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

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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.

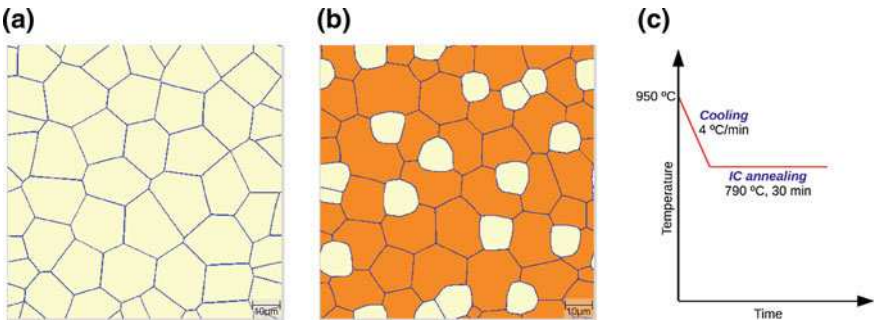

Fig. 1 **a** Initial austenite microstructure. **b** Final microstructure. **c** Heat treatment cycle used for simulation

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

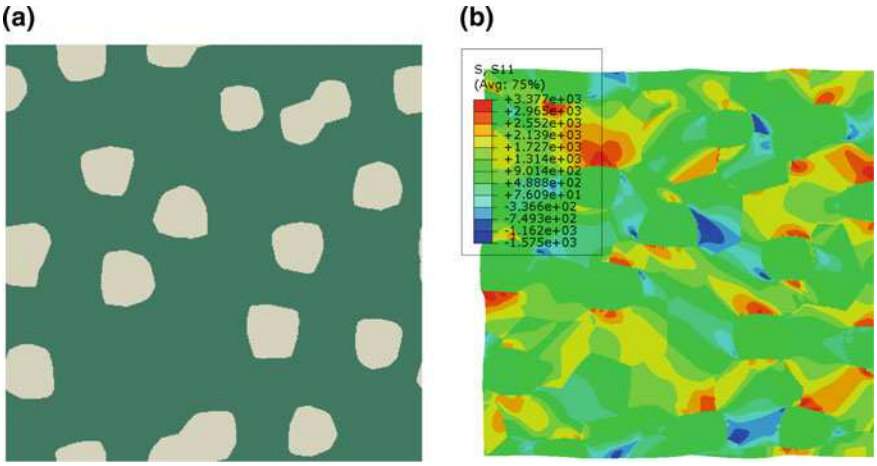

Fig. 2 **a** Initial microstructure for virtual testing. **b** Microstructure with 7% strain

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

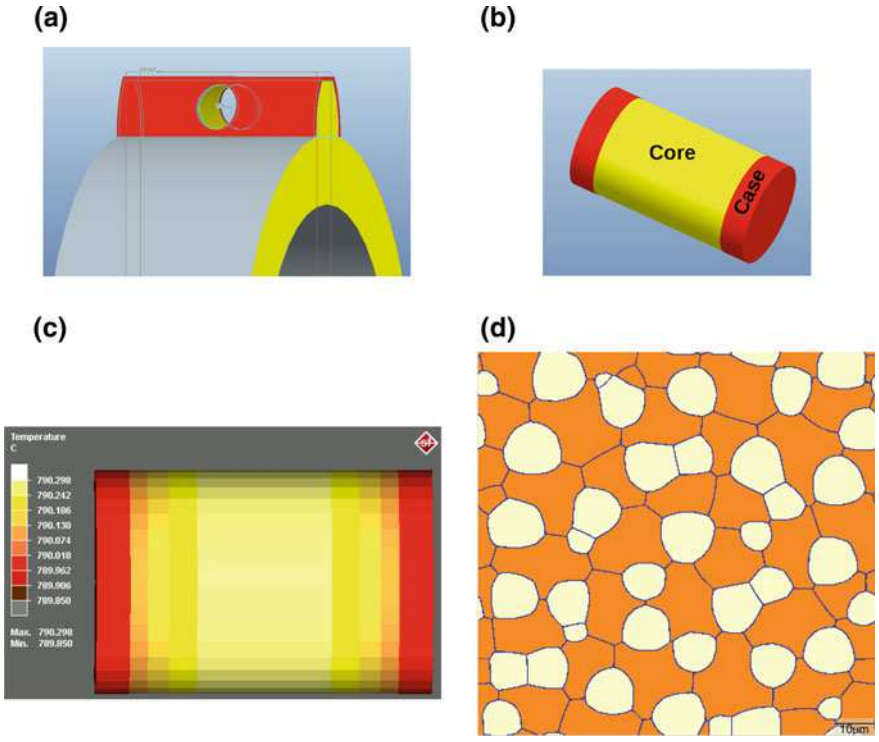

Fig. 3 **a** One tooth of a carburized gear. **b** Selected layered geometry. **c** Temperature distribution at an intermediate stage in Simufact. **d** Phase field simulated microstructure using the data from one of the tracking point in Simufact

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

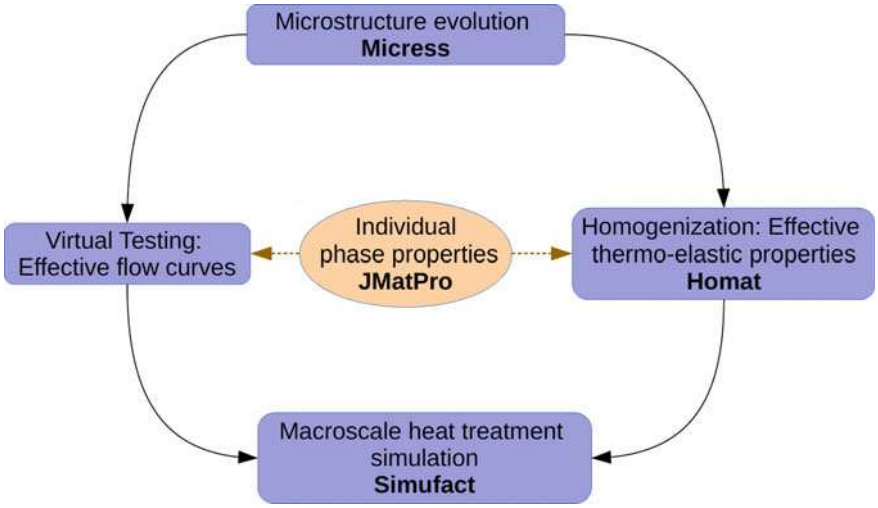

Fig. 4 Workflow for the multiscale simulation

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

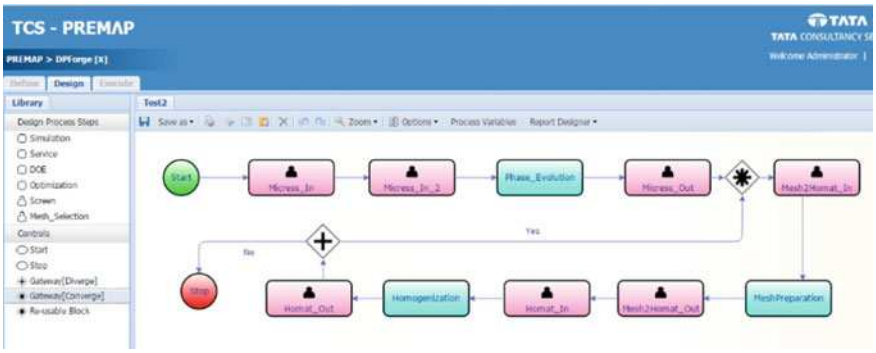

Fig. 5 Workflow implemented in PREMAP for micress and homat

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.

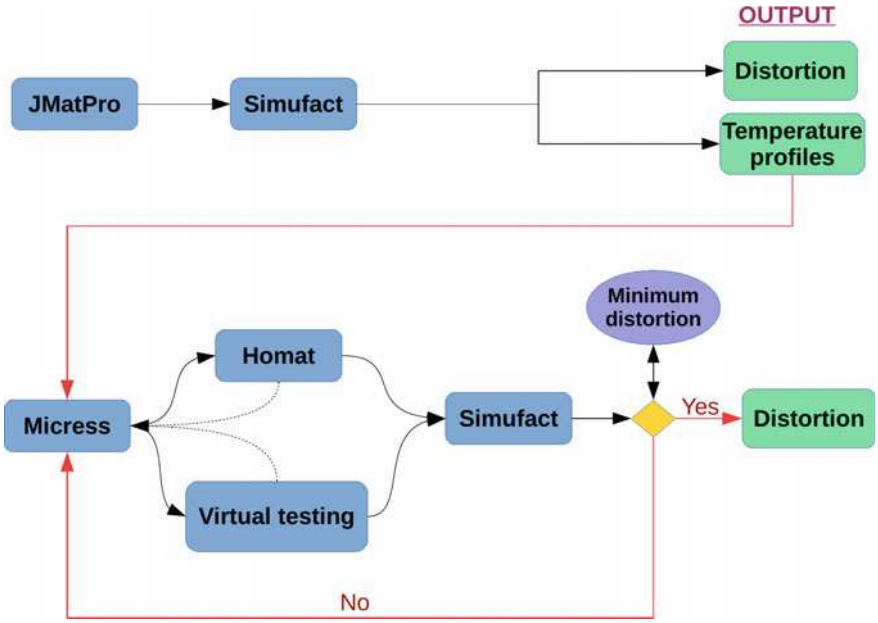

Fig. 6 Workflow for the implementation of a part of an ICME approach

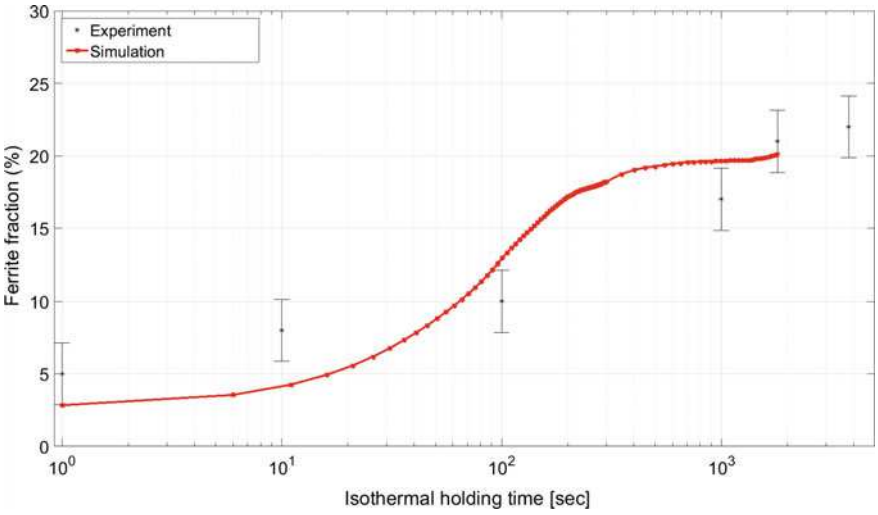

Fig. 7 Comparison of simulated ferrite volume fraction with experiments during isothermal holding at 790 °C

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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