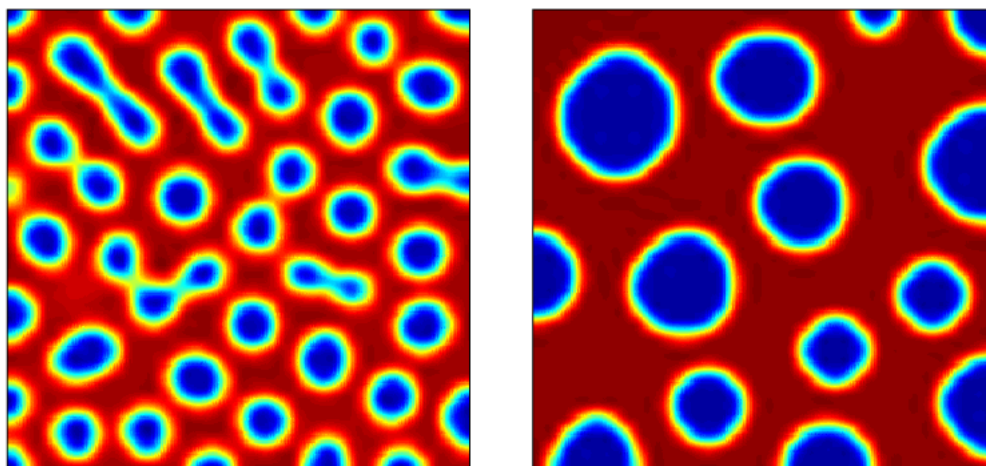
## SIMULATION VON ENTMISCHUNGSVORGÄNGEN IN ZWEIFHASIGEN LEGIERUNGEN

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### Abstract

Die für Lötverbindungen in mikroelektronischen Bauteilen verwendeten Materialien sind feste Mischungen aus mehreren Metallen. Im Laufe der Zeit weisen diese Legierungen eine Vielfalt an mikromechanischen Veränderungen auf. Typisch sind insbesondere Entmischungen der Legierungsbestandteile und eine anschließende Vergrößerung der einzelnen Phasen. Diese mikrostrukturellen Prozesse beeinflussen ihrerseits Belastbarkeit und Haltbarkeit der Lotverbindungen – und damit letztlich der mikroelektronischen Baueinheit. Die Gefügeveränderungen sind insbesondere deshalb interessant, weil auf Grund der Kleinheit der Verbindungselemente ihre Mikrostruktur sehr unmittelbaren Einfluss auf die Lebensdauer der gesamten Struktur hat. Um die Veränderungen der Mikrostruktur zu berechnen, verwenden wir hier eine Diffusionstheorie, die auf ein erweitertes Cahn-Hilliard-Modell führt. Die zugrundeliegenden Gleichungen sind partielle Differentialgleichungen 4. Ordnung. Die Standardtechniken der finiten Elemente Methode sind nicht unmittelbar anwendbar, weil für die Diskretisierung des variationellen Problems global  $C^1$ -stetige Approximationsfunktionen notwendig sind. In unserem Beitrag stellen wir deshalb eine Technik vor, die als FE-Ansatzfunktionen B-splines wählt. B-splines – normalerweise bekannt aus CAD-Anwendungen – erlauben die unmittelbare Erfüllung der notwendigen Stetigkeitsanforderungen und haben in der numerischen Lösung deutliche Vorteile gegenüber anderen Verfahren, wie z.B. gemischten FE-Methoden.



Wir illustrieren in unserem Beitrag die Vorteile der gewählten Methode anhand von Modellrechnungen. Darüber hinaus modellieren wir die Entmischung und Vergrößerung eines Silber-Kupfer-Hartlotes und vergleichen unsere Simulationen mit experimentellen Ergebnissen.

# NUMERICAL IMPLEMENTATION OF A MICROMECHANICAL MULTI VARIANT MODEL FOR TEXTURED POLYCRYSTALLINE SHAPE MEMORY ALLOYS

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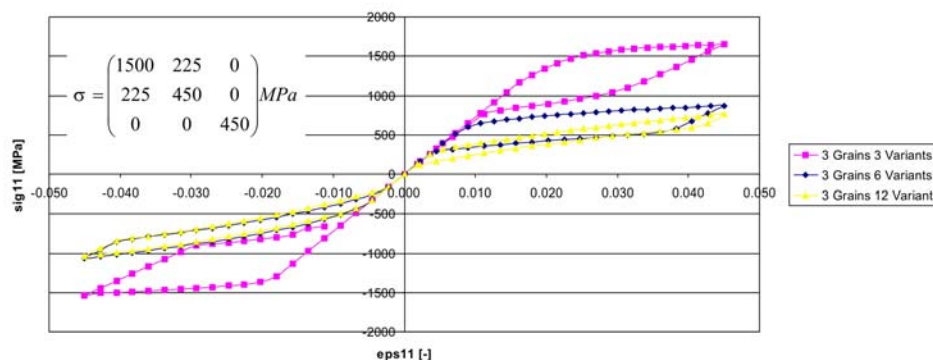
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## Abstract

Shape memory alloys have different material behaviour dependent on stress states such as tension, compression and shear. We call these observations of experimental results asymmetric effects. The local stress, occurring in the slip plane is the important factor for phase transformation. Thus a reason for the asymmetric effects is the microstructural occurrence of different variants for the multi-variant- and detwinned-martensite dependent on the stress state as well as preferred directions in textured materials.

The model presented in this paper enables to take into account all martensitic variants in different orientated grains. To this and the texture of a pseudoelastic NiTi wire is measured and the orientations and their weight/size are implemented in our model. Finally in a finite element example the superelastic behaviour of a stent with different stress states at different locations is investigated.

This model is based on the papers [1] and [2].



**Fig. 1 Comparison of simulations of polycrystals with 3 grains  
and 3, 6 and 12 martensitic variants**

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