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DESIGNING NITRIDING PROCESSES USING SIMULATOR OF THE KINETICS OF NITRIDED LAYER GROWTH

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Abstract

This article presents simulator of the kinetics of nitrided layer growth. Simulator of the kinetics of nitrided layer growth is an application, which supports new method of controlled gas nitriding called ZeroFlow. ZeroFlow method is used for nitriding selected car engine parts, such as crankshafts, camshafts, piston rings, poppet valve springs and discs, piston pins or nozzles for unit injectors. Through the use of simulation models, it is possible to develop the especially dedicated processes with specific parameters for each of this parts, which means that simulator of the kinetics of nitrided layer growth enables forming of nitrided layer with strictly defined properties: required phase structure with thicknesses of particular zones that occurs in it and required hardness distribution. Moreover, using simulation models this layers are obtained in the shortest possible time, which is connected with the lowest energy and gases consumption; therefore, nitriding process using ZeroFlow method (and simulator of the kinetics of nitrided layer growth) is both economical and environmentally friendly and meets with an increasing interest from the industrial consumers. Particular examples of industrial applications of simulator will be mentioned in article. Moreover, this article will show main functions, possibilities and advantages of simulator program; it will also present function called "simulation solver", which allows optimization of process parameters.

Keywords: *controlled gas nitriding, nitrided layer, process parameters, kinetics, simulator*

1. Introduction

Nowadays, simulations are commonly used during designing; usually they are used in the field of machine engineering and strength of materials. These simulations are carried out using programs such as AutoCAD, Matlab, Simulink, Patran or Femap. However, simulations can be carried out wherever it is possible to describe reality using mathematical models. In addition, some of heat treatment processes can be mathematically described, so it is possible to use simulations in designing new processes.

Simulations of heat treatment processes are a really important issue and they allow observing various phenomena, which usually are not perceived in industrial practice (sometimes even in experimental research). They can also be a part of regulation and control of the process. As an example of simulation of heat treatment, processes we can mentioned simulations of carburizing processes, successfully applied on a large scale in industry. Nevertheless, kinetics of nitrided layer growth is much more complicated than kinetics of carburized layer growth. Nitriding of iron can be accompanied by growth of the single-, double- or triple-phase layer (α, $\gamma'+\alpha$, $\varepsilon+\gamma'+\alpha$), where during carburizing only single-phase layer (austenite) is formed [4].

Based on his own research, L. Małdziński developed mathematical models of the kinetics of nitrided layer growth on iron and alloy steels; they are based on the phenomenological models of mass flow (nitrogen flow) and Fick's laws of diffusion [4]. Mathematical models describing kinetics of nitrided layer growth were imported into properly prepared application and as a result – simulator of the kinetics of nitrided layer growth has been created. It can be used to designing new processes of nitriding using ZeroFlow method.

2. Characteristics of ZeroFlow method

ZeroFlow is a new method of controlled gas nitriding, developed at the Poznan University of Technology, which enables precise forming of nitrided layers using nitriding kinetics. It is characterized by much lower consumption of gases, as well as simplification of the nitriding furnace and of the process itself, while full control over the kinetics of nitrided layer growth is still maintained. The same as in the traditional process, ZeroFlow method assumes the use of atmosphere consisting only raw ammonia. However, unlike to the traditional method, kinetics can be controlled by adjusting the chemical composition of the atmosphere in the furnace retort through the regulation of ammonia flow rate, or more precisely – through the regulation of ammonia inflow rate by stopping and reactivating ammonia feeding into the furnace retort. It is significant that in ZeroFlow method ammonia inflow rate is temporarily reduced to zero, which makes much easier to control the chemical composition of the atmosphere. To sum up, using a unary atmosphere makes the ZeroFlow method simpler than currently popular methods based on binary atmospheres, but simultaneously it allows controlling the kinetics of nitrided layer growth by regulating of ammonia inflow rate [5].

At average nitriding temperatures ammonia is in unstable thermodynamic state and because of the low durability of the molecules it disintegrate after contact with a metal surface, according to the following catalytic reaction of dissociation:

$$NH_3 \overset{Fe}{\Leftrightarrow} N + \frac{3}{2}H_2\,. \tag{1}$$

As a result of diffusion of atomic nitrogen into the steel surface, layer with different properties than original material (the material of the core) is formed. Its phase structure, zone thicknesses, and consequently – its properties – depend both on the type of the steel and the parameters of the nitriding process: temperature, nitriding potential of the atmosphere and time.

As a nitriding potential of the atmosphere we can describe a ratio of partial pressure of the atmosphere active ingredients. Atomic nitrogen and hydrogen, obtained by dissociation of ammonia, tends to recombine into diatomic molecules as soon as possible, whereas nitrogen diffusion occurs only when it is in atomic state – this means that is necessary to feed fresh amount of ammonia continuously into the furnace retort in order to carry out the process. Therefore, atmosphere in furnace retort during the process consist of nitriding gas NH_3 and denitriding gas H_2, which are the active ingredients of the atmosphere, and inert gas N_2 [1, 5, 9]. According to this, we can describe nitriding potential of the atmosphere as a following formula:

$$N_p = \frac{p_{NH_3}}{{p_{H_2}}^{3/2}}\,. \tag{2}$$

Depending on the activity of nitrogen in the atmosphere (which is connected with nitriding potential), nitriding of steel may be accompanied by growth of the single-, double- or triple-phase layer (α, γ'+α, ε+γ'+α). The connection between phase structure and parameters such as nitriding potential and temperature is shown on T-N_p-N phase equilibrium diagram (Fig. 1) [2, 4, 5].

Thus, parameters of nitriding process have significant influence on the nitriding layer structure and through their regulation and control it is possible to form the nitrided layer precisely with respect to the required phase structure, zone thickness, hardness distribution, and as a result – to obtain nitrided layer which fulfil the requirements imposed on them. Among most important parameters we rate time, temperature and nitriding potential of the atmosphere, however, these are not all of factors which determine the kinetics of nitrided layer growth [2, 4]. For example, T-N_p-N phase equilibrium diagram concerns only raw iron, when in fact especially his alloys with carbon (carbon steels) and alloy elements (alloy steels) are nitrided. L. Małdziński proved that T-N_p-N phase equilibrium diagram could be used only for steels containing Cr, Mn, Mo, V, because content of these elements do not change its shape [4, 5]. A large number of factors, which are relevant to the course of nitriding process, make use of mathematical models necessary for precise forming of nitrided layers. Mathematical models of the kinetics of nitrided layer growth can be applied in simulations of nitriding processes, where they enable prediction of the kinetics of nitrided layer growth as a function of process parameters: time, temperature and nitriding potential of the atmosphere. They also take into account the cumulative effect of alloying elements and carbon on diffusion streams of nitrogen atoms into ε, γ' and α phases, and as a result – on the speed of growth of these phases. Furthermore, they allow controlling growth of the ε and γ' phases as a function of nitriding potential and temperature not only in simple single-stage processes, but also in more complicated multi-stage processes. To sum up, these models enables forming phase structure of nitrided layer by adjusting the process parameters. What is more, through the use of mathematical models layers are produced in the shortest possible time, which is connected with the lowest energy consumption [3-5].

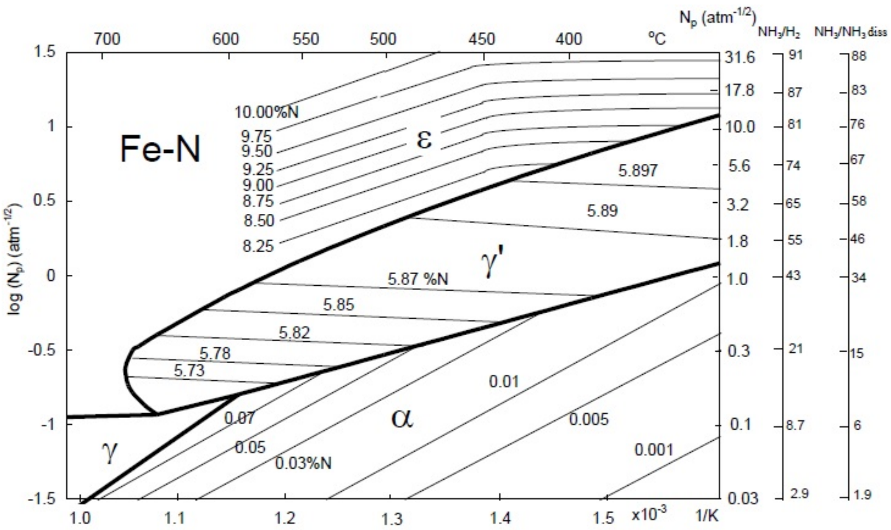

Fig. 1. T-N_p-N phase equilibrium diagram

On the basis of mathematical models has been developed the simulator of the kinetics of nitrided layer growth, which is a program that supports designing new processes of nitriding using ZeroFlow method. Application of mathematical models describing the kinetics of nitrided layer growth in designing nitriding processes is particularly important from the industrial point of view, where through obtaining properly formed layers it is possible to provide required properties and to increase the durability of the nitrided parts, and as a result – to increase durability of machines and vehicles [3]. Therefore, simulator of the kinetics of nitrided layer growth and controlled gas nitriding ZeroFlow meet with an increasing interest from the industrial consumers. Until now, ZeroFlow nitriding method has been introduced in 26 industrial plants in Poland and many other countries worldwide, such as Italy, Great Britain, Canada, Sweden, Singapore, South Korea, Germany, Czech Republic, Belarus, Russia, India, Pakistan, and Switzerland. 36 industrial installations have been constructed and implemented so far, another 4 are launched. Several thousands of nitriding processes for various parts of machines and vehicles have been conducted with positive results, and most of them were designed using mathematical models (simulator) of the kinetics of nitrided layer growth.

3. Simulator of the kinetics of nitrided layer growth

Simulator of the kinetics of nitrided layer growth (Fig. 2) is a computer programme which enables graphical and computational prediction of the growth of nitrided layer thickness and particular phases that will occur in it (ε, γ', ε+γ', α), effective case depth and hardness distribution as a function of process parameters: time, temperature and nitriding potential of the atmosphere. In practice it means that by using a simulator of the kinetics of nitrided layer growth, it is possible to form the nitrided layer precisely and as a result – to obtain nitrided layer with strictly defined, required properties [3].

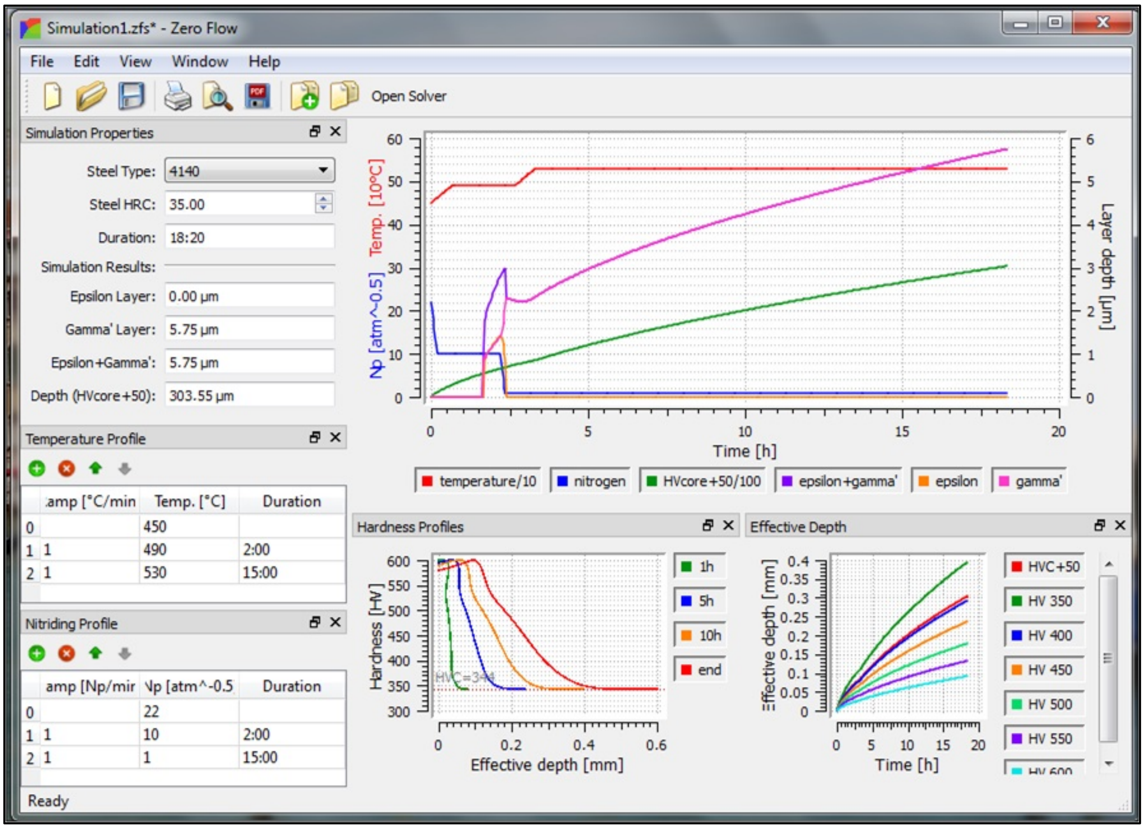

Fig. 2. Simulator of the kinetics of nitrided layer growth, main view

Main simulator window consists of two major parts on the left side we can recognize a number of cells, which are intended for nitriding parameters input, and on the right side – graphs showing the results of conducted simulation. Simulation is carried out automatically after entering data about the simulated process, such as simulation properties, temperature profile or nitriding profile. Simulation properties allow choosing the type of steel or determining core hardness (steel HRC). Currently simulator contains models for Armco iron and 12 types of steel, including 1020 and 1050, low-alloy steels 4140, 5140, 4340, N135M, 18HGT, 8620, medium-alloy steels 32CVD13, H11, H13 and D2. Range of core hardness was based on hardness of steels used in experimental research and it is about 10HRC, however the minimum and maximum values are different for each type of steel. Moreover, in simulation properties we have also “Duration” cell, which shows overall time of nitriding process, computed based on temperature and nitriding profiles defined by user.

Temperature and nitriding profile have the form of tables, where each row represents one section of the profile. Every section can be edited, moved or added/deleted. One section corresponds to one stage of process and it is described by the following quantities: the duration of the section, its target value and a ramp (speed at which the target value is reached). Ramp is connected with actual conditions of heating and nitriding potential reduction, resulting, among others, from the size of the furnace (or more precisely – from the size of its retort) or batch size. Each of these values is entered into another column.

Any change in parameters (time, temperature, nitriding potential of the atmosphere, as well as the properties of the steel) will restart the simulation and automatically perform calculations for the new input parameters. Results of the simulation are presented both in numerical and graphical form. Selected results in numerical form are presented under simulation properties and they contains following values:

– epsilon layer thickness,
– gamma' layer thickness,
– compound zone thickness (epsilon + gamma' layer), also known as a white layer,
– layer effective thickness with core hardness of +50HV (HVC+50).

As well as values in numerical form show only the final result of simulated nitriding process, graphs allow following the whole course of process and predicting on its basis specific values during the process. Main part of simulator window contains graph of ε, γ', ε+γ' layers thickness and effective case depth HVC+50 growth as a function of nitriding time, which also includes curves presenting changes of temperature and nitriding potential during nitriding process. Below are another two graphs. First of them shows hardness profiles on the cross-section of nitrided layer after different times of nitriding. Second graph shows growth of the effective case depth for specific values of hardness (e.g. HVC+50, HVC400, HVC500, HVC600) as a function of nitriding time.

To sum up, simulator of the kinetics of nitrided layer growth enables precise simulations of nitriding process as a function of process parameters: time, temperature and nitriding potential of the atmosphere. Parameters can be adjusted to suit actual conditions of nitriding process, which delivers detailed information about the growth of nitrided layer. Thus, simulator can function both as a regulatory and control. By regulatory is understood the ability to determine the process parameters in order to obtain specific properties of the layer; by control – the ability to compare layers obtained after nitriding process with simulation results. However, the most important advantage of simulator is the ability to optimize process parameters, and as a result – forming required nitrided layer in the shortest possible time and with the lowest energy and gases consumption. It is possible by using a simulation solver (Fig. 3).

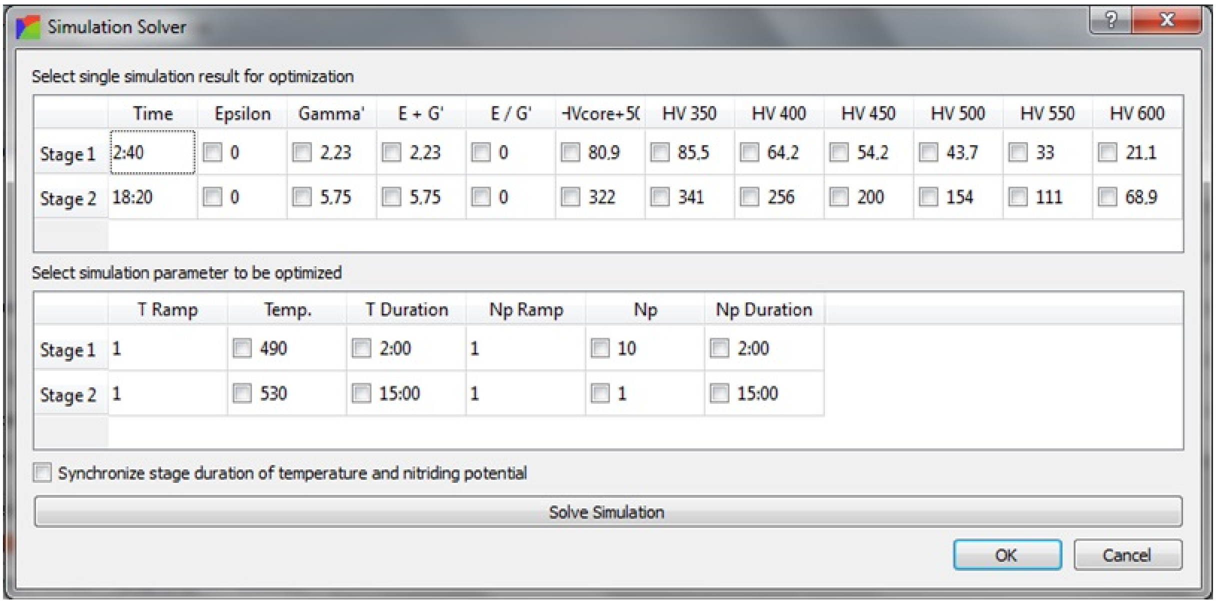

Fig. 3. Simulator of the kinetics of nitrided layer growth, simulation solver

Main solver window consist of two groups of cells. First of them, described as a "Select single simulation result for optimization", contains results of simulation which is currently carried out. Among them we can distinguish: total duration of each stage of the process, ε, γ', ε+γ' layers thickness, ε/γ' ratio, effective case depth HVC+50 and others. In second group, described as a "Select simulation parameter to be optimized", we have process parameters – time, temperature, nitriding potential of the atmosphere, which are optimized in order to obtain required layer structure and properties. To optimize the parameters, we have to select single cell from the first group and set its target value, and then select parameter from the second group, which will be changed. After pressing the button “Solve simulation”, new value of selected parameter will be shown instead of previous one. Without no doubt, solver is one of the most important functions of simulator of the kinetics of nitrided layer growth, because it is an essential factor determining economical and environmentally friendly character of nitriding uses ZeroFlow method.

Gathered industrial experience not only confirmed the effectiveness of ZeroFlow method, but they also confirmed the effectiveness of using a simulator of the kinetics of nitrided layer growth as an application that supports precise forming of nitrided layer with respect to the required phase structure, zone thicknesses and hardness distribution.

4. Practical applications of the simulator in designing nitriding processes

Forming of nitrided layers occurs on steels that are most commonly used in transport machines engineering, like vehicles and aircrafts, or in technological machines and tools (used for example for the wood industry) engineering. Therefore, ZeroFlow nitriding is used for parts of machines and vehicles such as toothed wheels or inlet sleeves with the pushing piston. In addition, many processes were conducted for parts of car engines: crankshafts, camshafts, piston rings, poppet valve springs and discs, piston pins or nozzles for unit injectors. Many examples of industrial applications of nitriding processes using ZeroFlow method (and simulator of the kinetics of nitrided layer growth) were described in literature [3, 5-8].

Among most interesting examples of simulator applications in designing nitriding, processes can be mentioned:

- nitriding of crankshafts for sport car engines – due to application of crankshafts and working conditions, requirements for treated parts were set high, regarding nitrided layer phase structure, thickness of layer zones, thickness of effective precipitate zone, hardness, as well as dimensional and geometrical changes; all of requirements were obtained in specially designed triple-stage process,
- nitriding of toothed wheels for wind power plants – due to high surface pressure on the teeth, a thick nitrided layer without the white layer was required; for this case was used similar method as that for nitriding of crankshafts (with small modifications),
- nitriding of plates for casting glass bulbs for lamps,
- nitriding of dies for pressure aluminum casting.

Without using mathematical models, fulfilment of all the requirements in the cases described above would be much more difficult and would need to carry out many experimental researches, which would involve additional costs. Through the use of simulator nitrided layers not only fulfil all the requirements imposed on them, but they also were obtained in the shortest possible time and with the lowest energy and gases consumption.

5. Summary

Simulator of the kinetics of nitrided layer growth is an application, which supports nitriding using ZeroFlow method. Despite of many advantages and proven effectiveness it still requires further development and research – including verification and modification of the existing models and development of models for new types of steel. However, it should be noted that limitations of the simulator does not preclude from using them, both in experimental and industrial scale. The necessity of continuous development of simulator results from increasing demands of industrial consumers, which are determined by constant advances in technology and increasing interest in new, ecological and environmentally friendly technologies, machines and tools supporting production of layers with strictly defined properties.

Gathered experience has shown that simulator of the kinetics of nitrided layer growth allows precise forming of nitrided layers with respect to the required phase structure, zone thicknesses and hardness distribution; simulator enables forming of nitrided layer phase structure with thicknesses of particular phases that occur in it as a function of process parameters: time, temperature and nitriding potential of the atmosphere. Furthermore, through the use of mathematical models these layers are produced in the shortest possible time, which is connected with the lowest energy and gases consumption.

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