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The Evolution of Microstructure for Carburizing and Quenching 17CrNiMo6 Steel: Forecasting and Experimentation

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Abstract: This paper investigates the evolution of the microstructure of 17CrNiMo6 steel produced by carburizing and quenching through computer-aided engineering (CAE) and experimental study. The chemical composition, microstructure, and properties vary from surface to the core during the carburizing and quenching, which makes the CAE simulation of temperature field and microstructure evolution more complex. The performance–temperature and field performance–microstructure iterations using different simulation methods are applied. The results showed that the CAE forecast microstructure evolution is consistent with the experiment. The error between the predicted and experimental values from the surface to 2000 µm is 5%–9%, and the predicted results are consistent with the experiment at the depth of 2000 µm.

Keywords: carburization; quench; simulation; temperature field

1. Introduction

This gear is generally used for transmission devices. According to the service condition of the gear, it should be capable of frequently withstanding great force and braking load shocks. On this basis, the level of endurance, fatigue strength, and impact toughness for gear steel should meet these requirements [1,2]. 17CrNiMo6 steel is a kind of high-strength low carbon alloy steel used for gear steel. The chemical components of the 17CrNiMo6 steel sample were measured with Spectro type M10, as shown in Table 1.

Carburizing heat treatment is a type of chemical heat treatment. When carbon is diffused into the steel surface through carburizing heat treatment, martensite will form during subsequent quenching. The formation of a hard superficial layer leads to the improvement in wear and fatigue properties due to the hardening with a compressive state on the surface [3–5]. In addition, discovering the accurate physical model is difficult [6,7]. As computer technology is constantly progressing, it has been used to analysis the microstructure and stress of the materials after heat treatment. Nowadays, CAE has been used in the designation of new materials or new alloys, simulation of the process of research, and observation of the microstructure and composition. Multiple CAE methods including thermodynamic analysis and the finite element method are used to calculate the microstructure and the property of materials. Some researchers [8–14] have proposed several numerical simulations using the finite element method (FEM) to solve this problem. Consequently, the use of numerical simulation with thermal-mechanical-metallurgical coupling is essential to achieve a better understanding of the effects of quenching heat treatment on the quality of cooled parts, allowing for the evaluation of properties that cannot be measured experimentally. Based on the above research, the present work aims to use the combination of various CAE methods, using the method of cyclic iteration, the...
material properties, and temperature field, and the precision of microstructure calculation is improved.

Table 1. Chemical components.

| Element | C      | Cr      | Ni      | Mo     | Mn     |
|---------|--------|---------|---------|--------|--------|
| Standard (wt.%) | 0.15–0.20 | 1.5–1.80 | 1.4–1.70 | 0.25–0.35 | 0.40–0.60 |
| Sample (wt.%)   | 0.17   | 1.65    | 1.60    | 0.30   | 0.50   |

2. Experimental Method

The carburizing 17CrNiMo6 steel specimen consists of two steps; see Figure 1. The specimen has a size of 50 × 50 × 30 mm. JMatPro (version 5.0), a software for the calculation of thermodynamics, has been used in the simulation of the carburizing process [15–17]. Calculating the quenching properties makes it possible to find the overall cooling rate of the specimen from the surface to the core. Cycle methods require the calculation of properties from surface to core. MSC.Marc version 2017 software (MSC Corporate, Irvine, USA) was used for the finite element simulation of the quenching heat treatment of a steel specimen with the geometry shown in below; MSC.Marc [18] was used to model the distribution of temperature during quenching. The boundary conditions and thermal quantities of the model are mentioned below. Finally, the cooling curve was derived from the case to the core [6]. To obtain microstructure distribution, the curve must first be fit before calculating the properties. Meanwhile, metallographic and phase analyses of the material are carried out from the case to the core, including metallographic test and phase analysis.

Figure 1. Carburizing and quenching process chart.

3. Experimental Procedure of Simulation

3.1. Procedure of Simulation on Carburizing

The thickness of the carburized layer can be measured using two standards [19,20]. The first one is the chemical composition and the other one is the effective depth of the hardened layer. According to the standard, the effective hardening depth of 17CrNiMo6 steel is about 3.05 mm. JMatPro software (version 5.0) is a simulation software for material properties, which can simulate the gradient distribution of carbon concentration and thickness of the metal material carburizing layer. It can also simulate the changes of microstructure and properties of materials under different heat treatment processes. It classifies computing modules by material type, including nickel-based superalloy, aluminum alloy, magnesium alloy, steel, and so on. In this paper, the steel module of JMatPro software is used to
simulate the microstructure evolution during the quenching process of 17CrNiMo6 steel. The carbon amounts from the case to the core, as below.

Figure 2 shows that the depth of the carburized layer is about 3.9 mm. Based on the chart, the chemical composition of different layers is achieved. From the surface to 2 mm, the amount of carbon changes rapidly. It is basically flat with the base metal at the depth of 3.5 mm, which has been ready for the property. This is because of the great importance of the cooling rates on the microstructure and property of the steel. The hardness of the steel will be higher with the increase in the cooling rate, and the toughness will be lower [21–23]. Therefore, to achieve more accurate results, during the calculation of the properties of the steel, it is necessary to use the methods of performance–temperature field and performance–microstructure iterations [24]. For the first time, the calculation of the properties from the case to the core is achieved through the steady-state module. Figures 3 and 4 are the thermal conductivity and specific heat of the surface calculated by JMatPro software. At the critical point of phase transition, the thermal conductivity and specific heat capacity will decrease significantly.

![Figure 2. Carbon amount.](image1)

![Figure 3. Thermal conductivity of the surface.](image2)
3.2. Procedure of Simulation on the Temperature Field during Quenching

The quenching temperature field is simulated by the software MSC.Marc, which is based on the finite element [25]. The mesh distribution of finite element is shown in Table 2.

Table 2. Sets’ distribution.

| Set Number | 1   | 4   | 6   | 7   | 10  |
|------------|-----|-----|-----|-----|-----|
| Depth (µm) | 0–200| 200–400| 400–600| 600–800| 800–1000 |
| Set number | 11  | 12  | 13  | 14  | 15  |
| Depth (µm) | 1000–1500 | 1500–2000 | 2000–2500 | 2500–3000 | 3000–core |

After simulation, the cooling rates of quenching will be obtained according to the chemical composition of different layers. To obtain the more precise result, three surfaces are divided into smaller sets, as in Table 3.

Table 3. The fitting function of node 1.

| Temperature Interval | Intercept | Slope |
|----------------------|-----------|-------|
|                      | Value     | Standard Error | Value     | Standard Error |
| 830–700              | 798.29    | 24.39     | –168.54  | 6.66      |
| 700–600              | 720.26    | 1.76      | –36.89   | 3.74      |
| 600–500              | 688.50    | 0.48      | –20.69   | 2.63      |
| 500–400              | 635.54    | 0.22      | –16.41   | 2.49      |
| 400–300              | 596.03    | 0.21      | –13.69   | 3.88      |
| 300–200              | 525.58    | 0.22      | –10.55   | 5.85      |
| 200–100              | 350.89    | 0.31      | –5.14    | 16.34     |
| 100–65               | 92.46     | 0.08      | –0.21    | 7.79      |

From Figure 5, the changes in temperature and time will be achieved. The distribution curve shows the variation trend of every node. For a better view, we set node 1 as an example. The cooling condition is shown in Figure 6. For the first node, as an example, the temperature changes rapidly at the beginning of quenching, and slowly as time passes.
Table 2. Sets’ distribution.

| Set Number | Depth (μm) |
|------------|------------|
| 1          | 0–200      |
| 4          | 200–400    |
| 6          | 400–600    |
| 7          | 600–800    |
| 10         | 800–1000   |
| 11         | 1000–1500  |
| 12         | 1500–2000  |
| 13         | 2000–2500  |
| 14         | 2500–3000  |
| 15         | Core       |

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Figure 5. Temperature field cloud picture and cooling curve of nodes. (a) $t = 0$ s, (b) $t = 2.43$ s, (c) $t = 31.16$ s, and (d) cooling curve.

Figure 6. Cooling curve of node 1.
3.3. Calculate the Properties Cyclicly

Quenching is a meta stable state. To obtain the more precise results of the properties, the method of cycling was used. When the cooling curves of different layers were obtained, they were fitted into functions on account of the cooling profile wizards where needed.

Comparing the original cooling curve to the curve that has been fitted, the trend of both curves is the same in general. The fitted function is input into the meta stable state of JMatPro to calculate the properties from the case to the core for the second time. The thermal conductivity and specific heat of different layers were calculated in a more accurate way, as shown in Figures 7 and 8.

![Figure 7. Thermal conductivity of node 1 after one cycle.](image)

![Figure 8. Specific heat of node 1 after one cycle.](image)

3.4. Simulation of the Temperature Field after a Cycle

The temperature field through MSC.Marc was simulated a second time, applying the properties calculated in the cycle method. Then, the same model was taken advantage of with the first simulation. The cooling curves were set as follows (Figure 9).
Figure 8. Specific heat of node 1 after one cycle.

3.4. Simulation of the Temperature Field after a Cycle

The temperature field through MSC.Marc was simulated a second time, applying the properties calculated in the cycle method. Then, the same model was taken advantage of with the first simulation. The cooling curves were set as follows (Figure 9).

Comparing the curve of node 1 before to the cycle, we can see that the trend of the curve is the same in general, but there is also something different, which can prove that the curve using the cycle method is more accurate.

3.5. Calculate the Microstructure Field

When the curves achieved the second time were fitted as shown in Table 4, JMatPro was used to calculate the microstructure field, including the distribution and the variation during the quenching. The curves of different layers were fitted and the functions were obtained, as well as the cooling rates. Table 5 shows the cooling rate of the node on the core.

Table 4. Cooling rate of the node on the surface.

| Temperature Interval | Intercept | Slope |
|----------------------|-----------|-------|
|                      | Value     | Value |
|                      | Standard Error | Standard Error |
| 830–700              | 806.58   | 5.49  |
| 700–600              | 731.49   | 4.35  |
| 600–500              | 657.73   | 4.71  |
| 500–400              | 592.91   | 4.98  |
| 400–300              | 464.45   | 9.63  |
| 300–200              | 395.34   | 3.32  |
| 200–100              | 305.43   | 8.34  |
| 100–65               | 89.65    | 6.95  |

Table 5. Cooling rate of the node on the core.

| Temperature Interval | Intercept | Slope |
|----------------------|-----------|-------|
|                      | Value     | Value |
|                      | Standard Error | Standard Error |
| 830–700              | 825.40   | 1.16  |
| 700–600              | 813.29   | 2.59  |
| 600–500              | 770.99   | 5.71  |
| 500–400              | 664.91   | 11.25 |
| 400–300              | 529.92   | 3.58  |
| 300–200              | 483.56   | 6.83  |
| 200–100              | 360.03   | 14.69 |
| 100–65               | 82.81    | 6.05  |
The calculation of the microstructure field and the variation in microstructure are shown in the following charts. From the chart, we can obtain the temperature and the time at which martensite occurs.

Figures 10 and 11 show the temperature and the time at which phases like martensite and bainite occur on the surface. Similar to martensite, which occurs at 165 °C and 40.98 s, when the time goes to 53.86 s, the temperature drops to 122.5 °C and the content of martensite reaches 50%. After quenching, the final structure is 9.65% austenite and 90.35% martensite, among which there is a very small amount of bainite. According to the cooling curve and CCT continuous cooling transformation curve, there should be no bainite at the surface cooling rate. The tissue content calculated by software is 0.01% bainite, and the content is extremely small. Compared with the charts that show the cooling curves and continuous cooling transformation curves, it is easy to illustrate that there is little bainite existing on the surface and a little bainite in the core of the model. Comparing the tissue composition obtained by calculation and simulation with that obtained by the cooling curve and CCT diagram, it can be seen that the tissue obtained by simulation and that deduced by the cooling curve and CCT diagram are approximately the same (Figures 12 and 13).

![Figure 10](image1.png)

**Figure 10.** Phases changes with time.

![Figure 11](image2.png)

**Figure 11.** Phases changes with temperature.
4. Results and Discussion

4.1. Simulation Results

The distribution of the microstructure field is shown in the following charts. It indicates which microstructure occurs at what temperature and when. The time and temperature at which martensite starts to occur, as well as when and at what temperature the martensite goes to 50% from the case to the core, are chosen.

We can see that different layers have different sequence of martensite and bainite, as well as the final distribution of every type of microstructure. From Table 6, dynamic distribution of the microstructure from the case to the core is achieved. In general, the temperature at which martensite occurs has a rising trend, and when it comes to a depth of 4000 μm, the temperature remains steadily at 369 °C. The carbon content is the main reason for the change in the starting temperature of martensite. At the same time, that is, the time that the microstructure occurs, martensite occurs firstly at a depth of 4000 μm.

Table 7 shows the final distribution of the steel from the case to the core. As shown in Figure 14. As time passes, martensite occurs at a depth closer to the surface. Because of heat conduction, martensite finally occurs in the steel at the core. The transformation
rate of steel at the core is much slower than that near the surface, so martensite finally occurs here.

Table 6. Dynamic distribution of the microstructure from the case to the core.

| Depth (µm) | Martensite Start (s) | Martensite 50% |
|------------|----------------------|----------------|
|            | Time t(s) Temp T (°C)| Time t(s) Temp T (°C) |
| 0          | 41.19 164.37         | 53.86 122.5     |
| 200        | 39.84 168.75         | 52.96 125.46    |
| 400        | 39.56 169.68         | 51.94 128.82    |
| 600        | 40.07 174.53         | 52.08 132.5     |
| 800        | 30.45 187.5          | 42.17 145.0     |
| 1000       | 35.19 203.43         | 44.93 161.25    |
| 1500       | 27.69 254.68         | 33.89 216.25    |
| 2000       | 21.69 303.12         | 27.41 265.0     |
| 2500       | 19.90 334.37         | 24.14 296.25    |
| 3000       | 18.61 353.75         | 22.92 316.25    |
| 4000       | 18.76 369.06         | 23.48 331.25    |
| 6000       | 22.64 369.76         | 27.47 335.0     |
| 8000       | 25.76 369.76         | 30.59 335.0     |
| 10,000     | 28.74 369.76         | 33.37 335.0     |
| 15,000     | 33.93 369.76         | 38.91 334.37    |

Table 7. Final distribution of steel from the case to the core.

| Depth (µm) | Austenite% | Martensite% | Bainite% |
|------------|------------|-------------|----------|
| 0          | 9.64       | 90.34       | 0.01     |
| 200        | 9.14       | 90.85       | -        |
| 400        | 8.57       | 91.42       | -        |
| 600        | 7.99       | 91.99       | 0.01     |
| 800        | 6.20       | 93.79       | -        |
| 1000       | 4.54       | 95.44       | 0.01     |
| 1500       | 1.46       | 98.50       | 0.03     |
| 2000       | 0.49       | 99.36       | 0.14     |
| 2500       | 0.23       | 99.16       | 0.60     |
| 3000       | 0.14       | 98.71       | 1.14     |
| 4000       | 0.09       | 97.98       | 1.92     |
| 6000       | 0.08       | 98.21       | 1.69     |
| 8000       | 0.08       | 98.08       | 1.83     |
| 10,000     | 0.08       | 97.97       | 1.932    |
| 15,000     | 0.08       | 97.37       | 2.54     |

Figure 14. The content of microstructure of different layers.
On the other hand, the content of martensite has a rising trend from the case to the core. On the contrary, the content of austenite declines. From the chart, we also know that there is a little bainite existing near the core and little bainite near the surface, which is the same as in the simulation of JMatPro mentioned above.

4.2. Experiments Results of Microstructure and Phase

Layer by layer, metallographic experiments were performed from the case to the core. A Carl Zeiss Axiovert 200 MAT metallographic microscope (Carl Zeiss Microscopy GmbH, Germany) was used. The carburized samples were cut into samples of $10 \text{ mm} \times 10 \text{ mm} \times 15 \text{ mm}$ by electric spark wire cutting machine, and specimens were ground by 180 to 1200 grit sandpapers, polished with chromic oxide, and subsequently etched by 5% Nital. The following chart is the carbon distribution shown in the model. The picture shows that the carbon has a trend from the case to the core (Figure 15).

Moreover, the microstructure is shown on the metallograph from the case to the core. It shows the case, as well as depths of 20, 40, 60, 80, 100, 120, 160, 180, 200, and 600 $\mu m$, and the core.

The metallograph of Figure 16a is the microstructure of the depth of 20 $\mu m$. According to the carbon contribution, there is a higher carbon content than that near the core. Corrosive liquid is a solution of nitric acid alcohol of 4%. Because the cementite is corroded easily by this type of solution, cementite will appear as a small white shape under the metallographic microscope. Thus, the small white shapes in the metallograph in Figure 16 are the microstructure—cementite. Figure 16b,c shows that there are more white small shapes in (b) than in (l), and the small white shapes in Figure 16d–j also show a downtrend, which proves that, the deeper the depth, the lesser cementite content there will be.

From Figure 16a, it is not very easy to clearly make out the outline of the martensite. When the depth is deeper in Figure 16d–f, the outline of the martensite becomes clearer. In the Figure 16h, when the depth is 120 $\mu m$, the outline of martensite is clear enough. In Figure 16h, where the depth is about 600 $\mu m$, the number of small white shapes reduces and the martensite is the acicular martensite. Figure 16l shows the micrographic of the core, where the shape of martensite is oversized because of the cooling rates.

Thus, according to the experiments on metallography, the carbon content, as well as the cementite, reduces from the case to the core, and the outline of martensite becomes more clear. The carbon martensite in the core is low.

At the same time, phase analysis was carried out on the workpiece layer by layer. X’Pert PRO multifunctional X-ray diffractometer (Cu target Kα ray, $\lambda = 0.154 \text{ nm}$) was used to analyze the phase of carburized samples. The operating voltage and current were 40 KV and 40 mA, respectively, and the scanning range was $20^\circ$–$140^\circ$. The XRD patterns were analyzed by the software Highscore. Compared with the standard of PDF card, the answers are showed in Figure 17.
Figure 16. The metallograph layer by layer: (a) case, (b) depth of 20 µm, (c) depth of 40 µm, (d) depth of 60 µm, (e) depth of 80 µm, (f) depth of 100 µm, (g) depth of 120 µm, (h) depth of 160 µm, (i) depth of 180 µm, (j) depth of 200 µm, (k) depth of 600 µm, and (l) core.

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Figure 17. The content of the microstructure from XRD.

Figure 18 shows that there are seven peaks at each depth of the workpiece. Four of them are peaks of austenite and the others are martensite. The double peaks at the large degree were taken into consideration in the calculation and the content of different layers from the case to the core was obtained using the direct and contrast method. Table 8 displays the answer, and the table is displayed as a chart. The chart shows that the content of martensite presents an increasing trend and the austenite presents a reducing trend, which is same as the result of the simulation.

Table 8. The content of the microstructure from XRD.

| Depth (µm) | Martensite (%) | Austenite (%) |
|-----------|----------------|---------------|
| 20        | 95.99631845    | 4.003681549   |
| 60        | 78.00152027    | 21.99847973   |
| 120       | 83.2360707     | 16.7639293    |
| 190       | 82.97027584    | 17.02972416   |
| 280       | 88.87531497    | 11.12468503   |
| 500       | 95.60167217    | 4.398327833   |
| 580       | 98.990674      | 1.009326002   |
| 1000      | 99.50605689    | 0.493943112   |
| 2000      | 99.44403915    | 0.555960854   |

Figure 17. The content of the microstructure from XRD.
Figure 18 shows that there are seven peaks at each depth of the workpiece. Four of them are peaks of austenite and the others are martensite. The double peaks at the large degree were taken into consideration in the calculation and the content of different layers from the case to the core was obtained using the direct and contrast method. Table 8 displays the answer, and the table is displayed as a chart. The chart shows that the content of martensite presents an increasing trend and the austenite presents a reducing trend, which is same as the result of the simulation.

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| Depth (µm) | Martensite %  | Austenite %  |
|-----------|---------------|--------------|
| 20        | 95.99631845   | 4.003681549  |
| 60        | 78.00152027   | 21.99847973  |
| 120       | 83.2360707    | 16.7639293   |
| 190       | 82.97027584   | 17.02972416  |
| 280       | 88.87531497   | 11.12468503  |
| 500       | 95.60167217   | 4.398327833  |
| 580       | 98.990674     | 1.009326002  |
| 1000      | 99.50605689   | 0.493943112  |
| 2000      | 99.44403915   | 0.555960854  |

4.3. Comparison of the Simulation and Experimental Results

Taking the results of both the simulation and the experiments into consideration shows that the trends of the two results are the same in general; that is, the content of austenite has a reducing trend and the content of martensite has an increasing trend from the case to the core. Moreover, there is little bainite that exists near the core.

Inevitably, a computation error exists in the process of the whole simulation, including the cycle method as well as experiments. However, the evolution of the steel during the carburizing and quenching was also proven (Figure 19).
Figure 18. X-ray diffraction pattern from 20°~130°.

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Figure 19. The content of the microstructure from XRD.

5. Conclusions

Comparing the simulation results with the experimental results can provide a reference for the evolution of microstructure forecast and text for carburizing and quenching 17CrNiMo6 steel. The main conclusions can be summarized as follows.

(1) The carburized layer depth obtained from the simulation is 3.9 mm, which conforms to the contribution of carbon content from the case to the core.

(2) The cycle method helps to calculate the properties from the case to the core and simulate the temperature field in quenching as well as the microstructure field, which has proved that the martensite starting temperature becomes higher as the carbon content becomes lower. Thus, from the surface to a depth of 4000 µm, $M_S$ has a downwards trend and, when it comes to a depth of 4000 µm or even further, $M_S$ becomes steady because of the same carbon content. Thus, the depth at which martensite occurs is 4000 µm, thus it occurs near the surface. On account of the conduction of heat transfer, martensite occurs lastly in the part near the core. From the case to the core, the martensite content becomes higher and little bainite occurs.

(3) The metallographic test shows the microstructure condition of layers from the case to the core, which helps to analysis the contribution of the microstructure. The low carbon martensite in the core appears to have a clearer outline than that of other layers. The content of cementite is greater at the surface of the carburized layer than at that of base metal, which is suitable for regular carburizing.

(4) The X-ray diffraction experiment shows that both austenite and martensite exist in the 17CrNiMo6 steel after carburizing and quenching. The content of martensite increases and the content of austenite decreases from the surface to the core, which is the same as the results of the simulation.

(5) The CAE forecast microstructure evolution is consistent with the experiment. The error between the predicted and experimental values from the surface to 2000 µm is 5%–9%; the predicted results are consistent with the experiment at a depth of 2000 µm.
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