Mathematical Model of Heat Treatment and Its Computer Simulation

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Abstract : Computer simulation on heat treatment is the foundation of intelligent heat treatment. The simulations of temperature field , phase transformation , stress/strain complicate quenching operation were realized by using the model of three dimensional non-linear finite element method and the treatment methods of abruptly changing interface conditions. The simulation results basically fit those measured in experiments. The intelligent sealed multipurpose furnace production line has been developed based on the combination of computer simulation on gaseous carburizing and computer control technology. More than 3000 batches of workpieces have been processed on this production line , and all are up to standard. The application of computer simulation technology can significantly improve the loading ability and reliability of nitriding and carburizing workpieces , reduce heat treatment distortion , and shorten carburizing duration. It is recommended that the reliable product design without redundancy should be performed with the combination of the CAD of mechanical products , the CAE of materials selection and heat treatment , and the dynamic evaluation technology of product reliability.

Key words :heat treatment ; mathematical model ; computer simulation ; intellectualization

1 Introduction

Heat treatment is the principle process used to improve the loading capacity , durability and reliability of the products. However , because the complicated phenomena happened during heat treatment are quite difficult to be observed and measured directly , the quality of the treated workpieces is often hard to be ensured ; or because the full latent capacity of the materials is not utilized , the volume , mass and etc. of the workpieces have to be increased. Therefore , heat treatment has become a bottleneck to limit the level of the manufacturing.

With the assistance of computers , multidisciplinary knowledge including materials , heat transfer , elastic-plastic mechanics , fluid mechanics and mathematics can be integrated to build the quantitative mathematical models describing the various phenomena and their interactions , which can be used to understand the overall process , to control precisely the quality of heat treatment , to optimize the techniques and develop novel techniques and equipments. Therefore , mathematical modeling and computer simulation of heat treatment are the foundation of intelligent (knowledge intensive) heat treatment , and also the leading edge of this field in the world[1-3] .

2 Retrospection

The microstructure transformation , stress and strain behavior during heat treatment have already been studied since the early 1970s[4] . A temperature-microstructure model was established in the 1980s , followed by a temperature-microstructure-stress/strain model[2,5] , as shown in Fig. 1 , where ① represents the effects of temperature on microstructure transformation ; ② is the effects of transformation latent on temperature field ; ③ is the effects of temperature on stress field ; ④ stands for the stress induced by phase transformation ; ⑤ is the effects of stress on transformation rate (dynamics) ; and ⑥ represents the effects of stress on temperature field.

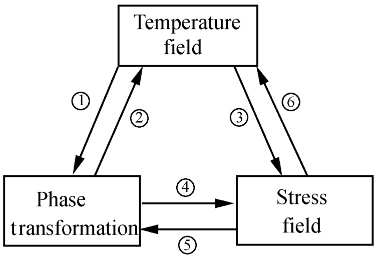

Fig. 1 The relationship between temperature field , stress field , phase transformation during heating or cooling

①—The effects of temperature on microstructure transformation ; ②—The effects of transformation latent on temperature field ; ③—The effects of temperature on stress field ; ④—The stress induced by phase transformation ; ⑤—The effects of stress on transformation rate (dynamics) ; ⑥—The effects of stress on temperature field

With the efforts of scholars from all over of the world , the mathematical modeling and computer simulation have been greatly developed , and the numerical methods used to solve the nonlinear transient temperature field have also been well established[6] . The research results such as phase transformation during non-isothermal continuous cooling and heating , coupling model between temperature and microstructure have provided good conditions for the computer simulation[7,8] . In the calculation of thermal and structural stress , FE methods and thermal elastic-plastic model were adopted recently. During strain analysis the elastic strain , plastic strain , thermal strain , phase transformation strain and transformation plasticity strain were considered. The exceeding yield limit , mathematical models considering yield function and strain strength have already been developed[2,9,10]. The effects of stress on transformation dynamics were even reported[9,11]. The above researches have built a good basis for the modeling of coupled temperature-microstructure-stress/strain fields.

However , the application of heat treatment simulation is developed so slowly that there is no definite report on its large-scale application in production so far. According to the analysis , the main obstacles lie on that (1) most simulation works are based on one-or two-dimensional model , whereas the practical workpieces are three-dimensional ; (2) in most quenching simulations single quanchant is only considered , whereas different quenchants are frequently used in different stages of cooling ; (3) the precision of simulation is not satisfying ; (4) most simulation works are not incorporated tightly with computer control and equipment design.

3 Achievements

In order to improve the present situation , Shanghai Jiaotong University has done a series of researches on the computer simulation of heat treatment.

3.1 Computer simulation on heat treatment of workpieces with complex shapes and complex quenching operations

In the early 1990s , a three-dimensional model was established to simulate the heating process , and the simulated results were in good agreement with the experimental results in salt-bath furnace , electric resistance furnace and large gas furnace. The heating-up period of the stepped shaft in the large gas furnace was shortened from the previous 20 h to 14 h.

In the 1990s , the project "Computer simulation on quenching with abruptly changed interface conditions and quenching technique CAD" supported by National Natural Science Fund was completed , and the temperature , microstructure , stress/strain variations during complex quenching operations were successfully simulated. For example , the temperature distribution in a jack catch during quenching is very complicated (as shown in Fig. 2). Because the thickness of the jack catch is quite different in different section , the catch has high tendency to generate quenching crack , therefore , a complicated operational process such as pre-cooling → water quenching →oil quenching or pre-cooling →water quenching →self-tempering should be adopted to cool the catch. In different stages of cooling , the surface heat transfer coefficients have difference of several orders in magnitude , so the cooling process can only be simulated by the method of abruptly changing boundary conditions to correctly predict the microstructure and performance distributions. The simulated results agreed well with the experimental results (see Fig. 3)

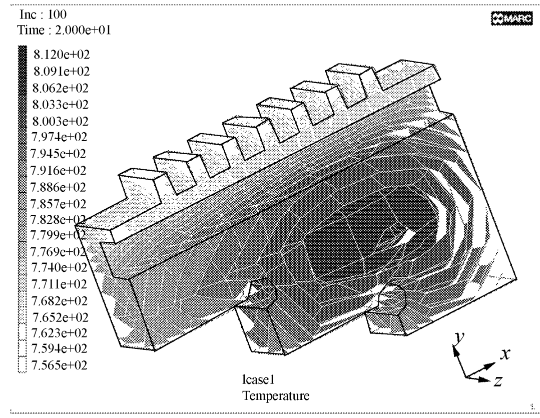

Fig. 2 Temperature field in austenized jack catch after pre-cooling 20 s in air

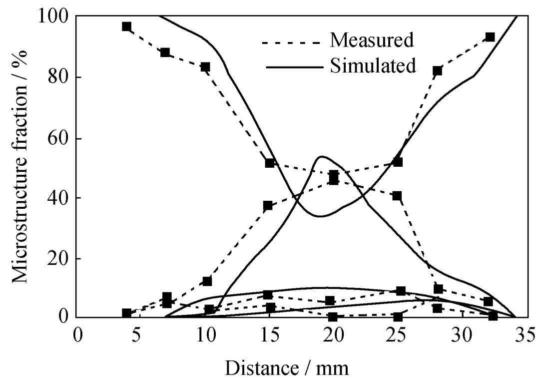

Fig. 3 Microstructure distribution on the section of jack catch after quenching

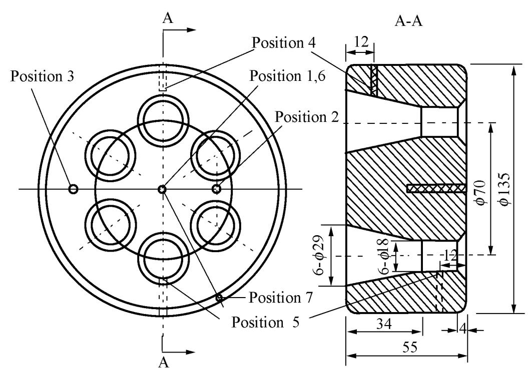

Fig. 4 Schematic of anchor ring part

1 —Temperature measuring hole Φ2. 5 mm , depth 27. 5 mm ; 2 —Temperature measuring hole Φ2. 5 mm , depth 53 mm ;3 —Temperature measuring hole Φ2. 5 mm , depth 27. 5 mm ; 4 —Temperature measuring hole Φ2. 5 mm , inner surface of hole ; 5 —Inner surface of hole ; 6 —Central point on the face with little peristome of hole ;7 —Middle point on side surface with height of 27. 5 mm

The inner hole of an anchor ring(see Fig. 4) is required to have enough hardness ,but the thin wall between neighboring holes makes quenching crack form easily. Fig. 5 is the contour of the simulated microstructure distribution in the anchor ring during quenching. The simulated temperatures are in accordance with the experimental results in different positions of the anchor ring during quenching with pre-cooling →water quenching →self-tempering (Fig. 6) , and so is the microstructure distribution after quenching.

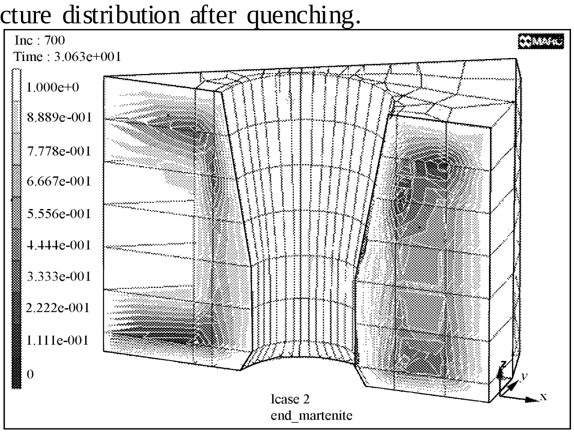

Fig. 5 Simulation on martensite transformation process in anchor ring during quenching

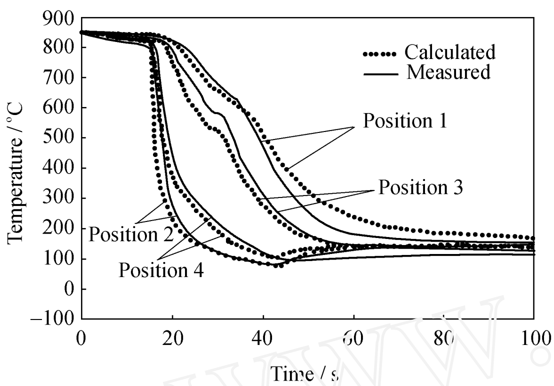

Fig. 6 Comparison of cooling curves between simulation results and measured values in different positions of anchor ring during complicated quenching operation (pre-cooling → immersed quenching →self-tempering)

Contact fatigue failure is among the significant failure patterns of the high hardness cold roller. After heat treatment , it is required not only that the surface of the cold roller possesses high hardness , but also that residual compressive stress is formed in the surface layer to counteract the contact stress. Fig. 7 shows the simulated residual stress distribution in the

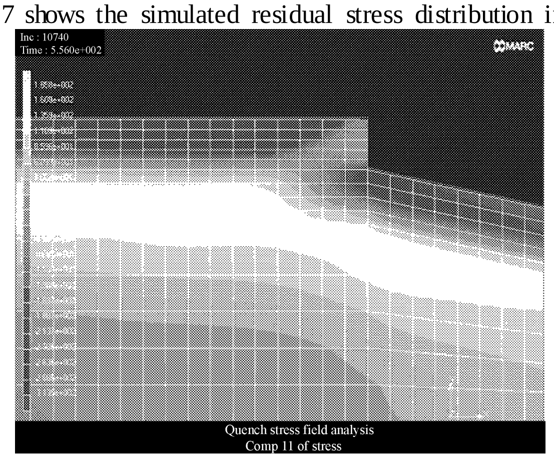

Fig. 7 Computer simulation on stress field of high hardness cold roller during quenching

cold roller (ϕ170) after quenching , which agrees well with the experimental results (Fig. 8) . According to the simulated results , proper quenching medium and method can be chosen to get a reasonable residual stress distribution of the cold roller.

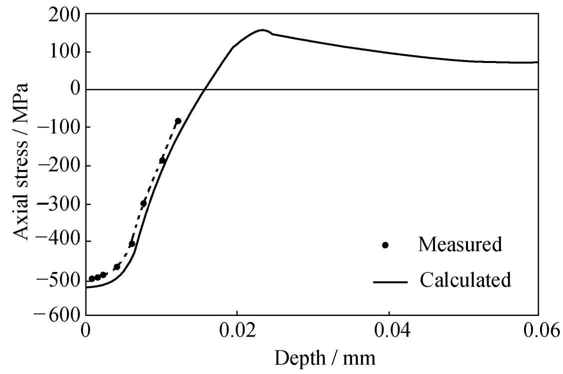

Fig. 8 Comparison of residual stress distribution between simulated results and experimental values on the cold roller (ϕ170) after quenching

3. 2 Mathematical modeling and computer simulation of carburizing (or nitriding)

The research and application of mathematical modeling and computer simulation of carburizing and nitriding in China have the following features , compared to the same work abroad.

(1) The furnace temperature , furnace gas composition , carbon or nitride potential , diffusion coefficient transfer coefficient and so on are regarded as the functions of time to well simulate the real manufacture. The simulated and measured results were in accordance (see Fig. 9) .

(2) The influence of shape factors on the concentration distribution in the layers is indicated (Fig. 10) .

(3) Computer simulation and process control are integrated into intelligent automation control technology. The carburizing process is automatically simulated , the techniques are automatically optimized and the process is automatically controlled. No paper is required in production (Fig. 11) .

(4) Traditional control technology of gas carburizing can only eliminate the difference between acquired and set values (Fig. 12a) . The dynamic carbon potential control technology with on-line calculation of mathematical model (Fig. 12b) can eliminate the influence of these differences on the final carburizing results and guarantee the quality and reproducibility of carburizing.

3. 3 Application

3. 3. 1 Development of automatic production line of intelligent hermetic chamber furnace Collaborating with Fengdong Heat Treatment LTD , Shanghai Jiaotong University applied some of these achievements into automatic production line of intelligent hermetic chamber furnace , which has already put into operation and treated over 3000 batches of workpieces so far without error and condemned stores. Moreover , the heat

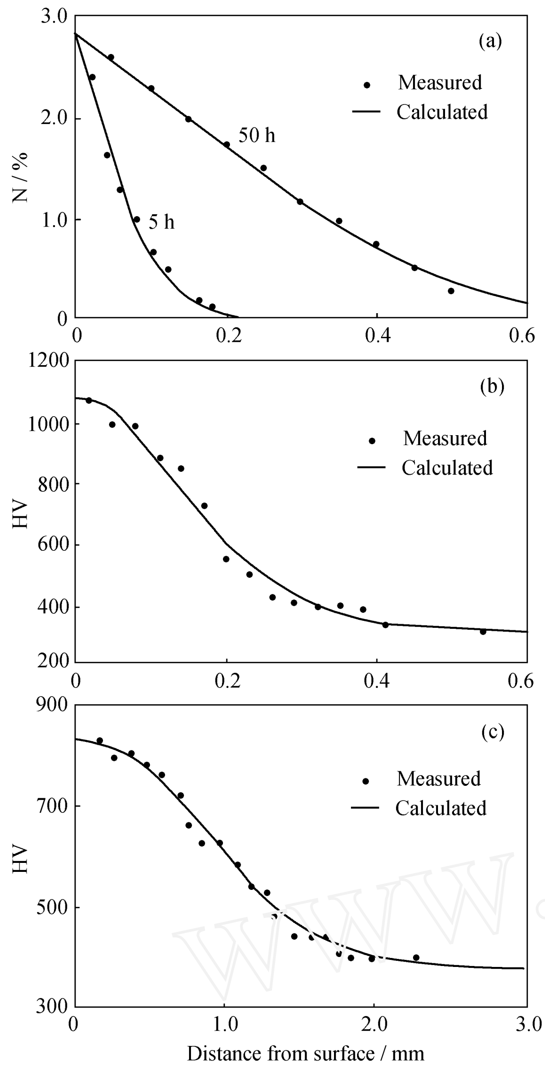

Fig. 9 Simulated and measured nitrogen profile and hardness distribution

(a) Nitrogen profile of 38CrMoAl steel after controlled nitrided at 510 ℃; (b) Hardness profile of 38CrMoAl steel after nitrided at 510 ℃for 50 h ; (c) Hardness distribution in carburized 20CrMnTi steel

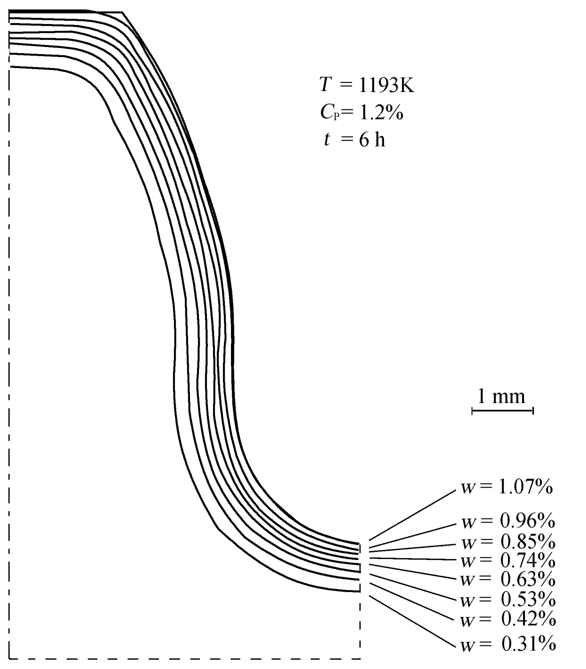

Fig. 10 Computer simulation on carbon concentration profile of surface carburized gear

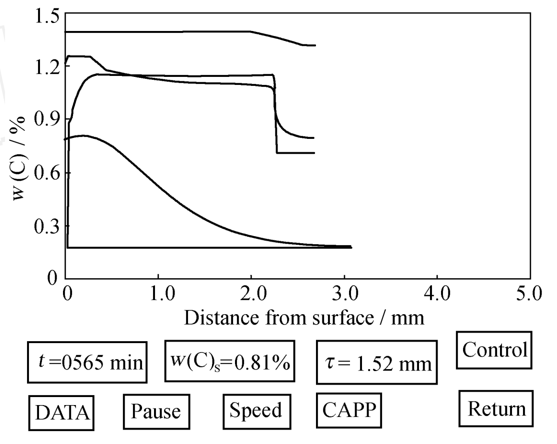

Fig. 11 Simulation on carburizing process and optimum technology parameters programming automatically performed by computer control system

treatment quality was highly improved and the carburizing period was shortened from 6. 5 h to 5. 75 h per batch.

3. 3. 2 Improvement of the service properties of case-hardened parts High-speed heavy-loaded gear treated by traditional technology in the power station boiler , with the rotation speed of 6000 r/min and the power of 4600 kW , was easily damaged and the speed change box was broken. After dynamic carbon potential control technology was employed , a flat concentration distribution curve was acquired and the loading capacities of the gears were well improved. Now the gears treated by this technology have already been in mass production and in safe operation.

The mechanical downdraught cooling tower used in large petrochemical or steel enterprises , serving in formidable conditions due to its limited installation space , was damaged frequently when treated by traditional technology. However , the reduction gear in the cooling tower treated by dynamic carbon potential control technology is all in safe operation and has already been in mass production and exportation.

Treated by high concentration carbrizing and dynamic carbon potential control technology , the high-power diesel engine cam produced in Guangdong Diesel Engine Corp. has a steady hardness higher than the upper limit in normal carburizing (> 62HRC) , and its service life is greatly prolonged.

3. 3. 3 Improvement of the service properties of nitrided parts

The wear resistance of the nitriding layer treated by this technology was doubled , as shown in Fig. 13 , and its contact fatigue strength was also improved from 1400 MPa to 1700 MPa. In another case , the load factor of the bi-arc gear of speed change box for ship treated by this technology reached 735 MPa , which is 25 % higher than that of normal nitriding.

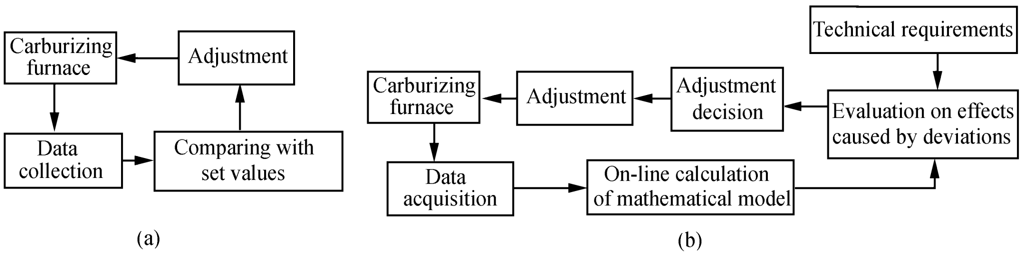

Fig. 12 Comparison between (a) traditional technology of carbon potential control and (b) dynamic carbon potential control technology

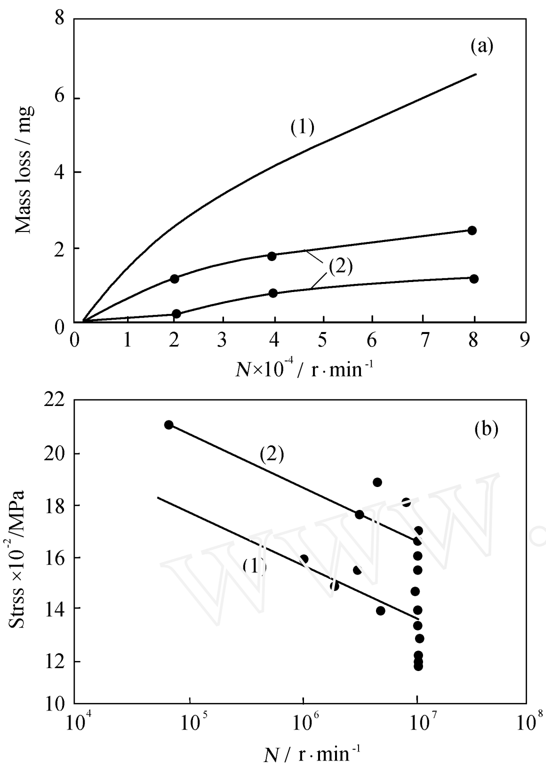

Fig. 13 Test results of specimens treated by dynamic controlled nitriding technology and traditional nitriding technology

(a) Wearing testing; (b) Contact fatigue testing

(1) Traditional nitriding; (2) Dynamic controlled nitriding

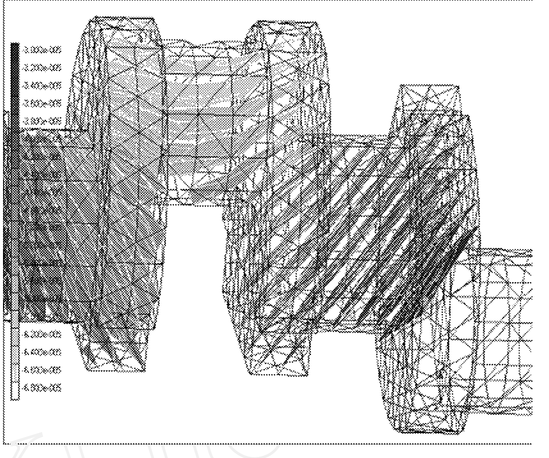

Fig. 14 Computer simulation on deformation of nitriding heavy power high-speed diesel crankshaft made by 35CrMo steel

3.3.4 Deformation control of nitriding for a heavy power diesel crankshaft Computer simulation was employed to study the deformation of nitriding a crankshaft (Fig. 14), and thus the method was obtained to control the deformation in production.

3.3.5 Fluid dynamic simulation and furnace chamber design of an extra-large pit furnace for gaseous carburizing Fig. 15 shows the largest pit furnace for gaseous carburizing in Asia. The reasonability of gas flow in the furnace and temperature uniformity are the key points of furnace design and fabrication. After the problems of the schemes provided by several foreign electric furnace manufactures were pointed out, the furnace with the fluid dynamic simulation and furnace chamber design has already been built and put into production by China. Altogether, the fabrication cost was reduced by 11 $\times10^6$ RMB, whereas the temperature uniformity in the furnace chamber was less than ±3.5 ℃, better than the highest national standard (≤ ±5 ℃). Hundreds tons of parts treated in this furnace were all qualified, including the gear used in ship elevators in Shukou, Fujian province (with the diameter of 2800 mm, the largest case-hardened gear at that time), gears in 300 t main speed reducer pulling machine and extra-large rolling machine.

Fig. 15 Extra-large pit furnace for gaseous carburizing at Luoyang Mineral Machinery Factory

4 Conclusion

Mathematical modeling and computer simulation of heat treatment, as the basis of virtue production of heat treatment, has shown great potential. However, it should be pointed out that, because of its incompleteness and immature, the precision of simulation is still not satisfying so far and the models have to be modified by experimental results. The application scope of the models is restricted even under modification and validation. Further improvement of the simulation precision relies on the more difficult fundamental research. For instance, the calculation of the relationship between phase transformation and stress depends on the empirical formulation, which is only suitable to the particular types of steel. Without the breakthrough in relevant theoretical research, the adaptability of the model will not be broadened and the simulation precision will not be improved greatly either. Furthermore, the heat exchange of boiling medium and solid, combination of electromagnetic field, plasma field, multi-coupling simulations in different dimensions and so on are still under further investigation. If the achievement of mathematical modeling and computer simulation is benefit from the effective use of the fundamental theoretical knowledge with the aid of computer, its development will depend to a great extent on the acquisition of new knowledge, that is, the development of fundamental research.

Another important problem is that mathematical modeling and computer simulation technology should not be only restricted within production, and should be integrated with design and manufacturing. For example, product CAD and materials selection should be integrated with computer simulation of heat treatment and product reliability evaluation to construct a novel design base (see Fig. 16), carrying out high reliable, redundant free product design. It can be predicted that mathematical modeling and computer simulation will play more and more important role in the advanced manufacturing technologies.

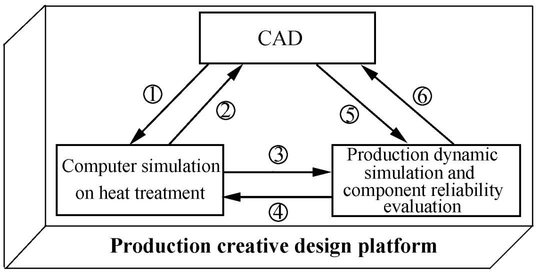

Fig. 16 Effect of heat treatment computer simulation on optimum products design

①Property index and dimension/ shape of component, ②Design rationality, ③Residual stress distribution and strength of component after heat treatment, ④Rationality of materials selection and heat treatment, ⑤Products design and serving conditions, ⑥Reliability and redundancy

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