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Microstructure based simulations for prediction of flow curves and selection of process parameters for inter-critical annealing in DP steel

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Abstract. Dual phase steels are versatile advanced high strength steels that are being used for sheet metal applications in automotive industry. It also has the potential for application in bulk components like gear. The inter-critical annealing in dual phase steels is one of the crucial steps that determine the mechanical properties of the material. Selection of the process parameters for inter-critical annealing, in particular, the inter-critical annealing temperature and time is important as it plays a major role in determining the volume fractions of ferrite and martensite, which in turn determines the mechanical properties. Selection of these process parameters to obtain a particular required mechanical property requires large number of experimental trials. Simulation of microstructure evolution and virtual compression/tensile testing can help in reducing the number of such experimental trials. In the present work, phase field modeling implemented in the commercial software Micress® is used to predict the microstructure evolution during inter-critical annealing. Virtual compression tests are performed on the simulated microstructure using finite element method implemented in the commercial software, to obtain the effective flow curve of the macroscopic material. The flow curves obtained by simulation are experimentally validated with physical simulation in Gleeble® and compared with that obtained using linear rule of mixture. The methodology could be used in determining the inter-critical annealing process parameters required for achieving a particular flow curve.

1. Introduction

Dual phase steels(DP steel) are advanced high strength steels that consists of hard martensite and soft ferrite phases in their microstructure. DP steel sheets are used in automobile industry due to the combination of high strength and formability, high crashworthiness, high tensile to yield strength ratio, high work hardening rate and good ductility and hence can help in automobile weight reduction [1, 2]. In future cars, it may occupy up to 80% of the total weight of car [3]. The DP steels used for sheet metal applications typically consists of around 0.2 and 0.8 volume fractions of martensite and ferrite respectively [4]. Thus, it contains hard martensite islands in soft ferrite matrix. DP steels also have high potential for application in bulk components like gear. DP steel has shown improved fatigue strength and decrease in heat treatment distortion of carburized gears and hence reduce the noise in automotive applications.

It also has added advantages that the existing manufacturing lines can be used without major modifications [3]. The DP steel that is to be used in such an application should typically have 0.8 and 0.2 volume fractions of martensite and ferrite respectively. Thus it contains soft ferrite islands in a hard martensite matrix. The present work focuses on this type of DP steel, that could be used for automotive gear applications.

Microstructure plays a major role in governing the properties of dual phase steels, especially the phase fractions, morphology and distribution of the phases [4]. The phase transformation happening during inter-critical annealing in DP steel has a major role in governing the microstructure of the material. Phase field modeling is a versatile tool that can be used to simulate the microstructure evolution [5–7]. It had been used previously to perform the simulation of phase transformation during inter-critical annealing in DP steel [1, 9]. The ability to predict mechanical properties from microstructure is of high demand as it can lead to predictive capability that can help in reducing the number of experimental trials required or to help in designing careful experiments. Among the various approaches that can perform this, Finite Element Method (FEM) is of special interest, as it takes into account the morphology of the phases [2, 4]. Ramazani et.al had used virtual tensile test using FEM to predict the macroscale flow curve from the microstructure [3]. This methodology can also be used to predict the high temperature flow curves of a material to judge the capability of a material for high temperature application. Attempts have also been made to couple phase field modeling and FEM to analyse the microstructure evolution and deformation behaviour [10–14].

In the present work, phase field simulation is used to simulate the microstructure evolution during the heat treatment process. Virtual tests are performed on the simulated microstructure to obtain the effective macroscopic flow curves and the obtained flow curve are compared with the ones obtained by using linear rule of mixture(ROM). Physical simulation in Gleeble® is used to validate the virtual test results.

2. Phase field simulation of microstructure evolution
The austenite to ferrite transformation during inter-critical annealing in DP steel was simulated using the multi phase field model(1) implemented in the commercial software Micress® [15].

$$\dot{\phi}_\alpha = \sum_{\beta=1,\dots,N} \mu_{\alpha\beta} \left\{ \sigma_{\alpha\beta} \left[\phi_\beta \nabla^2 \phi_\alpha - \phi_\alpha \nabla^2 \phi_\beta + \frac{\pi^2}{2\eta^2} \left(\phi_\alpha - \phi_\beta \right) \right] + \frac{\pi}{\eta} \sqrt{\phi_\alpha \phi_\beta} \Delta g_{\alpha\beta} \right\}, \quad (1)$$

where, ϕ_α and ϕ_β are the order parameters, $\mu_{\alpha\beta}$ is the interface mobility, $\sigma_{\alpha\beta}$ is the surface energy, $\Delta g_{\alpha\beta}$ is the thermodynamic driving force and η is the thickness of the diffuse interface. The multi phase field equation is coupled with the diffusion equation(2), since the driving force($\Delta g_{\alpha\beta}$) depends on the local concentration [9].

$$\dot{c} = \nabla \sum_{i=1}^{N} \phi_i D_i \nabla c_i \ , \quad (2)$$

where, D_i is the multi-component diffusion coefficient matrix. The thermodynamic and the diffusion data required for the simulation were obtained from the ThermoCalc® databases TCFE7 and MOBFE1 using the Micress® TQ interface. The heat treat treatment cycle, the chemical composition, simulation conditions and the experimental validation of the Micress® simulation is discussed in one of the work by the authors [16].

3. Physical simulation of high temperature compression test using Gleeble®
In order to obtain the flow curve, a compression test was performed on the material using Gleeble 3800®. A cylindrical specimen of 6mm radius and 9mm length was used for this purpose. The

specimen was prepared using Electrical Discharge Machining(EDM) and thermocouples were welded on to it. Then it was solutionized and heat treated before the start of the compression test, so as to obtain the required dual phase microstructure in the material. Solutionizing was performed at 950 °C followed by cooling to the inter-critical annealing temperature of 790 °C at a cooling rate of 4 °C/min. It was then held at this temperature for 30 minutes, following which the compression test was performed at a strain rate of 0.001 s^{-1}. Figure 1 shows the overall thermal cycle that was used in Gleeble$^{\circledR}$ and figure 2 shows the flow curve obtained.
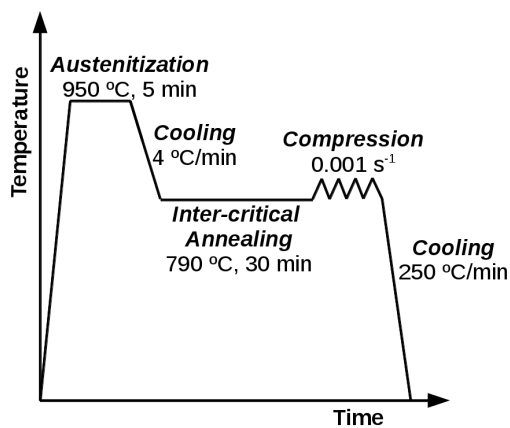
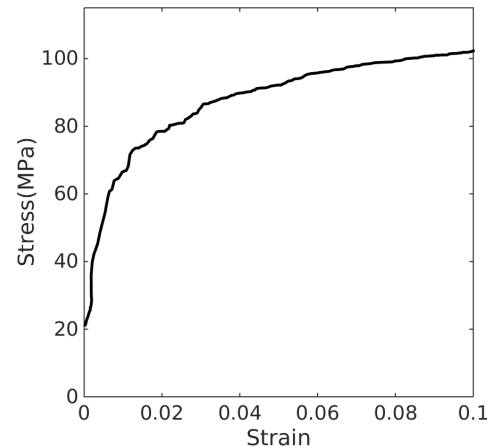**Figure 1.** Overall heat treatment cycle.

Figure 2. Flow curve obtained from Gleeble$^{\circledR}$.

4. Virtual testing for flow curves

In order to obtain the effective macroscale flow curve, virtual compression tests were performed on the phase field simulated microstructure using FEM implemented in the commercial software Abaqus$^{\circledR}$. The phase field simulated microstructure was assumed to be the Representative Volume Element (RVE). Figure 4 shows a phase field simulated microstructure in which the white colour represents the ferrite phase and the grey colour represents austenite phase. The RVE was meshed with C3D8 elements and periodic boundary conditions were applied. The properties of the individual phases, ferrite and austenite were obtained from JMatPro$^{\circledR}$ database, for an austenitization temperature of 950 °C and an initial grain size of 10 μm. The initial grain size input was based on the experimentally observed initial austenite grain size, taken by averaging the data from several optical micrographs. Figure 3 shows one such optical micrograph of the initial austenite grains. The RVE was uniaxially loaded at 790 °C and the average von Mises stress and effective strain of all the elements in the microstructure were recorded to obtain the effective macroscopic flow curve. Figure 5 shows the von Mises stress distribution in the microstructure for an applied strain of 2%.

Linear rule of mixture (ROM) is one of the methods for obtaining the macroscale properties from the properties of individual phases and their phase fractions. The flow curve for the material can be calculated using ROM with the following equations:

$$\sigma = \sigma_\gamma V_\gamma + \sigma_\alpha V_\alpha \,, \tag{3}$$

$$\varepsilon = \varepsilon_\gamma V_\gamma + \varepsilon_\alpha V_\alpha \,, \tag{4}$$

where σ_γ and σ_α are the true stress, ε_γ and ε_α are the true strain and V_γ and V_α are volume fraction for austenite and ferrite phase respectively. This approach is also used in some of the
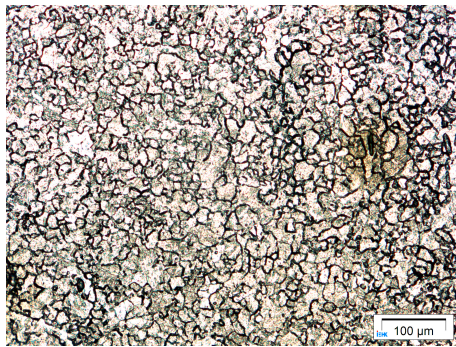
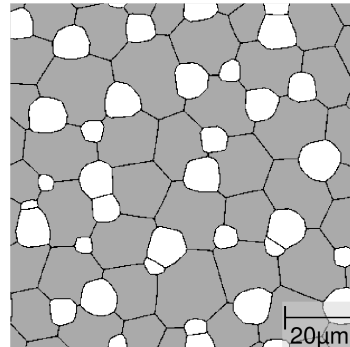**Figure 3.** Representative light optical micrograph showing the prior austenite grains austenitized at 950 °C .

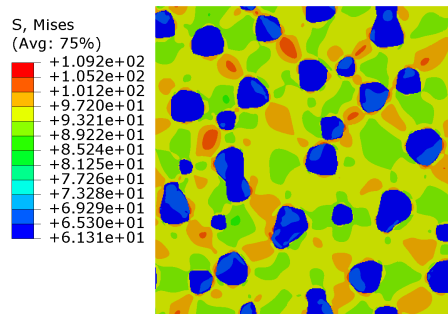**Figure 4.** Phase field simulated microstructure in Micress®.

Figure 5. von Mises stress distribution during virtual test, for an applied strain of 2%.

commercial softwares for the calculation of properties. Hence, in the present work the results obtained from virtual tests are also compared with that obtained using ROM.

4.1. Simulations with and without consideration of grain orientations
While performing the virtual test simulations, the orientation of the grains are important, especially to distinguish two grains of same phase. Hence, a study was conducted to see the effect of the grain orientation assignment on the virtually obtained flow curve. Figure 6 shows the flow curves obtained when the orientation of the grains are not taken into account, along with the flow curve of austenite and ferrite phases, flow curve obtained with ROM and the macroscopic flow curve obtained from experiment. The microstructure was loaded in X and Y directions and both yielded same results. When the orientation of the grains are not taken into account, the virtually simulated flow curve matched closely with that of ROM, but both of these showed considerable deviation from the experimentally obtained flow curve. In order to consider the grain orientations, a random orientation was assigned to the grains using Micress® and these orientations were exported to the FEM software. Though the orientations were assigned to the grains, the material properties assigned were isotropic. Figure 7 shows the virtually obtained flow curve, along with the experimentally obtained flow curve and the one obtained by ROM. The virtually simulated flow curve deviated from ROM and moved closer to the experimentally obtained flow curve.

4.2. Simulations with varying initial grain size in JMatPro^®
For obtaining the flow curves for the individual phases(austenite and ferrite) from JMatPro^®, the austenitization temperature and the initial austenite grain size are to be provided as the inputs. The austenitization temperature in the present study is 950 °C and the initial austenite grain size is 10 μm. But, the model used in JMatPro^® predicted an initial austenite grain size of 30 μm for an austenitization temperature of 950 °C. Hence, a study was conducted to see the effect of varying the initial grain size in JMatPro^® on the final flow curves obtained by virtual test. The grain size was varied from 10 μm to 30 μm. Figure 8 shows the flows curves obtained for initial grain sizes of 10, 20 and 30 μm. The difference in the flow curves is due to the difference in the properties of the individual phases predicted by JMatPro^®, when the initial grain size is varied. It was observed that for the grain size predicted by JMatPro^®, the simulated flow curves matched very closely to that of the experiment. Though the matching with experiment is better for the grain size predicted by JMatPro^®, in the following studies a grain size of 10 μm is used, since it is the actual grain size in the material.
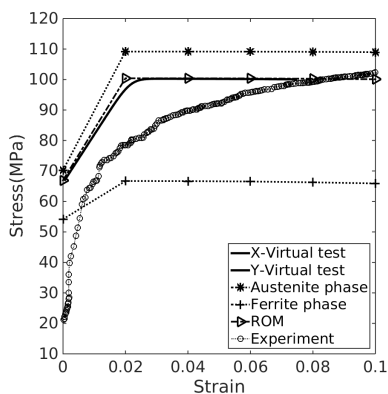

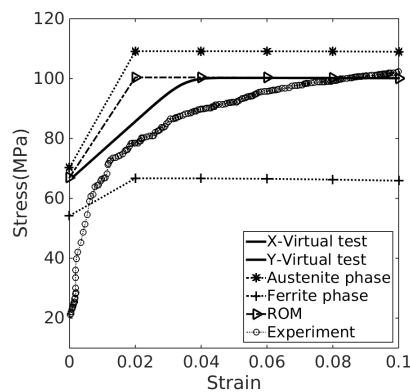**Figure 6.** Virtual test without considering grain orientations.

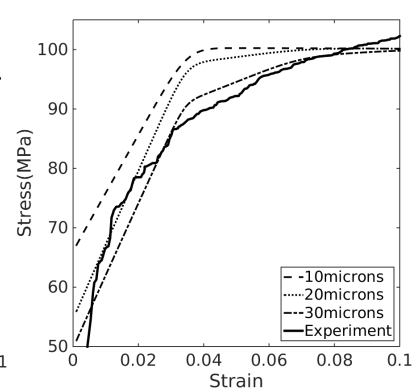**Figure 7.** Virtual test with random orientations assigned to grains.

Figure 8. Virtual test with varying initial grain size in JMatPro^®.

5. Towards the use of microstructure simulations for selection of process parameters for inter-critical annealing

The above simulation chain was repeated for different process parameters. The inter-critical annealing temperature and time was varied and the effect of these parameters on the virtually simulated flow curves was studied.

5.1. Flow curve variation with inter-critical annealing temperature
The inter-critical annealing temperature was varied between 720 °C and 780 °C in steps of 20 °C, for a constant holding time of 30 minutes. For each of these temperature, a phase field simulation was performed to predict the microstructure evolution during the cooling and holding after the solutionizing at 950 °C. Figure 9 shows the final microstructure obtained for various temperatures. White colour represents ferrite phase and grey colour represents austenite. With decrease in holding temperature, the final volume fraction of ferrite increased.

Virtual compression test was performed on each of the above simulated microstructure to obtain the flow curve. The properties of austenite and ferrite phases were obtained from JMatPro^® for an initial grain size of 10 μm and austenitization temperature of 950 °C. Figure 10 shows the variation of flow curves with annealing temperature. With increase in temperature,
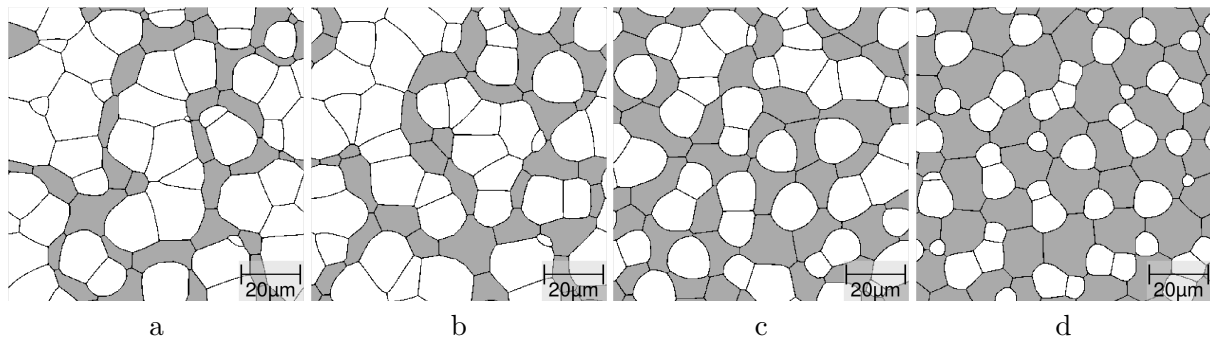
Figure 9. Final microstructure after 30 minutes holding at various temperatures: (a) 720 °C (b) 740 °C (c) 760 °C (d) 780 °C.

the flow curve shifted down. This decrease in the flow property is due to the combined effect of change in phase properties with temperature, change in volume fraction of phases and change in morphology. These combined effects are captured in the present methodology for obtaining the flow curves.

5.2. Flow curve variation with inter-critical annealing time
The inter-critical annealing time was varied for a constant holding temperature of 740 °C. The phase field simulated microstructure for each of the holding time was used to perform the virtual test for obtaining the flow curve. Figure 11 shows the flow curves obtained for various holding time. With increase in holding time, the flow curves shifted down. The primary reason for this decrease in flow property is the variation in the volume fraction of phases with time. There was only a slight change in the morphology with time during the isothermal holding.
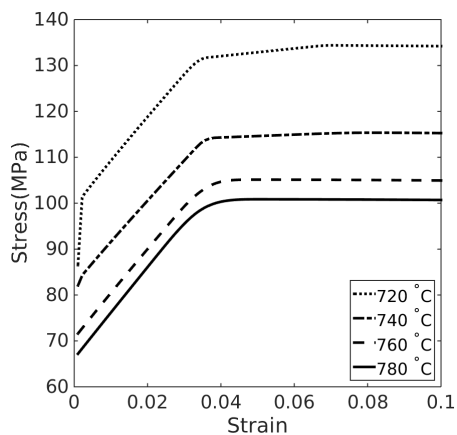

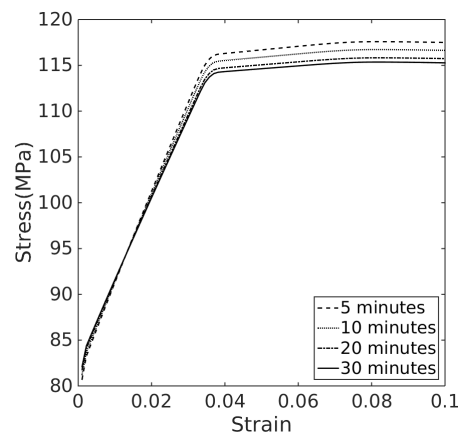**Figure 10.** Flow curve variation with inter-critical annealing temperature for a constant holding time.

Figure 11. Flow curve variation with inter-critical annealing time for a constant holding temperature.

6. Conclusions
The microstructure evolution in dual phase steel during heat treatment was simulated using phase field simulation. Virtual test was conducted on the simulated microstructure to obtain the

flow curve and a Gleeble$^{\circledR}$ simulation was performed to validate the virtual test results. It was observed that the orientation of the grains do play a role in obtaining an accurate prediction of flow curve using virtual test. On comparing the obtained flow curves with ROM, it was observed that when the orientation of grains were not considered, the virtual test results came very close to ROM, but both deviated from experimental results. On assigning random orientation to grains, it was observed that the virtual test results deviated from the ROM and came closer to the experimental results. The properties of the individual phases required for the virtual test were obtained from JMatPro$^{\circledR}$. These properties varied on varying the initial grain size input to JMatPro$^{\circledR}$. On using the initial grain size predicted by the model in JMatPro$^{\circledR}$ it was observed that the virtual test results came vary close to the experimentally obtained flow curve. The simulations were repeated for various inter-critical annealing temperatures and times. The methodology can be used in determining the inter-critical annealing process parameters required for achieving a particular flow property in a material. The present methodology is able to capture the combined effects of change in phase properties, change in volume fraction of phases and change in morphology with the variation in process parameters, within the limits of a two dimensional microstructure simulation.

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