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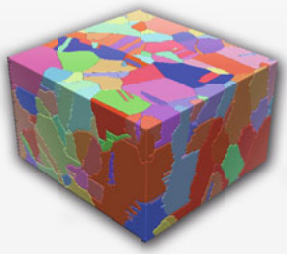

Proceedings of the 4th World Congress on Integrated Computational Materials Engineering (ICME 2017)

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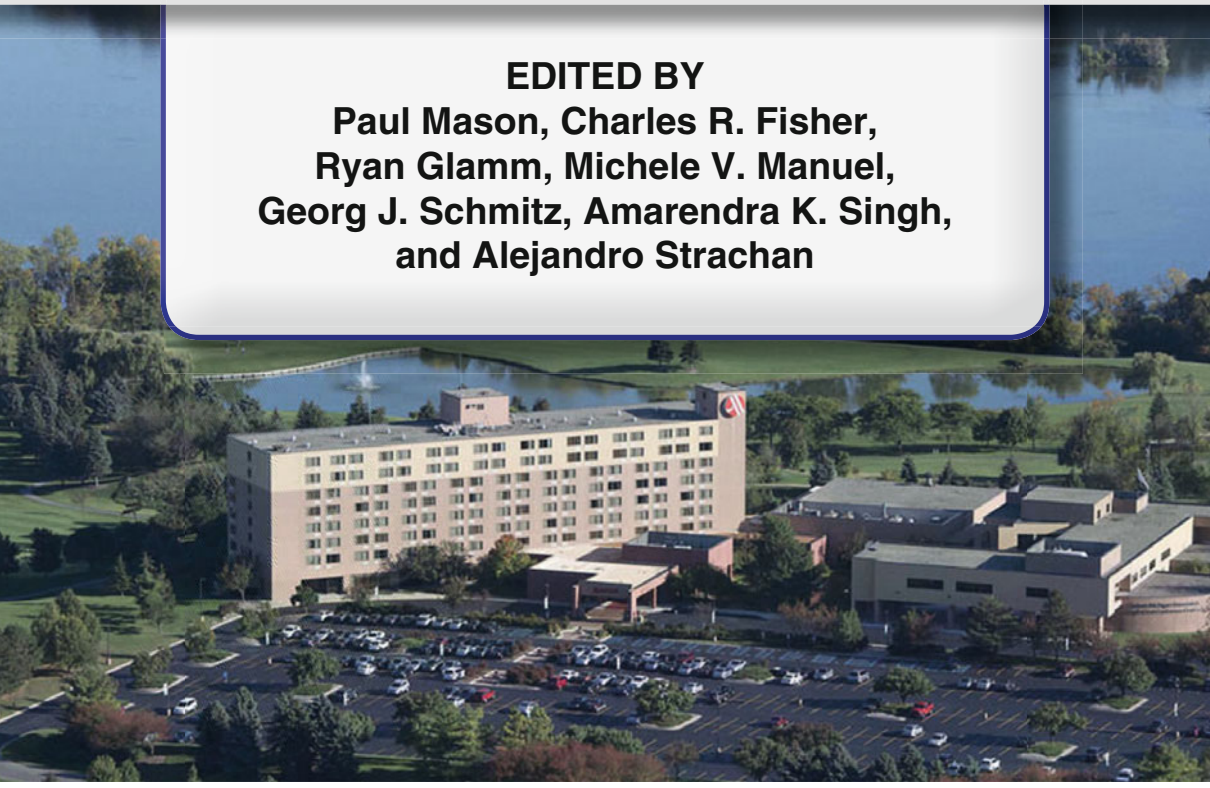
Paul Mason, Charles R. Fisher, Ryan Glamm, Michele V. Manuel, Georg J. Schmitz, Amarendra K. Singh, and Alejandro Strachan



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The Minerals, Metals & Materials Series

Paul Mason · Charles R. Fisher · Ryan Glamm
Michele V. Manuel · Georg J. Schmitz
Amarendra K. Singh · Alejandro Strachan
Editors

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Preface

This is a collection of manuscripts presented at the 4th World Congress on Integrated Computational Materials Engineering, a specialty conference organized by The Minerals, Metals & Materials Society (TMS) and the seven conference organizers, and held in Ypsilanti, Michigan, USA, on May 21–25, 2017.

Integrated computational materials engineering (ICME) has received international attention as it has been proven to shorten product and process development time, while lowering cost and improving outcomes. Building on the great success of the first three World Congresses on Integrated Computational Materials Engineering, which started in 2011, the 4th World Congress convened researchers, educators, and engineers to assess the state-of-the-art ICME and determine paths to further the global advancement of ICME. More than 200 authors and attendees from all over the world contributed to this conference in the form of presentations, lively discussions, and manuscripts presented in this volume. The international advisory committee members representing 11 different countries actively participated and promoted the conference.

The specific topics highlighted during this conference included integration framework and usage, ICME design tools and application, microstructure evolution and phase field modeling, mechanical performance using multiscale modeling, ICME success stories and applications, and a special focus on additive manufacturing. The conference consisted of integrated all-conference plenary talks, invited talks, contributed presentations, and a number of excellent poster presentations.

The 34 papers presented in this volume represent a cross section of the presentations and discussions from this congress. It is our hope that the 4th World Congress on ICME and these proceedings will further the global implementation of ICME, broaden the variety of applications to which ICME is applied, and ultimately help industry design and produce new materials more efficiently and effectively.

Paul Mason
Charles R. Fisher
Ryan Glamm
Michele V. Manuel
Georg J. Schmitz
Amarendra K. Singh
Alejandro Strachan

Acknowledgements

The organizers/editors would like to acknowledge the contributions of a number of people without whom this 4th World Congress, and the proceedings, would not have been possible.

First, we would like to offer many thanks to the TMS staff who worked tirelessly to make this an outstanding conference and an excellent proceedings publication.

Second, we want to thank the international advisory committee for their input in the planning of the conference, the promotion of the conference, and their participation in the conference. This international committee included the following: Dipankar Banerjee, Indian Institute of Science, India; Annika Borgenstam, KTH—Royal Institute of Technology, Sweden; Masahiko Demura, University of Tokyo, Japan; Dennis Dimiduk, BlueQuartz, LLC, USA; B.P. Gautham, Tata Consulting Services, India; Liang Jiang, Central South University, China; Kai-Friedrich Karhausen, Hydoaluminium, Germany; Peter Lee, Imperial College, UK; Mei Li, Ford Motor Company, USA; Baicheng Liu, Tsinghua University, China; Javier Llorca, IMDEA, Spain; Jiangfeng Nie, Monash University, Australia; Warren Poole, University of British Columbia, Canada; Antonio J. Ramirez, The Ohio State University, USA; James Warren, National Institute of Standards and Technology, USA; and Erich Wimmer, Materials Design, France.

Finally, we would especially like to acknowledge the financial support of all our sponsors. We are also grateful for the participation and contributions of all of the attendees.

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About the Editors/Organizers

Paul Mason graduated in 1989 from South Bank University in London, UK, with an Hons degree in physical sciences and scientific computing. On graduation, he joined the Atomic Energy Research Establishment at Harwell and worked in the area of civil nuclear power for 14 years focusing on materials R&D issues, particularly at high temperatures. Paul began his career mostly involved in experimental work and then moved into the modeling realm. In 2004, Paul was appointed President of Thermo-Calc Software Inc when the Swedish-based Thermo-Calc Software AB started a US subsidiary. Since that time Paul has been responsible for the marketing and sales, technical support, training, and customer relations for the North American market which includes the USA, Canada, and Mexico. Paul has been actively involved in the TMS ICME Committee since its formation and was Chair of the Committee from 2014 to 2016.

Charles R. Fisher is a Materials Scientist in the Welding, Processing, and Nondestructive Evaluation (NDE) Branch at the Naval Surface Warfare Center, Carderock Division (NSWCCD) near Bethesda, Maryland. Charles has been with the US Navy for 4 years working in computational weld mechanics (CWM) and ICME-related programs, with a focus on residual stress and distortion analysis in welded structures. He holds a B.S. in materials engineering from Iowa State University and a M.S. and Ph.D. in materials science and engineering from the University

of Florida. He first became involved with TMS as a student member of Material Advantage in 2005, and has been a continuous and active member since.

Ryan Glamm is a Materials and Processes Engineer for Boeing Research and Technology focused on developing novel alloys and processes for structural airframe applications. He has a B.S. in materials science and engineering from The Ohio State University and a Ph.D. in materials science and engineering from Northwestern University. He has lead the introduction of integrated computational materials engineering for metals within Boeing and has authored numerous internal and four external publications and has two patents under review. Additionally, he has had assignments supporting KC-46, 777X, and the qualification of fastening assembly automation. He has interest in utilizing computational methods for accelerating technology implementation and in solving in-production engineering challenges. Ryan is active in the Puget Sound ASM International Chapter as the Education Chair.

Michele V. Manuel is a Professor and Chair in the Department of Materials Science and Engineering at the University of Florida. She received her Ph.D. in materials science and engineering at Northwestern University in 2007 and her B.S. in materials science and engineering at the University of Florida. She is the recipient of the 2013 Presidential Early Career Awards for Scientists and Engineers (PECASE), NSF CAREER, NASA Early Career Faculty, ASM Bradley Stoughton Award for Young Teachers, AVS Recognition for Excellence in Leadership, TMS Early Career Faculty, TMS Young Leaders Professional Development, and TMS/JIM International Scholar Awards. Her research lies in the basic understanding of the relationship among processing, structure, properties, and performance. She uses a system-based materials design approach that couples experimental research with theory and mechanistic modeling for the accelerated development of materials. Her current research is focused on the use of system-level design methods to advance the development of new materials through microstructure optimization. Of specific

interest are lightweight alloys, self-healing metals, computational thermodynamics and kinetics, shape-memory alloys, and materials in extreme environments—specifically under high magnetic fields and irradiation.

Georg J. Schmitz obtained his Ph.D. in materials science in 1991 from RWTH Aachen University in the area of microstructure control in high-temperature superconductors. At present, he is senior scientist at ACCESS e.V., a private, nonprofit research center at the RWTH Aachen University. His research interests comprise microstructure formation in multicomponent alloys, modeling of solidification phenomena, phase field models, and thermodynamics. He is the official agent for Thermo-Calc Software AB in Germany and provides global support for MICRESS®. He has been appointed as expert by several institutions and is an active member of the committee on "Digital Transformation in Materials Engineering" of the Association of German Engineers (VDI), member of the TMS Integrated Computational Materials Engineering (ICME) Committee, and member of the European Materials Modelling Council (EMMC). He is editor and reviewer for a number of journals and has published more than 150 scientific articles, a book on a platform concept for ICME, and a recent Handbook of Software Solutions for ICME.

Amarendra K. Singh received his B.Tech. degree in metallurgical engineering in 1987 and M.Tech. and Ph.D. degrees in metallurgical engineering and materials science from the Indian Institute of Technology, Kanpur. He is currently a Professor with the Department of Materials Science and Engineering at the Indian Institute of Technology, Kanpur. Prior to joining IIT Kanpur in April 2015, he was with TCS Innovations Lab-TRDDC, Pune, for 23 years where he had successfully demonstrated the power and utility of mathematical modeling in optimization manufacturing operations leading to significant productivity gains, quality improvements, energy saving, and/or environment compliance. Dr. Singh has actively carried out research in number of areas including liquid metal

processing (steelmaking, copper, and aluminum), solidification processing (ingot and continuous casting of steel/aluminum), and combustion and multiphase reacting flows (power plant boilers and metallurgical furnaces). Professor Singh's current research focus is on the areas of mathematical modeling of metallurgical operations with special focus on steelmaking and processing operations and integrated computational materials engineering (ICME). Dr. Singh has received many awards and honors, including being selected for the AICTE-INAE Distinguished Visiting Professorship at IIT Bombay from 2009 to 2011, TCS Distinguished Scientist Award in 2011, and the Metallurgist of the Year Award from the Ministry of Steel, Govt. of India, in 2014.

Alejandro Strachan is a Professor of materials engineering at Purdue University and the Deputy Director of the Purdue's Center for Predictive Materials and Devices (c-PRIMED) and of NSF's Network for Computational Nanotechnology. Before joining Purdue, he was a Staff Member in the Theoretical Division of Los Alamos National Laboratory and worked as a Postdoctoral Scholar and Scientist at Caltech. He received a Ph.D. in Physics from the University of Buenos Aires, Argentina, in 1999. Among other recognitions, Prof. Strachan was named a Purdue University Faculty Scholar (2012–2017), received the Early Career Faculty Fellow Award from TMS in 2009 and the Schuhmann Best Undergraduate Teacher Award from the School of Materials Engineering, Purdue University, in 2007. Professor Strachan's research focuses on the development of predictive atomistic and molecular simulation methodologies to describe materials from first principles, their application to problems of technological importance, and quantification of associated uncertainties. Application areas of interest include coupled electronic, chemical and thermo-mechanical processes in devices of interest for nanoelectronics and energy as well as polymers and their composites, molecular solids and active materials, including shape memory and high energy density materials. He has published over 120 articles in peer-reviewed scientific literature.

Part I
Integration Framework and Usage

An Attempt to Integrate Software Tools at Microscale and Above Towards an ICME Approach for Heat Treatment of a DP Steel Gear with Reduced Distortion

Deepu Mathew John, Hamidreza Farivar, Gerald Rothenbucher, Ranjeet Kumar, Pramod Zagade, Danish Khan, Aravind Babu, B.P. Gautham, Ralph Bernhardt, G. Phanikumar and Ulrich Prahl

Abstract Finite element simulation of heat treatment cycles in steel could be challenging when it involves phase transformation at the microscale. An ICME approach that can take into account the microstructure changes during the heat treatment and the corresponding changes in the macroscale properties could greatly help these simulations. Dual phase steel (DP steel) are potential alternate materials for gears with reduced distortion. Inter-critical annealing in DP steel involves phase transformation at the microscale and the finite element simulation of this heat treatment could be greatly improved by such an ICME approach. In the present work, phase field modeling implemented in the software package Micress is used to simulate the microstructure evolution during inter-critical annealing. Asymptotic Homogenization is used to predict the effective macroscale thermoelastic properties from the simulated microstructure. The macroscale effective flow curves are

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obtained by performing Virtual Testing on the phase field simulated microstructure using Finite Element Method. All the predicted effective properties are then passed on to the macro scale Finite Element simulation software Simufact Forming, where the heat treatment cycle for the inter-critical annealing is simulated. The thermal profiles from this simulation are extracted and passed on to microscale to repeat the process chain. All the simulation softwares are integrated together to implement a multi-scale simulation, aiming towards ICME approach.

Keywords DP steel · Multi phase field modeling · Homogenization · Inter-critical annealing · Gear · Finite element method · Micress · Simufact

Introduction

Production of tailored components with improved properties is one of the primary aims of the industry at present. This requires materials with complex microstructures and strategic process design and control. Integrated computational materials engineering (ICME) is one of the present areas of interest for both academic and industrial research, as it uses physics based models, empirical models and human expertise in an integrated manner to significantly reduce the time and cost of development of new materials and their manufacturing processes. ICME had been successfully used for materials design, development and rapid qualification [1, 2]. Dual phase steel (DP steel) is one of the potential alternate materials for gears as it shows improved fatigue life and decrease in heat treatment distortion [3]. Low pressure vacuum carburizing (LPC), along with high pressure gas quenching (HPGQ) can be used to produce carburized components with less distortion, compared to other heat treating methods. ICME tools can help in controlling the gear distortion in such a heat treatment [4]. ICME approach had also been applied to optimize the metallurgy and improve the performance of carburizable ferrium steels, which are now commercially available for gear and bearing applications [5]. Multiscale modeling can be used to achieve ICME in order to assess the effects of constituent properties and processing on the performance of materials [6]. The present work aims towards an ICME approach for the design of a DP steel gear with reduced distortion. Vertical integration (multiscale modeling) is one of the aspects of an ICME approach. The present work addresses this aspect for the micro and macro scales. The data input-output of all the simulation tools was modeled on an ICME platform. LPC with HPGQ was used to carburize and heat treat the DP steel gear. A chemical composition selected using Calphad tools for carburized DP steel gear with maximum hardenability and maximum difference between Ae_3 and Ae_m was used for the simulations.

Simulations at Different Length Scales

Microscale: Phase Field Simulation

Phase field modeling is one of the widely used technique to predict the microstructure evolution during diffusional phase transformations. It had been used successfully to simulate the austenite to ferrite transformation in DP steels [7–9]. In the present work, phase field modeling implemented in the commercial software package Micress® was used to simulate the microstructure evolution during phase transformation. The austenite to ferrite transformation during inter-critical annealing in DP steel was simulated at the microscale. In order to simulate this phase transformation, a two dimensional multi-phase field simulation was performed on a multi-component system with chemical composition Fe-0.35Cr-0.75Mn-0.5Mo-0.4Si-0.1Ni-0.18C. An initial synthetic microstructure was created using voronoi tessellation, using the initial austenite grain size obtained by averaging the grain size from several experimental micrographs. Figure 1a shows the initial austenite microstructure with an average grain size of 10 μm. For simulating the nucleation of ferrite, seeds were defined at the triple junctions. The thermodynamic and the kinetic data required for the phase field simulation was obtained from ThermoCalc database, using the TQ coupling feature of Micress. Periodic boundary conditions were defined in all directions and the local equilibrium negligible partitioning (nple) approach was used to simulate the redistribution of the alloying elements. Simulations were run with 12 threads on an Intel Xeon E5-2630 processor and the average simulation time was around 9 h. The other simulation parameters used are reported in Table 1. Some of these parameters are taken from literature [10].

The simulation was performed for the heat treatment cycle consisting of cooling and holding (inter-critical annealing) as shown in Fig. 1c. The inter-critical annealing (IC annealing) time chosen for the simulation was 30 min. Figure 1b shows the final microstructure after the 30 min of holding. The white colour represents the ferrite phase and the remaining region represents the austenite phase.

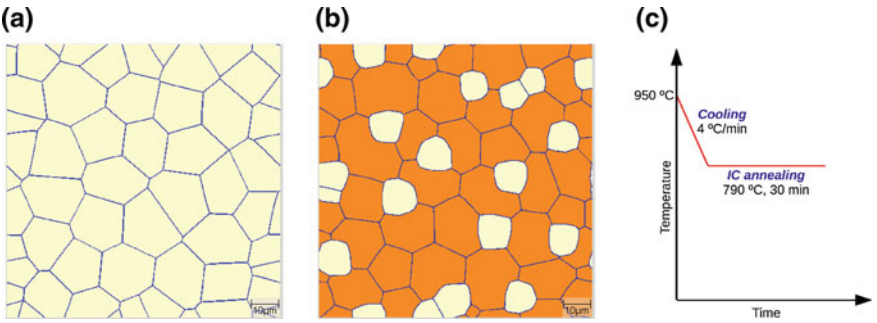

Fig. 1 **a** Initial austenite microstructure. **b** Final microstructure. **c** Heat treatment cycle used for simulation

Table 1 Micress simulation parameters

Simulation parameter		Value
Interfacial mobility: cm^4/Js	$\gamma-\gamma$, $\alpha-\alpha$	1×10^{-5}
	$\gamma-\alpha$	2×10^{-5}
Interfacial energy: J/cm^4	$\gamma-\gamma$, $\alpha-\alpha$	2×10^{-5}
	$\gamma-\alpha$	4×10^{-5}
Domain size		100 × 100 μm
Grid size		0.25 μm
Time step		Automatic (based on stability criterion)

Effective Properties: Asymptotic Homogenization

Asymptotic homogenization could be used to predict the effective thermo-elastic properties of an RVE (Representative Volume Element). The method uses assumption of microstructure periodicity and uniformity of the macroscopic fields within a unit cell domain [11]. In the present work, in order to predict the effective thermo-elastic properties from the phase field simulated microstructure, asymptotic homogenization implemented in the commercial software tool Homat® was used. The simulated microstructure in Micress (RVE) was meshed with C3D8 (8 node linear) hexahedral elements using Mesh2Homat tool. The meshed microstructure was passed on to Homat tool for performing the asymptotic homogenization. In order to perform the homogenization, Homat requires the geometric description and the properties of the individual phases. Geometric description (microstructure) was obtained from Micress whereas the properties of individual phases were obtained from JMatPro® database. Thermo-elastic homogenization was performed at 790 °C to obtain the effective macroscale elastic modulus, poissons ratio, density, specific heat capacity, thermal expansion coefficient and thermal conductivity.

Virtual Testing: Effective Flow Curve

Virtual testing on an RVE can be used to predict the effective flow curve of the macroscopic material [12]. Ramazani et al. [13] have successfully used virtual tensile testing on RVE in two and three dimensions to predict the flow curves of DP steel. In the present work, in order to predict the effective flow curve from the phase field simulated microstructure (RVE), a uniaxial tension test was performed on the microstructure using finite element method. The phase field simulated microstructure was meshed with C3D8 hexahedral elements. The microstructure consisted of two phases, austenite and ferrite as shown in Fig. 2a. White region represents ferrite phase and the remaining portion represents austenite phase. The properties of ferrite and austenite phases obtained from JMatPro® database were used for performing the finite element simulations. The meshed microstructure was

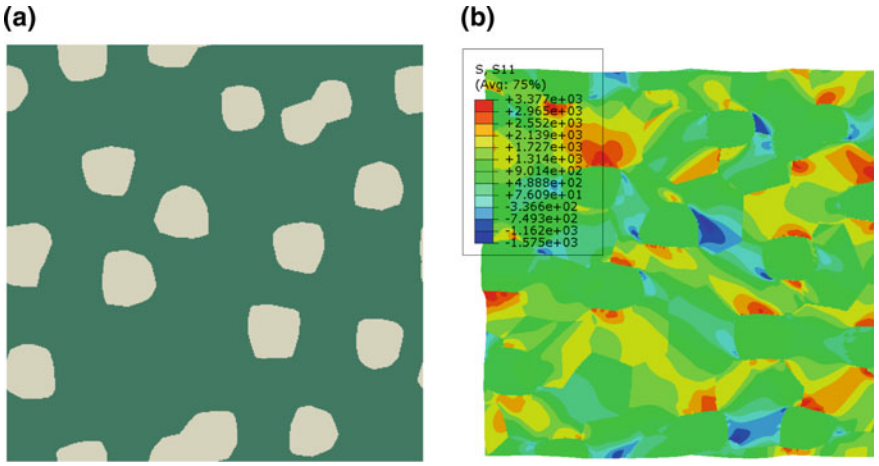

Fig. 2 **a** Initial microstructure for virtual testing. **b** Microstructure with 7% strain

loaded uniaxially in x direction to 7% strain and the average stress-strain response from the entire microstructure was recorded. Figure 2b shows the distribution of stresses in x direction for a strain of 7%. All operations were performed using commercial finite element tools. The average stress-strain response of all the elements in the RVE was used to obtain the effective flow curve of the macroscopic material. This flow curve is passed on to the software Simufact Forming® to start the macroscale simulation.

Macroscale Simulation of Heat Treatment

The inter-critical annealing heat treatment was simulated at the macroscale using finite element method, implemented in the commercial software package Simufact Forming®. Two dimensional axisymmetric simulation was performed on a cylindrical layered geometry. The geometry is assumed to be extracted from one tooth of a carburized gear as shown in Fig. 3a, b. The outer layer corresponds to the carburized layer (case of the gear). It is assumed that this layer has a uniform carbon composition of 0.7% throughout. The inner layer corresponds to the core of the gear with 0.18% carbon. The austenite to ferrite phase transformation is assumed to happen only in the core region. For the case region, no phase transformation happens during the inter-critical annealing. A fully austenite microstructure as shown in Fig. 1a is used to assign the effective macroscale material property for this layer. The material properties are assigned separately for the core and the case layers. The macroscale heat treatment cycle shown in Fig. 1c is simulated on the layered geometry. 2D quadrilateral elements were used for the simulation. Figure 3c shows the temperature distribution at an intermediate stage of the simulation

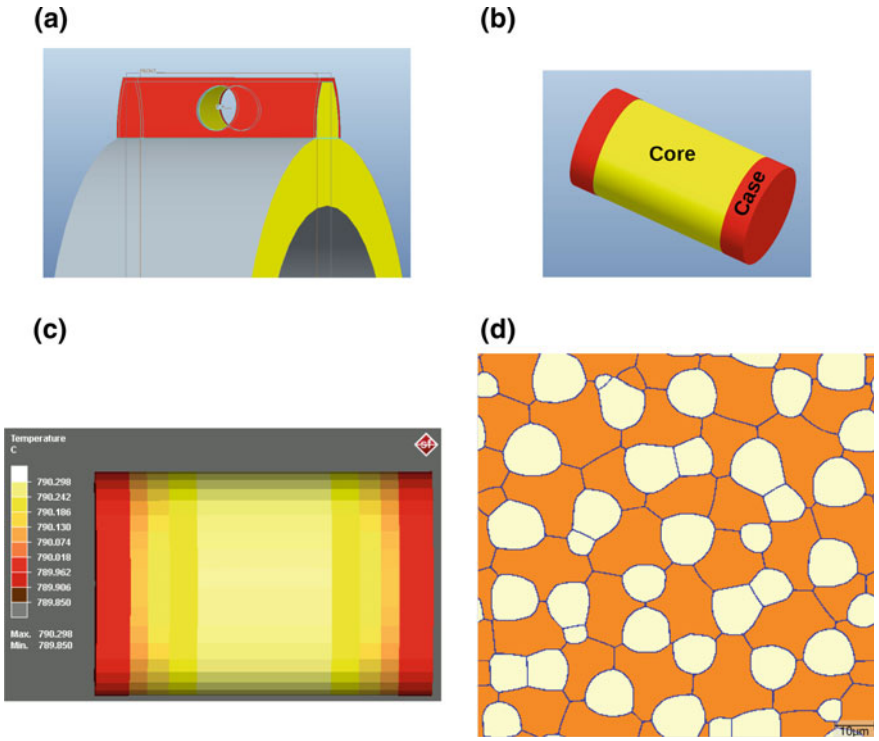

Fig. 3 **a** One tooth of a carburized gear. **b** Selected layered geometry. **c** Temperature distribution at an intermediate stage in Simufact. **d** Phase field simulated microstructure using the data from one of the tracking point in Simufact

in Simufact. Tracking points were used in the simulation to extract the thermal profile across the geometry during the simulation. The data from these tracking points were used to start a phase field simulation to obtain the microstructure evolution across the macroscale geometry. Figure 3d shows the phase field simulated microstructure using the data from one of the tracking points. The phase fraction from this simulated microstructure was compared with experimental data and was found to be matching well.

Multiscale Simulation Chain

A multi-scale simulation chain as shown in Fig. 4 was completed. For implementing this simulation chain, homogenization and virtual testing was performed for the phase field simulated microstructure at various instants along the heat treatment cycle. The effective macroscale properties calculated were fed to the macroscale heat treatment simulation in Simufact. The tracking point data in

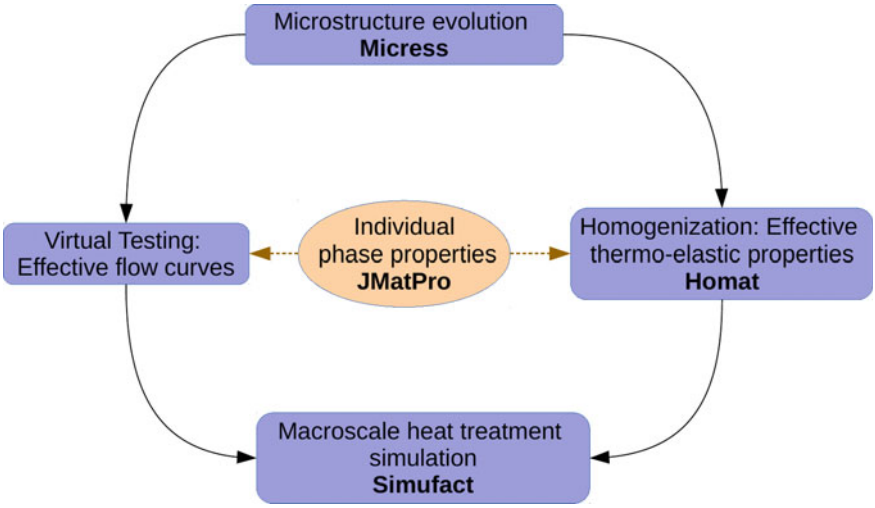

Fig. 4 Workflow for the multiscale simulation

Simufact was used to start a phase field simulation to obtain the microstructure evolution at the tracking point during the macroscale heat treatment process. In this way, the microstructure evolution at various points across the geometry was calculated and the corresponding effective macroscale material properties were obtained using homogenization and virtual testing. These properties were in turn fed to macroscale heat treatment simulation in Simufact to repeat the multiscale simulation chain.

ICME Platform

ICME approach requires an efficient information exchange between the simulation tools at various length scales. An ICME platform can greatly help in facilitating this information exchange and can also help in tracking the results along the process chain. This in turn eases the effort required and also gives a better understanding of the mechanisms by tracking the simulation results along the production chain [14]. In the present work, the data input-output of all the simulation tools was modeled on the ICME platform PREMAP (Platform for Realization of Engineered Materials and Products). PREMAP is an IT platform from Tata Consultancy Services (TCS) that facilitates integration of models, knowledge, and data for designing both the material and the product [15]. PREMAP requires ontological definitions of various entities including for product with requirements, manufacturing processes and material description at different scales. It essentially provides semantic bases which can be used for working with different tools through a unified semantic

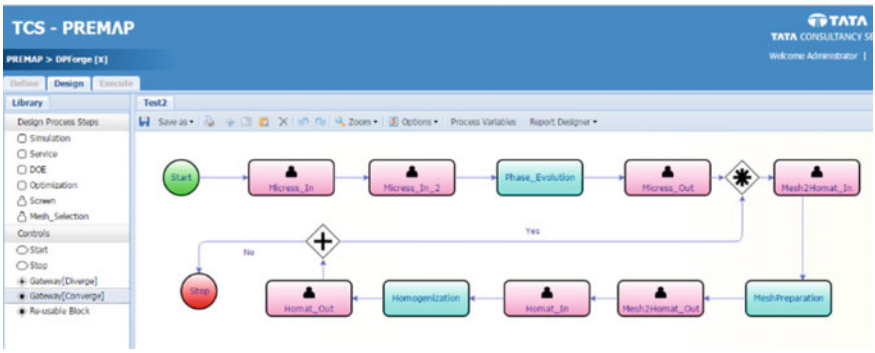

Fig. 5 Workflow implemented in PREMAP for micress and homat

language. This enables extensibility as well as use of different tools within an engineering workflow. This ontology can be used to express various forms of knowledge in forms or rules, expressions, etc. to help take engineering decisions. In the present work, the platform is used to help in repeating the multi scale simulation chain for various conditions, across the macroscale geometry, in order to arrive at the best possible process conditions. Figure 5 shows a snapshot of the simulation chain implemented in PREMAP for micress and homat. With the help of the ICME platform, several runs with different conditions could be made across the simulation chain to arrive at microstructure which gives minimum distortion and best possible combination of mechanical properties at the macroscale.

ICME Implementation Strategy

In order to start the multi-scale simulation chain to implement ICME approach, a starting temperature profile was required. In order to obtain this profile across the macroscale geometry, a Simufact simulation was performed using the material property data obtained from JMatPro database. The temperature-time data from the tracking points in this simulation was used to start a phase field simulation in Micress, as shown in Fig. 6. The simulated microstructure was then used to perform homogenization and virtual testing to obtain the macroscale effective properties. These properties were then fed to Simufact to start the macroscale simulation of heat treatment. This process chain was repeated until the target values for the desired properties were achieved. Once all the simulations are calibrated with experiments, this strategy could be used to obtain the microstructure and the process conditions corresponding to minimum distortion and best possible combination of mechanical properties at the macroscale.

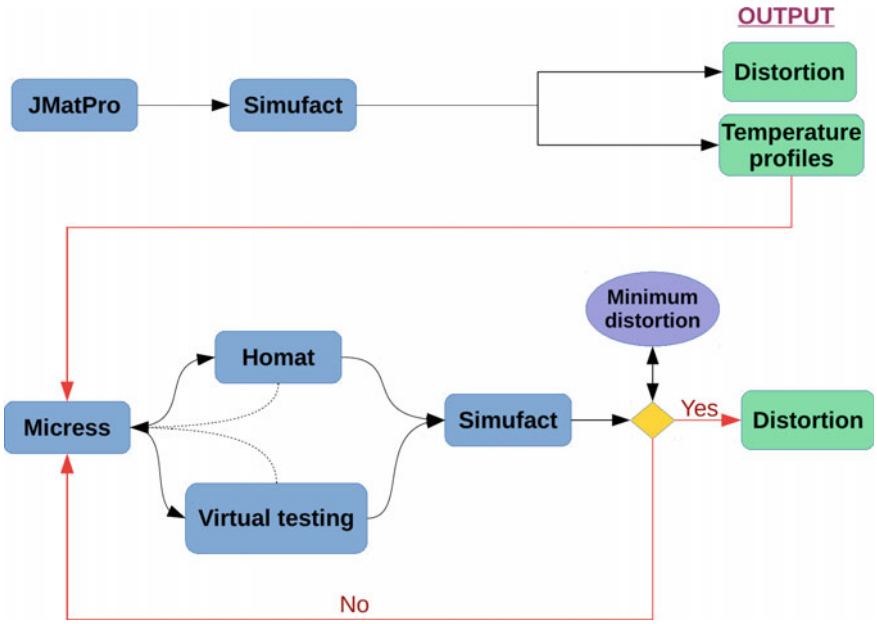

Fig. 6 Workflow for the implementation of a part of an ICME approach

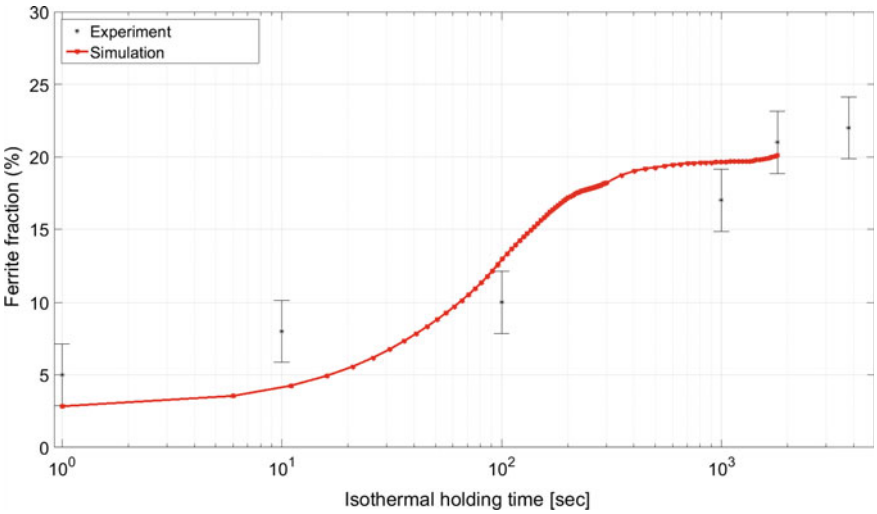

Fig. 7 Comparison of simulated ferrite volume fraction with experiments during isothermal holding at 790 °C

Experimental Validation

In order to validate the Micress phase field simulations, the macroscale heat treatment process was physically simulated on cylindrical samples in Baehr® Dilatometer and the phase fractions were obtained from the optical micrographs. The phase fraction evolution during the inter-critical annealing, obtained from these experiments were compared with that simulated in Micress, as shown in Fig. 7. The carburizing process and the final distortion at macroscale are simulated on Navy C-Ring specimens and experimentally validated in another work by the authors [16].

Conclusion

The present work implements the vertical integration aspect (multi-scale modeling), aiming towards an ICME approach for the microstructure and process design of a DP steel gear with reduced distortion. The microstructure and property evolution during inter-critical annealing heat treatment in DP steels were simulated using commercial software tools. The macroscale heat treatment was simulated on a layered cylindrical geometry to mimic the heat transfer across the cross-section of one tooth of a carburized gear. The data input-output of all the software tools was modeled on an ICME platform. The simulation chain implemented in this work could be used to obtain the microstructure with minimum distortion and best possible combination of macroscale material properties. In this way, the number of experiments required for such a microstructure and process design could be reduced.

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Integrated Microstructure Based Modelling of Process-Chain for Cold Rolled Dual Phase Steels

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Abstract The properties of dual phase (DP) steels are governed by the underlying microstructure, the evolution of which is determined by the processing route. In order to design a dual phase steel with tailored properties, it is therefore important to model and design each of the process involved at the microstructure level in an integrated fashion. In this work, an integrated approach is used to predict the final microstructure and mechanical properties of dual phase steels through microstructure based modelling of cold rolling, intercritical annealing and quenching processes. Starting with a representative volume element (RVE) of initial ferrite-pearlite microstructure, cold-reduction during rolling is simulated in a FEM based micromechanics approach under appropriate boundary conditions. The deformed microstructure with plastic strain energy distribution after cold-reduction serves as input for modelling static recrystallization and ferrite/pearlite to austenite transformation during intercritical annealing using a phase-field approach. A micromechanics based quenching simulation is then used to model austenite to martensite transformation, related volume expansion and evolution of transformational stress/strain fields. The resultant microstructure with its complete state is used to evaluate the flow behavior under uniaxial loading conditions in a FEM based micromechanics approach under periodic boundary conditions. Property variation for different initial microstructure, composition and processing conditions are studied and discussed.

Keywords Micromechanics · Phase-field · Intercritical annealing · Process integration · Microstructure modelling · Phase transformation · Property prediction

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Introduction

Cold rolled dual phase steels are known for their high strength, high toughness and high formability. This makes them a suitable candidate for producing strength-relevant and crash-relevant body-in-white components having complex geometries such as cross-beams, pillars and other reinforcements [1]. This has been possible due to the multiphase nature of these steels wherein the different microstructure constituents impart varied properties to the steels. The constant pursuit of the auto-makers to cater to the increasing fuel-efficiency demands and safety regulations have led to the necessity of continual improvement and optimization of the properties and hence the microstructure of these steels.

Researchers have continuously tried to optimize the properties of the dual phase steels with new processing routes and processing conditions [2, 3]. The final properties of dual phase steels not only depend upon the individual properties of these micro-constituents but also on their morphology and distribution. On the other hand, the properties of the individual phases, their morphology and distribution depend upon the processing history of the steel. Therefore, in order to optimize the final properties of steels in a systematic way, it is not only important to optimize the individual processes involved but also the entire process-chain with explicit tracking of the microstructure evolution. With the advent of microstructure based process-structure [4, 5] and structure-property [6, 7] modelling techniques, it is now possible to model the evolution of microstructure and properties with the processing conditions. Apart from that, with more efforts being put towards solving problem through ICME route, optimizing the entire process-chains of the products in a closed-loop with systematic decision making at each decision point is the need of the hour.

The final steps of a typical processing route for the production of cold-rolled dual phase steels is shown in Fig. 1. There has been number of attempts in past for sequential integration of microstructure based process models as well as integration of process-property models. Madej et al. [8] carried out microstructure based modelling of cold-rolling of ferritic-pearlitic steels using FEM and used its plastic energy distribution output for modelling static recrystallization (SRX) during inter-critical annealing (ICA) using cellular automata in a digital material

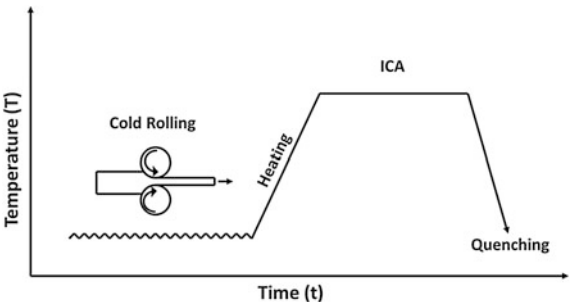

Fig. 1 A typical processing route for cold-rolled dual phase steels

representation framework. Rudinizki [9] on the other hand studied the through process modelling of production of dual phase steels by modelling ICA using phase-field approach followed by property prediction of the microstructure thus obtained using FEM based micromechanics approach. Ramazani et al. [10] modelled the process chain for dual-phase by integrating a similar phase-field approach based ICA model with FEM based micromechanics model of property prediction that took into account the effect of geometrically necessary dislocation formed during quenching on the final properties. However, none of these efforts attempt the integration of process-chain right from the cold-rolling till the final property-predictions in an ICME framework.

The present work involves the integration of microstructure based models of cold-deformation, inter-critical annealing and quenching processes to take into account the effect of each of them on the final microstructure and properties prediction of a cold-rolled dual phase steel. The focus is on the integration of models on an ICME-enabling platform that allows running the process-chain simulations in a loop with decision-making at each stage, thereby opening up the opportunity for optimizing the process-chain in a closed-loop.

Integrated Numerical Models

Figure 2 shows the integration of various micro-scale process models used in this study along with relevant phenomena modelled and related information exchange. The process-chain simulation starts with a 2D RVE of ferritic-pearlitic microstructure having certain statistics defined in terms of ferrite grain size, pearlite colony size etc. This RVE represents a typical ferritic-pearlitic microstructure obtained at the end of runout table (ROT). A typical RVE used in this study is shown in Fig. 3a. The microstructure RVE was subjected to different mechanical and thermal boundary conditions of the subsequent processes and the essential physics involved was modelled to keep track of the evolution of microstructure along with its state of stress and strain. Following sections describe the details of the various microstructure-scale process and property models used.

Cold-Rolling

Cold reduction was modelled as a plain-strain compression of the RVE under homogenous boundary conditions using a FEM model in ABAQUS^{TM}. Chemical composition based flow curves for ferrite and pearlite [11], were used as input for the model. Based on the stress and strain partitioning between ferrite and pearlite phases, plastic strain energy was calculated at each material point of the RVE. A typical plastic strain energy distribution in a ferritic-pearlitic RVE having 14% pearlite, deformed to 50% cold reduction is shown in Fig. 3b.