Research on microstructure and hardness of AISI1050 disk based on FDM and FEM methods during quenching process

Yishuai Zhang¹,a, Jia Fu ²b*, Hongxing Sun¹,³,c, Hua Liu ¹,d*

¹ Zhengzhou Research Institute of Mechanical Engineering, Co.,Ltd., China Academy of Machinery Science and Technology, Zhengzhou, 450001, China;
² School of Materials Science and Engineering, Xi'an Shiyou University, Xi'an, 710065, China
³School of Mechanical Engineering, Xi'an Jiaotong University, Xi'an, 710049, China
a email: zhangyishuai@bit.edu.cn, cemail: sunhx@zrime.com.cn
* Corresponding author: bemail: fujia@xsyu.edu.cn, demail: liuhua@zrime.com.cn

Abstract: Microstructures of AISI1050 disk during quenching were simulated by DEFORM-HT, and corresponding parameters of mechanical properties were investigated by applying the algorithm of finite difference method (FDM). Above all, thermo-physical parameters and diagrams of CCT curve were calculated by JMATPRO. Besides, the simulation of multi-phase microstructure considering initial thermo-physical parameters was realized by DEFORM-HT. The volume fraction of single phase were obtained by the FDM method, and then a weight function considering carbon equivalent of phases was introduced to predict the final hardness of multi-phase and according to the quenched microstructure and independent single phase hardness simulated. Temperature field, stress field and microstructure change of an AISI1050 disk under different quenching processes were studied by using the DEFORM-HT software numerical simulation calculation, combined with the continuous cooling transition curve (CCT curve) of AISI1050 steel. The martensite transformation of the disk tread during the quenching process can increase the wear resistance. According to the actual working conditions combined with the CCT curve of AISI1050 steel, the hardness of the disk rim surface is 54.8 HRC, which can meet the requirements of 51-56 HRC. It is concluded that the maximum equivalent stress of the disk (the equivalent stress after unloading is the residual stress) is distributed near the disk inner layer in the inside of the plate to hand over the location. The microstructure of the specimen is observed and compared with the simulation results, which prove that the simulation results are reliable. The simulated hardness by using both JMATPRO and DEFORM-HT can provide some basis to predict the hardness on certain degree.

1. Introduction

In the process of quenching, microstructure can be seen as temperature’s derivatives [1], quantitative analysis of quenching process can be simplified and possible, and mechanical properties are inseparable both microstructure and temperature thus can be obtained by a series of algorithm. Microstructure research of quenching nowadays is mainly concentrated in metallographic observation, heat-transfer coefficient [2-3], phase-field model [4], martensitic transformations theory [5], temperature
field calculation [6], TTT/CCT diagrams simulation [7] and a kind of the phase-field simulation [8]. During quenching process, phase transformation is accompanied by the changes of temperature field, which can be investigated to provide useful information for calculation of phase volume fractions.

JMATPRO is commonly used to calculate TTT/CCT diagrams and thermo-physical properties of carbon steel, low alloy steels, Cr–Mo steels [9], aluminum alloys [4], multi-component alloys [10,11] and nickel-based super alloys [11]. It can also be enlarged to investigate high temperature deformation behavior [13,14], to establish the phase-field model [4] and to predict mechanical properties [15].

The phase transformation of low carbon bainitic martensitic steel wheel and the residual stress of wheel rim during quenching were studied and analyzed by using DANTE and ABAQUS softwares [16]. Nejad et al. [17] simulated the heat treatment of the wheel with the finite element method, the effects of creep, latent heat of phase change, surface temperature and heat transfer coefficient on the residual stresses of wheel. In this paper, the temperature, residual stress, hardness of the wheel quenched by Deform-HT software are studied, and the microstructure was simulated by finite element method, and the microstructure was analyzed by experiment. In previous research, we have investigated microstructures of 316LN by the experiment [14] and hardness of AISI1050 steel by the nano-indentation simulation [15], which helps us to investigate another medium-carbon alloy steel -AISI1050 steel. As a kind of medium-carbon alloy steel, AISI1050 steel is mainly used to produce the disk of train wheel, gear, gear as a kind of medium-carbon alloy steel shaft, friction disk and mandrel [18]. Sunay [19] has studied microstructures and mechanical properties of AISI1050 steel during quenching process and it holds a higher wear resistance under complicated load condition. AISI1050 steel disk during quenching process in this work is aim to get the relationship between multiple-phase hardness and single-phase hardness, and then provide the quenched hardness model of AISI1050 steel.

This work is done based on the proposed assumption that hardness is the function of phase hardness and its volume fraction. The phase volume fractions are calculated by the finite difference method (FDM) and thus the hardness model is proposed. The hardness prediction model was verified by hardness experiment. Metallographic observation and hardness experiment were carried out and a kind of hardness model was given out by using finite difference method (FDM). The investigation provides a great significance for the practical application.

2. Method and procedure

2.1 Microstructure simulation by FEM

Quenching process is in accordance with heat transfer theory, Fourier theorem and Newton's cooling law, so temperature change meets the Eqs. as follows:

\[
\begin{align*}
\rho c \frac{\partial T}{\partial t} + \nabla \cdot (q) &= H \\
q &= -k \nabla T = h(T_s - T_a)
\end{align*}
\]

(1)

Where \( \rho \) represents the density, \( c \) is the heat capacity, \( T \) is the temperature, \( H \) is the heat generation rate per unit volume, \( \nabla \) is the gradient operator, \( q \) is the heat flow, \( k \) is the thermal conductivity, \( q_e = h(T_a - T_s) \) is heat convention boundary condition [20].

The temperature field distribution accompanied by time and internal thermal stress field can be obtained by the finite element method based on calculating Eqs. (1) from reference [17].

Assuming that the initial volume fraction of austenite is 1 and each phase transformation is independent, so only one phase transformation occurs in a certain temperature range. Transformation models of martensite, bainite and pearlite can be calculated by using the following Eqs.s from Eqs. (2) to Eqs. (5).

Lee et al. [21] has obtained martensitic transformation model to calculate volume fraction from austenite to martensite in low alloy steels. And the phase transformation model considering the effect of austenite grain size (AGS) can be modified by reference [22, 23]:
\[
\xi_M = \int 0.8435 \xi_M^{0.6587} \cdot (1 - \xi_M)^{1.2906} \, dT
\]  
(2)

Where \(\xi_M\) represents the volume fraction of martensite, and \(T\) is the transformation temperature.

For volume fractions of ferrite/pearlite and bainite, the values of \(\log f_\ell(T)\) and \(n\) can be obtained by coefficients of \(C_{ij}\) and \(D_{ij}\).

Bainite transformation model to predict volume fraction from austenite to bainite is proposed by Garrett et al. [24], which is shown in Eq. (3):

\[
\xi_B = \int A \exp\left(\frac{T^* - T}{B}\right) \left(1 - \xi_B^*\right)^n \exp\left(-\frac{G^*}{RT}\right) \, dt
\]

(3)

Where \(\xi_B\) represents the volume fraction of bainite; \(A, B, n, \gamma\) are material constants, within these constants; \(r^*\) represents the critical bainite radius; \(G^*\) is the critical value at which nucleation may take place; \(T^*(\varepsilon)\) is the experimental data, \(t\) represents the growth time.

Pearlite transformation model drawn from theoretical calculation by Capdevila et al. [25] is shown in Eqs. (4) as follows:

\[
\xi_P = 1 - \exp\left(-\frac{3.35}{d_a^2} \left(1 - F\right)^2 \cdot G \cdot t \cdot f(G, I, t)\right)
\]

(4)

Where \(\xi_P\) represents the volume fraction of pearlite; \(d_a\) is the austenite grain diameter; \(F\) is the volume fraction of pro-eutectoid ferrite transformed before pearlite reaction starts; \(G\) is particles growth rate; \(f(G, I, t)\) is the ratio of extended area of pearlite on one plane; \(t\) represents the growth time.

Johnsen-Mehl-Avrami Eqs. [26] has described the transformation from austenite to ferrite + pearlite and to bainite, which is shown in Eqs. (5) as follows:

\[
\xi_{\alpha} = 1 - \exp\left(-f_\ell \left(T(t)\right)\right) \cdot t^r
\]

(5)

Where \(\xi_{\alpha}\) is the volume fraction of austenite transformed; \(f_\ell(T)\) and exponential \(n\) are both functions of temperature \(T\); \(t\) is transformation time.

Values of \(n\) and \(f_\ell(T)\) derive from isothermal phase transformation diagrams and can be expressed as:

\[
\begin{align*}
\log f_\ell(T) &= C_{w_i} + C_1 T + C_2 T^2 + C_3 T^3 \\
2n &= D_{w_i} + D_1 T + D_2 T^2 + D_3 T^3
\end{align*}
\]

(6)

Volume fractions of martensite, bainite and pearlite in a unit can be obtained if other material constants in corresponding Eqs.s are known to us. Volume fraction of pro-eutectoid ferrite below \(A_{c1}\) is determined by an extended line of equilibrium phase boundary of austenite and austenite/cementite [27] and thus calculated by \(A_{cm}\) temperature curve [28]. Here \(C_{ij}\) and \(D_{ij}\) can be calculated by using finite difference method (FDM).

2.2 Calculation of Multi-phase properties

Maynier [29] has proposed that phase hardness of alloy steel is the function of cooling rate \(V_r\) and its composition by experiment, and each phase hardness quotation is given out as follows:

\[
\begin{align*}
HV_{C} &= 127 + 949 C + 27S + 11Mn + 16Cr + 21\log V_r \\
HV_{Si} &= 323 + 185C + 330Si + 153Mn + 144Cr + 191Mo + (89 + 53C - 55S - 22Mn - 20Cr - 33Mo)\log V_r \\
HV_{F-P} &= 42 + 223C + 55S + 30Mn + 7Cr + 19Mo + (10 - 19Si + 8Cr)\log V_r
\end{align*}
\]

(7)

Where \(V_r\) is the cooling rate, \(C, Si, Mn, Ni\) and \(Cr\) are separately for each weight percentage.

To describe the relationship between volume fraction of matrix phase and its hardness, weight function is introduced to reflect the contribution of each phase to hardness with considering carbon equivalent of phases. Supposing the volume fraction of retained austenite is less than 0.05 in low alloy steel, the carbide volume fraction is included in the volume fraction of martensite because the growth reaction of the transition carbide formed during quenching is controlled by the diffusion of the iron atoms through the dislocations of the martensitic structure [30]. Transforming the value of hardness from HV into HRC by Eqs.(7), quenching hardness model can be described by single phase (martensite \(M\), bainite \(B\) and ferrite-pearlite \(F-P\)) hardness and its weight coefficient, which is
described as follows:

\[
HRC = \beta_M HRC_M + \beta_B HRC_B + (\beta_F + \beta_B) HRC_F + \beta_a HRC_a
\]

Where \(\xi_M, \xi_B, \xi_F, \xi_B\) and \(\xi_{\text{ret}}\) represent volume fractions of martensite, bainite, ferrite, pearlite and retained austenite in a unit. \(\beta_M, \beta_B, \beta_F, \beta_B\) and \(\beta\) represent weight coefficients of martensite, bainite, ferrite and pearlite modified by the simulation results of DEFORM-HT. \(\beta\) is calculated by the total value of others phase’s. Amount of phase’s portions and weight’s portion s are equal to 100%, that is: 

\[
\xi_M + \xi_B + \xi_F + \xi_B + \xi_{\text{ret}} = 1, \quad \beta_M + \beta_B + \beta_F + \beta_B + \beta = 1.
\]

Critical cooling rates \(V_r\) of various phases can be obtained by simulated CCT curves, and then it is substituted to the Eqs. (7), thus the theoretical hardness of single phase can be calculated. By calculating the volume fraction and weight value of single phase, then substituting into Eqs. (2) (3) (4), the final hardness after quenching can be obtained.

2.3 Phase volume fraction calculation

Input parameter \(C_p\) (unit: J/kg·K) of 1050 steel obtained by reference [31], then substitute \(C_p\) into Eqs.(1) for heat transfer calculation, the relationship between cooling speed and temperature at various distance from surface can be obtained by finite difference method. The principle of finite difference method is described below.

For the axis-symmetric problem of heat transfer during quenching process, the Eqs.(1) can be simplified as the following Eqs. (10):

\[
\lambda \left[ \frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} \right] = c_p \rho \frac{\partial T}{\partial t}
\]

Where \(\rho\) is the density, \(T\) is the temperature, \(r\) is the radius of disk, \(t\) is the time, \(\lambda\) is the thermal conductivity coefficient related with temperature and phase volume fractions, \(c_p\) is the specific heat at constant pressure.

According to the nonlinear heat transfer mentioned in Eqs.(10), axisymmetric problem above can be solved by using FDM, and the finite difference scheme is obtained as follows:

\[
T_{i+1}^j = \Delta t \left[ \sum_{i=1}^{n} \xi_j (c_p \rho_i + \Delta H) \Delta r \right] \left[ \alpha_1 T_{i+1}^j + \alpha_2 T_{i}^j + \alpha_3 T_{i-1}^j \right]
\]

Where \(k_1, k_2, k_3\) and \(k_4\) separately represent austenitic, ferrite/pearlite, bainite and martensite, \(\Delta r\) is the space within internal nodes of difference mesh, \(\Delta t\) is the time step, \(r_j\) is the radial coordinates of node \(j\), \(\Delta H\) is the phase transaction latent. \(\lambda_j, \rho_j, c_p_j\) separately represent thermal conductivity coefficient, density and specific heat capacity at constant pressure of node \(j\) at moment \(i\). \(\alpha_1, \alpha_2\) and \(\alpha_3\) are corresponding coefficients related with thermal conductivity coefficient and phase volume fraction.

Coefficients of \(\alpha_1, \alpha_2, \alpha_3\) and \(\Delta t\) are described as:

\[
\alpha_1 = \lambda_j + \lambda_i \left[ \frac{1}{\Delta r} + \frac{1}{r_j} \right]
\]

\[
\alpha_2 = \sum_{i=1}^{n} \xi_j (c_p \rho_i + \Delta H) \Delta r \left[ \frac{\lambda_j + \lambda_i}{2 \Delta r} + \frac{\lambda_j + \lambda_i}{2 \Delta r} \right]
\]

\[
\alpha_3 = \lambda_i \left[ \frac{1}{\Delta r} + \frac{1}{r_{j+1}} \right]
\]

\[
\Delta t = 2 \Delta r \cdot c_p \rho / \left[ \frac{k_{j+1} + 2 k_j + k_{j-1}}{r} - \frac{k_{j+1} - k_{j-1}}{r} \right]
\]

The boundary condition simplified for calculation is shown in Eqs. (16):

\[
\lambda (T_{i+1}^j - T_{i}^j) / \Delta r = h (T_i^j - T_{\text{in}}) + c_p \rho (T_{i+1}^j - T_{i}^j) / (2 \Delta t)
\]

Where \(T_i^j\) is the temperature at moment \(i\) and node \(j\), \(T_{\text{in}}\) is the temperature of quenching medium, \(h_0\) holds its value 5.5 W/(K·m²).
transformation can be calculated on condition that the calculation of each temperature range is independent without other phase transition. In order to further verify the numerical algorithm and to analysis the simulation results, the quenching experiment is then carried out on HR-150A Rockwell tester and the microstructure is observed by VEX-600E metallographic microscope.

3. Results and Discussion

3.1 Calculation procedure
The initial conditions are as follows: averaged thermal transfer coefficient 27 N/(s·mm·°C), quenching temperature 880°C, time step 0.02s, step number 2500. Latent heat of phase transformation of ferrite/pearlite, bainite and martensite during simulation are 6.02×10^8 J/m³, 4.40×10^8 J/m³ and 6.28×10^8 J/m³ respectively. Convective heat is mainly considered, and ability data simulated by JMATPRO is obtained and then imported the simulated Jominy quenching harden curves into Deform-HT. Intensively mesh the nearby surface of disk and add material model and phase transformation models (Demo_Temper_Steel.KEY files), the simulated temperature field, hot stress field, microstructure distribution and hardened layer distribution are finally obtained and displayed.

3.2 Microstructure and hardness distribution
The simulated microstructure and hardness after quenching at step 2200 are shown in Fig.2.
As is shown in Fig.4, quenching at 880 °C in 6%AQ251, the surface is mixed microstructure of bainite-martensite in main, while the center is mixed ferrite-pearlite. Phase volume fractions under various phase transformations are observed in Fig.4 and shown in Tab.1).

| Distance from surface | 0mm | 10mm | 20mm | 25mm | 40mm |
|-----------------------|-----|------|------|------|------|
| Phase Fractions (%)   | F+P | B    | M    |      |      |
|                       | 0   | 0    | 100  | 0.008| 1.126| 4.923|
|                       | 1.126| 36.301| 51.263| 17.652|

These volume fractions of ferrite/pearlite, bainite and martensite are then substituted into the equation (7), and the theoretical hardness of multiple phases can be calculated.

The surface hardness is about 52.4HRC on average and the central part is about 27HRC, which is approachable to the surface hardness 54.8 HRC and center hardness 28.2 HRC calculated from Eqs. (7). To decrease the error, a proper weight function is introduced to modify the simulated hardness so as to predict the hardness, and phase transformation characterization is furtherly investigated by experiment below.

For comparison, the experimental hardness was tested on HR-150A Rockwell hardness tester, with the impact toughness was measured on JB-300B pendulum impact tester. The microstructure is lath martensite + lower bainite + carbide + a small amount of retained austenite. Within the lath martensite, there are retained austenite lamellae, which improves the toughness. The obtained fracture morphology is typical dimple fracture and belongs to ductile fracture. The comprehensive mechanical properties is the best when quenched at 880 °C, air-cooled and tempered at 250 °C. After tempering at 250 °C, the tempered martensite and lower bainite are uniformly distributed, and the hardness is even. The averaged experimental quenched hardness is 53.25 HRC at surface on average (impact toughness over 18J/cm²), which is close to the simulated hardness value of 52.40 HRC at surface on average. The relative error between measured average hardness and hardness calculated in equations are within 5%, indicating that numerical simulation to predict the hardness has certain guidance.

4. Conclusions

Based on the thermo-physical parameters calculated by JMATPRO, the quenching process (cooling from 880 °C to 150 °C by 6% AQ251 quenchant ) is simulated on DEFORM-HT software. Results are as follows:

(1) The simulated microstructures after quenching are mainly the type of martensite + bainite at surface and the type of pearlite + ferrite at centre.

(2) The average hardness is 54.8HRC on surface and average hardness 28.2HRC at centre based on the FDM, which are accord with the experimental ones with the relative error only 4.72% on surface and 3.57% at centre.
(3) The hardness fitting model after quenching based on the experimental value was put forward, which can help us to predict hardness distribution. This work is aim to explaining more about the relationship between final hardness and single phase by introducing the FDM method and a weight function.

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