International Journal of Mechanical Sciences 96-97 (2015) 47–57

Contents lists available at ScienceDirect

International Journal of Mechanical Sciences

journal homepage: www.elsevier.com/locate/ijmecsci

The numerical model prediction of phase components and stresses distributions in hardened tool steel for cold work

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ARTICLE INFO

Article history:
Received 10 September 2014
Received in revised form
18 February 2015
Accepted 17 March 2015
Available online 25 March 2015

Keywords:
Heat treatment
Tools steel
Phase transformations
Stresses
Isotropic or kinematics hardening
Numerical simulations

ABSTRACT

This study describes modelling of the processes of steel hardening. The first priority was given to a thermal phenomena, phase transformations in solid state and a mechanical phenomena. The issue of heat conductivity was based on the equation of transient heat conductivity with unit source. Numerical algorithms for kinetics of phase transformations and evaluation of fractions of phases were built on the diagrams of continuous heating and cooling of tool steel (CHT and CCT). The theoretical model of phase transformations was then verified by experiments. In modelling of mechanical phenomena, the equilibrium equations and constitutive relations were adopted in the rate form. Plastic strains are determined by the theory of non-isothermal plastic flow associated with the Huber-Mises condition. The model assumed isotropic and kinematics hardening and besides elastic, thermal, structural, plastic strains and transformations plasticity were included. Thermophysical properties including Young's modulus, tangent modulus and yield strength were directly dependent on temperature and material phase composition. The issues of thermo-elastic-plastic were solved using the finite element method. Implemented algorithms were applied in computer stimulation of hardening of non-alloy tool steel. Numerical analysis of thermal effects and phase transformations, i.e. stresses and strains in mechanical phenomena in a tool steel material undergoing hardening were made.

1. Introduction

Since the tools are used in very different operating environments and conditions, steel must meet a wide variety of requirements, of which robustness is always the primary criterion to be achieved. To obtain the best steel properties, proper thermal processes including hardening and tempering are required. Currently, numerical methods are increasingly often used in modelling of technological processes. They allow to analyse the process as far as complex shapes are concerned and to stimulate different starting and boundary conditions. Further, numerical approach is very flexible, as both an extension of the numerical algorithm and measuring of the outcomes for varying different thermal and physical parameters that may be possible, are enabled [1–5].

A complete analysis of the thermal process must consider appropriate mathematical and numerical models that allow tracing temporary temperature fields, changing in time components phase of material, distribution of temporary stresses, as a consequence the residual stresses (Fig. 1).

Numerical analysis of thermal treatment processes is an important issue to be considered by contemporary laboratories dealing with industrial designing in general (not only in the field of metallurgy). Phenomena associated with heat treatment are complex and not yet adequately explained. Improvement in this field of numerical solutions is particularly forced by industry which, striving for deployment of state-of-the-art technologies and reduction of costs, is demanding continuous enhancement of tool thermal treatment [4,6–8].

Quantitative evaluation of phase transformations, kinetics and analysis of the type of structure obtained as a result of cast steel cooling are required to calculate strains induced during the process. Current research of numerical modelling of heat processes tend to increase number of input parameters; in simulation of steel hardening, transformation plasticity are also taken into account [1,9–16].

Phase transformations, in particular in cooling processes, involve considerable changes in kinetics that are not always associated with external thermal impact. This phenomenon occurs for example during decomposition of austenite into pearlite, and - to a less extent - in formation of ferrite, bainite or martensite. The changes are associated with the latent heat of the transformation process [17–21].

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http://dx.doi.org/10.1016/j.ijmecsci.2015.03.013
0020-7403/

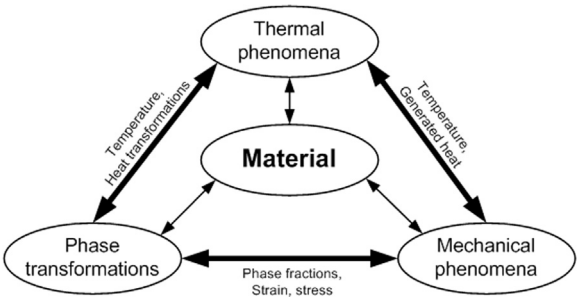

Fig. 1. Diagram showing relationships between thermal and mechanical phenomena in steel heat treatment.

Analyses of experimental data allowed developing many mathematical models to measure volume fractions of phase transformations in solid state. The Johnson-Mehl Avrami (JMA) equation [2] and generalised Kolmogorov equation [93] are the two primary models applied in almost all tests evaluating transformation of austenite into ferrite, bainite and martensite. In order to calculate the martensitic phase volume fraction, usually the Koistinen–Marburger (KM) equation, or any of its modified formulas, are used [22–25].

Models of phase transformations in solid state using the Avrami theory require thermal and physical parameters of the material to be hardened and CCT diagrams. Position and shape curves of the start and finish transformation depend on material chemical composition, austenitization temperature; hold time and austenite grain size. However, using of CCT diagrams that are available in the research databases is not sufficient to accurately stimulate the thermal process. Chemical composition of the investigated material of the same group can be so inconsistent that CCT diagrams display considerably different parameters for extreme chemical compositions of steel. This issue can be solved by using an available database of CCT diagrams to develop a separate CCT diagram for each steel alloy [19,25–27].

The outcomes of numerical simulation of steel hardening are also highly dependent on matching proper cooling environment that is modelled by boundary conditions. It was proved that a suitable fluid is a perfect medium to maintain adequate heating and cooling in thermal processes.

There are limited, non-comprehensive numerical models of tool carbon steel hardening. All models that are available in the research databases are somehow partial. They most often focus on analysing phase transformations during cooling and disregard stresses that are generated in this process. Transformation plasticity occurring in heat treatment (in particular during hardening) are also frequently ignored [28–33].

Thermal treatment processes are accompanied by considerable stresses. In order to assure the accuracy and efficacy of numerical simulations of mechanical phenomena, transformation plasticity have also been taken into account, apart from thermal, structural and plastic strains.

In numerical modelling of thermal treatment phenomena, finite-element, finite-difference and boundary-element methods are used. [1–4,21,34,35] The accuracy of numerical simulation often depends on the choice of calculation approach which is mostly a consequence of whether a variety of hardening related phenomena and their couplings were taken or not in the test. Therefore, in this study the finite element method has been applied.

In comparison to existing papers pertaining to thermal treatment modelling (hardening), the present work includes both the heating process and the cooling process. The CHT diagram was used in the simulation of heating transformation, and in the case of fast heating the modified equation KM was implemented. Simulations of mechanical phenomena were carried out with respect to two types of material strengthening, i.e., the isotropic hardening and kinematic hardening. A comparison of obtained findings was presented with reference to these two models of material. A generation history of stresses in heating and cooling processes was also revealed in connexion with information pertaining to phase transformation in the time cycle of hardening.

2. Thermal phenomena

Temperature fields are obtained with solved of transient heat equation (Fourier equation) with source unit:

$$\nabla \cdot (\lambda \nabla T) - C\frac{\partial T}{\partial t} = -Q \tag{1}$$

where: $\lambda=\lambda(T)$ is the heat conductivity coefficient [W/(mK)], $C=C(T)=\rho(T)c(T)$ is effective heat coefficient [J/m^{3}K], c - specific heat [J/(kgK)], ρ - density [kg/m^3], Q is intensity of internal source [W/m^3] (this can also be the phase transformations heat).

The Eq. (1) was completed with initial conditions

$$T(x_\alpha, t_0) = T_0(x_\alpha), Q(x_\alpha, t_0) = Q(x_\alpha) = 0 \tag{2}$$

Heating and cooling can be modelled using Neumann boundary condition (heating heat flux q_n on Γ_q) or Newton boundary (heat flux (q_n) on Γ_∞ depends on temperature of boundary elements and surrounding medium temperature), i.e:

$$q_n = -\lambda\frac{\partial T}{\partial n}\Big|_{\Gamma_q} = q^*\left(x_\alpha|_{\Gamma_q}, t\right) \tag{3}$$

$$q_n = -\lambda\frac{\partial T}{\partial n}\Big|_{\Gamma_\infty} = \alpha_\infty(T)\left(T|_{\Gamma_\infty} - T_\infty\right) \tag{4}$$

where q^* is a known performance of the surface heating source on the boundary part (Γ_q), $\alpha_\infty=\alpha_\infty(T)$ is the heat transfer coefficients [W/(m^{2}K)], and T_∞ is temperature of the surrounding medium (temperature of the surrounding environment from the side of Γ_∞).

3. Solid-state phase transformations

In both case the phase fractions transformed during continuous heating (austenite) is calculated using the JMA formula or modified KM formula (in relations on rate of heating) [22,24]:

$$\eta_A^h(T,t) = 1 - \exp(-b(t_s,t_f)(t(T))^{n(t_s,t_f)}) \tag{5}$$

$$\eta_A^h(T,t) = 1 - \exp\left(-\left(\frac{T_{sA}-T}{T_{sA}-T_{fA}}\right)^{m_H}\right) \text{ for } \dot{T} \geq 100\ K/s \tag{6}$$

where: η_A^h is austenite initial fraction nascent in heating process, T_{sA} is temperature of initial phase of austenite, T_{fA} – is final temperature for this phase, m_H is a power index measured experimentally (it is $m_H=2.5$ for the investigated steel sample) [19,25].

The coefficients $b(t_s,t_f)$ and $n(t_s,t_f)$ are obtained with (5) next assumption of initial fraction ($\eta_s=0.01$) and final fraction ($\eta_f=0.99$) and calculation are by formulas:

$$n(t_s,t_f) = \frac{\ln(\ln(0.01)/\ln(0.99))}{\ln(t_f/t_s)},\quad b(t_s,t_f) = \frac{-\ln(0.99)}{(t_s)^n} \tag{7}$$

Pearlite and bainite fraction (in the model of phase transformations upper and lower bainite is not distinguish) are determine by JMA formula.

$$\eta_i(T,t) = \chi(1 - \exp(-b(t(T))^n)) \tag{8}$$