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Microstructure based flow stress modeling for quenched and tempered low alloy steel

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ABSTRACT

Quenching and tempering (Q&T) process is commonly applied in part making industries for improving mechanical properties of carbon low alloy steels. After Q&T, microstructure of the steel consists of temper martensite and carbide precipitations. In this work, material modeling for describing flow stress behavior of the SNCM439 alloy steel under different tempering conditions was introduced. Microstructure based models were developed on both macro- and micro-scale. The models were afterwards applied in FE simulations for predicting stress–strain responses of the tempered steels. For the macroscopic model, the Ludwik equation was used, in which precipitation strengthening depending on particle size was incorporated by the Ashby–Orowan relationship. For the microscopic model, representative volume elements (RVEs) were generated considering microstructure characteristics of the examined steels. Flow curves of the individual constituents were described based on dislocation theory and chemical compositions. The FE simulations of tensile tests and RVE simulations under uniaxial tension were performed using the introduced models. The influences of the carbide precipitations on mechanical behavior of the tempered steels were investigated. The resulted effective stress–strain curves were determined and compared with the experimental ones. Both macroscopic and microscopic approaches accurately predicted mechanical properties and strain hardening behaviors of the tempered steels.

1. Introduction

To enhance mechanical properties of components made of low alloy steels with respect to application conditions are the main requisition of user. Several methods were developed and successfully integrated in the manufacturing process such as thermo-mechanical processing (TMP), warm and cold working with subsequent heat treatments. For example, rails steels for heavy haul are usually produced by the TMP, which significantly increases rolling contact fatigue and wear resistance [1]. Aeronautical bolts are manufactured by cold rolling and followed with heat treatment in order to maximize fatigue lifetime [2]. Quenching and tempering are one of the most frequently used heat treatment process for improving mechanical properties of carbon low alloy steels. As quenched microstructure of the steel consisted of almost complete martensite, which exhibited high strength and hardness, but very low ductility and toughness due to high dislocation density, elastic stress and complex morphologies [3]. Therefore, it was necessary to apply subsequent tempering to increase ductility of that as-quenched steel. Quenched carbon steels usually showed plate or lath martensite together with retained austenite depending on their carbon content [4]. For alloy steel, it was likely to obtain a fully martensitic structure, because alloying elements moved the diffusion-controlled transformation curves in transformation-time–temperature (TTT) diagram to longer time. By this manner, martensitic structure could be achieved at a slower cooling rate [5]. During the tempering of quenched alloy steel, various kinetic transformations took place and overlapped each other in four stages [5,6]. The first stage was around the temperature of 250 °C, at which the martensite (α' phase or supersaturated solution of carbon) transformed to a low carbon martensite (α'') by diffusion of carbon. It involved clustering of carbon to precipitation of iron carbide, especially the ε carbide ($Fe_{2.4}C$) [7,8]. The second stage was between 200 °C and 300 °C, during which retained austenite decomposed to bainite that was a form of α Fe with cementite needles (θ carbide, Fe_3C) [9–11]. By the third stage between 250 °C and 350 °C, the ε carbide was replaced by cementite, which started to coarsen and form a spheroid shape [12,13]. At the final stage, above 350 °C, growth and spherodization of cementite and other carbides occurred that

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followed by recovery or recrystallization of martensite above 600 °C [14,15].

The influences of tempering condition on microstructure developments and mechanical behaviors of quenched and tempered (Q&T) steels have been investigated in many works [16–21]. Otherwise, prediction of emerged microstructures and resulting mechanical properties by using empirical models and finite element (FE) simulation is challenging for the heat treatment process. Onel et al. [22] experimentally studied relationships between microstructure and mechanical properties of carbon steels after quenching and tempering. Three carbon steel grades were heat treated for producing microstructures consisting of ferrite and carbides at ferritic grain boundaries. Obtained results were analyzed in terms of the Hall–Petch equation for determining the effects of grain size as well as in term of the Ashby–Orowan relationship for evaluating the impacts of dispersed phases. Shi et al. [23] examined the effects of tempering on flow stress at elevated temperatures of a hardened steel and introduced then a quantitative model based on thermal history and material hardness. It was shown that modeling results agreed well with the experimental ones. By this model, the tempering effect on flow stress could be distinguished apart from softening mechanism because of the temperature rise. The model was also able to accurately predict hardness reduction caused by the tempering. Wan et al. [24] presented the effects of tempering time for quenched steel by using a mathematical model. This model was based on the Hollomon parameters, which correlated the hardness of the steel with the tempering time at different tempering temperatures. Smoljan [25] predicted mechanical properties and microstructure distribution of quenched and tempered work pieces with complex form. FE based simulations applying transient temperature fields were carried out. An algorithm for hardness prediction with regard to the Jominy test results was taken into account. Local hardness values of the specimen were determined by the conversion of calculated characteristic cooling time for phase transformation ($t_{8/5}$) to hardness. Smoljan et al. [26] described microstructure, hardness and threshold of fatigue crack initiation of quenched and tempered steel by means of FE simulations.

Currently, many researches focused on predicting flow stress behavior of steels with respect to their microstructure features. These approaches could be further connected with a through process modeling of the microstructure evolution of steels. By this manner, processing parameters for obtaining required mechanical properties of the steels could be optimized. Rodriguez et al. [27] predicted tensile curves of ferrite, pearlite, bainite and martensite of steels by using a unified formulation which was developed from the Voce type equation. This model was applied to fit the experimental tensile curves, which were associated with the different microstructures. The results were discussed in term of the characteristic sizes of each microstructure type. Uthaisangsuk et al. [28] characterized formability behavior of multiphase steels by using a micromechanical modeling. FE simulations of representative volume elements (RVEs) on the micro scale were conducted to describe influences of the heterogeneous microstructures on their mechanical properties. Sodjit et al. [29] predicted the overall stress–strain behaviors of dual phase steels. 2D RVE models, which were generated from real micrographs of the steels, were used. By this approach, dislocation theory, local chemical composition and geometrically necessary dislocations, which accumulate at the phase boundaries due to the austenite–martensite transformation during quenching process, were taken into account. Additionally, effects of microstructure banding, periodic boundary condition, 2D and 3D RVE models on calculated flow curves were examined by Ramazani et al. [30,31].

In this work, predictions of flow stress behavior of the JIS SNCM 439 steel under various Q&T conditions taking into account microstructure characteristics was aimed. By the experiments, the examined steel was austenitized, quenched in oil and subsequently tempered at five temperatures and two holding times. Metallographic analyses of these heat treated steels were performed using optical microscopy (OM), scanning electron microscopy (SEM). The X-ray diffraction (XRD) was used to identify occurred microstructure constituents. In addition, hardness and uniaxial tensile tests were carried out for determining mechanical properties of the steels. By the modeling, stress–strain behaviors of the Q&T steels were described on both macro- and micro-scales. The Ludwik's equation and Ashby–Orowan's equation [32] representing material strengthening due to carbide precipitation were applied for flow curve models in macroscopic FE simulations. In case of microscopic FE simulation, 2D RVEs were generated with respect to observed microstructures and flow stress models based on a dislocation strengthening theory and chemical compositions were applied for individual constituents [27]. Finally, the effective stress–strain responses predicted by both macroscopic and microscopic simulations were compared with the experimental results.

2. Experiments

2.1. Quenching and tempering

In this work, medium carbon low alloy steel grade JIS SNCM 439 supplied as hot rolled-round bar with the diameter of 25.4 mm in an as-annealed condition was used. The chemical compositions of the investigated steel are listed in Table 1.

First, the investigated steel was prepared for metallographic analyses and tensile tests. For the microstructure examination, specimens with a diameter of 10 mm and a height of 10 mm were used. For the uniaxial tensile test, tensile specimens according to the standard DIN EN ISO 6892–1:2009–12 [33] were machined in the longitudinal direction of the as-received hot rolled cylindrical steel bar. The specimens had a nominal gauge length of 25 mm, nominal width of 5 mm and 1 mm thickness. By quenching and tempering, as depicted in the temperature–time diagram in Fig. 1, all specimens were austenitized at the temperature of 870 °C about 10 min for obtaining a fully austenitic structure [34]. It was then followed by oil quenching to produce a martensitic structure [16]. Afterwards, quenched specimens were tempered at the temperatures of 450, 500, 550, 600 and 650 °C with the holding times of 1 and 3 h. After the heat treatments, specimens were ground, polished and etched for the metallographic analyses. A picric acid solution with 5 ml $C_6H_3N_3O$ acid, 2.5 ml $FeCl_3$, 2 ml HCl acid and 90 ml C_2H_5OH was used to reveal carbides and prior austenite grain boundaries in the emerged microstructures. The optical microscopy, SEM and XRD were applied for characterizing the microstructures and identifying the carbide precipitation of the steels under each Q&T condition.

2.2. Uniaxial tensile testing

Tensile tests with a crosshead speed of 0.5 mm min^{-1}, which corresponded to a quasi-static strain rate of 0.00033 s^{-1} were performed for the specimens under different Q&T conditions. Three repeated specimens of each condition were used. During the tests, force and displacement curves were recorded by means of a load

Table 1
Chemical compositions of the investigated steel, in weight fraction%.

Elements	C	Mn	Si	P	S	Ni	Cr	Mo
Wt.%	0.387	0.695	0.273	0.025	0.017	1.871	0.768	0.156