MATHEMATICAL MODELLING OF HOT PLASTIC DEFORMATION OF MICROALLOYED STEELS

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Abstract: *The article concerns the possibility to optimize the parameters of forging process with the method of thermo-mechanical treatment of microalloyed steels by means of mathematical modelling of yield stress obtained from conducted plastometric hot compression tests. To describe the yield stress, rheological model proposed by C.M. Sellars was used. Based on this model, the course of experimental and theoretical stress-strain curves has been verified using a minimum of goal function, for the most accurate matching of analyzed curves of investigated steels. Numerical calculations with the method of finite element method (FEM) were performed taking into consideration test results of compression of specimens in Gleeble 3800 simulator, in a temperature range of 900÷1100°C and at the strain rate of 1, 10 and 50* s^{-1}*. Obtained results allow to conclude that assumed rheological model along with coefficients, determined with the method of inverse analysis, describe satisfactorily the values of yield stress steels of studied steels.*

Keywords: RHEOLOGICAL MODEL, INVERSE ANALYSIS, MICROALLOYED STEELS

1. Introduction

Initially, the modelling was limited to a theoretical solution to the problem of force parameters of the process, i.e. determination of forces and moments, taking into account the phenomenon of material strengthening, as well as frequently adopting simplifying assumptions, lowering the accuracy of calculations [1,2]. The FEM method used nowadays allows modelling of mechanical, thermal and structural phenomena. The most important advantage of this method is the possibility to analyze local values of various parameters of these phenomena, taking into consideration heat exchange and the effect of strain rate in calculation of plastic flow of the material. Nevertheless, the effective use of this method for modelling of industrial processes of plastic working is mainly determined by the knowledge of yield stress, which depends mainly on the microstructural condition of hot deformed austenite. The necessity to include the impact of austenite microstructure on the value of yield stress in the thermomechanical model has led gradually to integration of these models, and additionally to the development of physical modelling with the use of torsion and compression plastometric tests [3-5]. However, it should be noted that in specimens subjected to torsion or hot compression, there is non uniformity of strain, strain rate, stress and temperature [1, 2, 6-10], caused by phenomena such as friction at the sample-tool interface, subsequently - heat generated as a result of strain and friction and also heat discharged to the tool and to the environment. In addition, the temperature of specimen changes during plastometric test, and its distribution is difficult to determine (e.g. with the use of thermomechanical simulators with working automatic control system and implemented resistance heating of samples). As a consequence, interpretation of direct test results is equivocal and requires further processing of obtained results. Application of the inverse analysis allows, in these cases, to effectively eliminate disturbances and determine adjusted values of yield stress, which may be the representative characteristic of investigated material, independent of the type of plastometric test, the shape of sample used, friction conditions, as well as heat exchange in a sample-tool system [11-15]. The essence of this method consists in numerical simulation of σ-ε flow curves obtained during performed laboratory tests, and successively in optimizing model parameters in such a way as to minimize the difference of the expected and measured parameters related to assumed rheological model [16,17].

The paper presents possibilities for the mathematical modelling of hot plastic deformation concerning some selected products obtained by forging structural steels with microadditions in the range of technological parameters simulating such processes in the plastometric compression test. Special attention was paid to the verification of the rheological model developed by Sellars et al. [3,18,19] describing the flow stress as a function of the deformation and temperature, as well as strain rate and the effect of dynamic recrystallization, which dominates in the hot deformation for the investigated structural steels with microadditions of Ti, Nb and V.

2. Experimental procedure

The test were carried out on laboratory melts of structural steels with microadditions, the chemical compositions of which is shown in Table 1.

Plastometric tests were carried out using the thermomechanical test simulator Gleeble 3800, in the Institute of Iron Metallurgy in Gliwice, Poland. Axisymmetrical samples 10 mm in diameter and 12 mm in length were used in this research study. Continuous compression tests of samples up to true strain ε=1 were conducted in order to obtain σ–ε curves and activation energy of plastic deformation. Specimens were resistance-heated in a vacuum at a rate of 3 °C/s to a temperature of 1150 °C. The samples were held at 1150 °C for 30 s and cooled to a deformation temperature of 1100, 1050, 1000, 950, and 900 °C.

Compression of specimens was done at a strain rate of 1, 10 and 50 s^{-1}. Tantalum foils were used to prevent sticking, and graphite foils were used as a lubricant to minimize the effect of friction on the flow curves. Additionally, both surfaces were covered with a nickel-based substance. Activation energy of the process of plastic deformation was calculated with the use of Energy 4.0 program [20, 21], basing on the following relationship:

$$\dot{\varepsilon} = A[\sinh(\alpha\sigma)]^n \exp(-Q/RT), \qquad (1)$$

where: $\dot{\varepsilon}$ – strain rate, σ – value of stress corresponding with the maximum value of flow stress, T – deformation temperature, R – the universal gas constant, A, α, n – constants.

In constitutive equations, actually applied for the purpose of modelling the processes of hot working, the effect of dynamic recovery and dynamic recrystallization are not always conveyed explicitly. The equation in wich both components are distinctly sepatated, elaborated at the University of Sheffield by Sellars et al. [3,18,19], takes the following form:

$$\sigma_p = \sigma_o + \left(\sigma_{ss(e)} - \sigma_o\right)\left[1 - \exp\left(\frac{\varepsilon}{\varepsilon_r}\right)\right]^{1/2} - R\,, \qquad (2)$$

where the respective variables are defined as follows:

$$R = 0 \qquad for\ \ \varepsilon \le \varepsilon_c\,, \qquad (2a)$$

$$R = \left\{\left(\sigma_{ss(e)} - \sigma_{ss}\right)\left\{1 - \exp\left[-\left(\frac{\varepsilon - \varepsilon_c}{\varepsilon_{xr} - \varepsilon_c}\right)^2\right]\right\}\right\} \qquad (2b)$$

$for\ \ \varepsilon > \varepsilon_c$,

Table 1: Chemical composition of the investigated steels

Steel	Concentration of the element in mass fractions, %											
	C	Mn	Si	P	S	Cr	Mo	Nb	Ti	V	Al	B
A	0.31	1.45	0.30	0.006	0.004	0.26	0.22	−	0.033	0.008	0.040	0.003
B	0.28	1.41	0.29	0.008	0.004	0.26	0.22	0.027	0.028	0.019	0.025	0.003

$$\sigma_o = \frac{1}{\alpha_o}\sinh^{-1}\left(\frac{Z}{A_o}\right)^{\frac{1}{n_o}}, \tag{2c}$$

$$\sigma_{ss(e)} = \frac{1}{\alpha_{ss(e)}}\sinh^{-1}\left(\frac{Z}{A_{ss(e)}}\right)^{\frac{1}{n_{ss(e)}}}, \tag{2d}$$

$$\sigma_{ss} = \frac{1}{\alpha_{ss}}\sinh^{-1}\left(\frac{Z}{A_{ss}}\right)^{\frac{1}{n_{ss}}}, \tag{2e}$$

$$\varepsilon_r = 0.31[q_1 + q_2(\sigma_{ss(e)})^2], \tag{2f}$$

$$\varepsilon_{xr} - \varepsilon_c = \frac{\varepsilon_{xs} - \varepsilon_c}{1.98}, \tag{2g}$$

$$\varepsilon_c = C_c\left(\frac{Z}{\sigma_{ss(e)}^2}\right)^{N_c}, \tag{2h}$$

$$\varepsilon_{xs} - \varepsilon_c = C_x\left(\frac{Z}{\sigma_{ss(e)}^2}\right)^{N_x}, \tag{2i}$$

$$Z = \dot{\varepsilon}\left(\frac{Q}{RT}\right) \tag{2j}$$

The variable in equation (2) are as follows:
σ_p – flow stress, σ_0 – the maximum stress when the plastic strain $\varepsilon = 0$, $\sigma_{ss(e)}$ – the onset of steady-state conditions in the extrapolated curve, σ_{ss} – the onset of steady-state conditions in the experimental flow stress curve, ε – plastic deformation, ε_c – strain for the onset of dynamic recrystallization, ε_r – the “transient strain constant” and effectively defines the curvature of the flow-stress curve between σ_p and $\sigma_{ss(e)}$ where the equation saturates, ε_{xr} – the strain required to reach a fixed amount of softening, measured in terms of $\Delta\sigma/\Delta\sigma_s$. This term effectively defines the rate of softening as a result of the dynamic recrystallization, ε_{xs} – the strain at the “onset” of steady-state when dynamic recrystallization occurs, R_x – a term expressing the dynamic recrystallization, Q – the activation energy for the deformation, A, α, n, q, C, N – constant for each characteristic stress σ_p.

The presented model illustrates more distinctly the behaviour of the material in the course of dynamic recrystallization [22], because it makes it possible to describe the point of deflection (ε_{peak}) on the curves σ–ε and the procedure of flow stress beginning at the peak strain up to the achievement of the value of the stresses in the steady state (σ_{ss}). The coefficients of this constitutive equation are usually determined based on the results of plastometric tests within a wide range of temperature and strain rates.

This allows us to model various structural materials over a wide range of conditions for hot plastic deformation. The main difficulty in applying this model lies in the large number of parameters, which have to be unambiguously identified. One of the main factors limiting the applications of the mode simulating the processes of plastic working is the difficulty in determining these coefficient, the values of which depend on the kind of applied material. Nevertheless, equation (2) has been used in this study for the investigated microalloyed steels.

For the optimization of the parameters of the applied model of Sellars [3,18,19], describing stress-strain curves, making use of the goal function Φ in the form:

$$\Phi = \sum_{i=1}^{N_p}\sqrt{\frac{1}{N_p}\left(\frac{\sigma_m - \sigma_c}{\sigma_m}\right)^2} \tag{3}$$

where: σ_m – measured stress, σ_c – calculated stress, N_p – number of measurement points of all the curves in the i-th experiment.

For the purpose of the minimum of equation (3), the Nelder and Mead Simplex [23] algorithm was used.

3. Results and discussion

The results of mathematical modelling of high-temperature process of plastic strain of studied microalloyed steels allowed for analytical verification of dependence proposed by C.M. Sellars, assumed for model analysis. This relation describes – possibly in the most precise way - the course of flow curves, obtained experimentally with plastometric method of axisymmetrical compression under tested conditions of deformation for metals and alloys with low stacking fault energy, exhibiting dynamic recrystallization phenomenon during plastic strain. Herein applied dependence, describing yield stress as a function of strain, strain rate and temperature together with the rheological model has been given in chapter II.

The inverse analysis method applied in the work consists of three basic elements: experiment, model of the experiment described as the model of direct task and optimization techniques. The model of direct task, simulating the experiment is most often the FEM option. In the simulation of experiment (direct solution), a computer program based on FEM was used for the purpose of compression of axisymmetrical samples.

Calculations with the use of FEM method were the basis for the inverse solution, which aims to define such rheological model of material which, when introduced into the model of direct task, will provide stress values that are closest to those obtained with the experiment. This boils to searching for a minimum, in respect to the parameters of rheological model, i.e. determination of the goal function. The next step of mathematical modelling was searching for a function, and in fact verifying assumed dependence according to C.M. Sellars, to describe in detail the changes of yield stress in a wide range of plastometric external variables present in tests, namely temperature and strain rate. Example of calculation results obtained basing on FEM in the form of dependence of yield stress versus deformation for investigated steels has been shown graphically in Fig. 1 and 2.

The numerically determined values of the coefficients assumed in the model, taking into account the Simplex algorithm concerning the analyzed stress-strain curves are shown in Table 2, which also contains the values of the energy of activation of the process of deformation and the final values of the goal function Φ, representing the accuracy of the modelling solution. Due to measurement errors and limitations with the model, different values were obtained for the goal function (equation 3) concerning of investigated steels.

However, the median square error of the calculation remains within 2-4% limits. This proves that the assumed model fits well with the experimental results. As apparent from the data presented in Table 2, higher accuracy of simulation, represented by lower value of the objective function ($\Phi = 0.0375$), was obtained for steel with Nb microaddition (steel B). The best matching accuracy of model and experimental curves was obtained for steel B, plastically deformed in a temperature range of 900÷1100°C at the strain rate of 1 and 10 s^{-1} (Fig. 2).

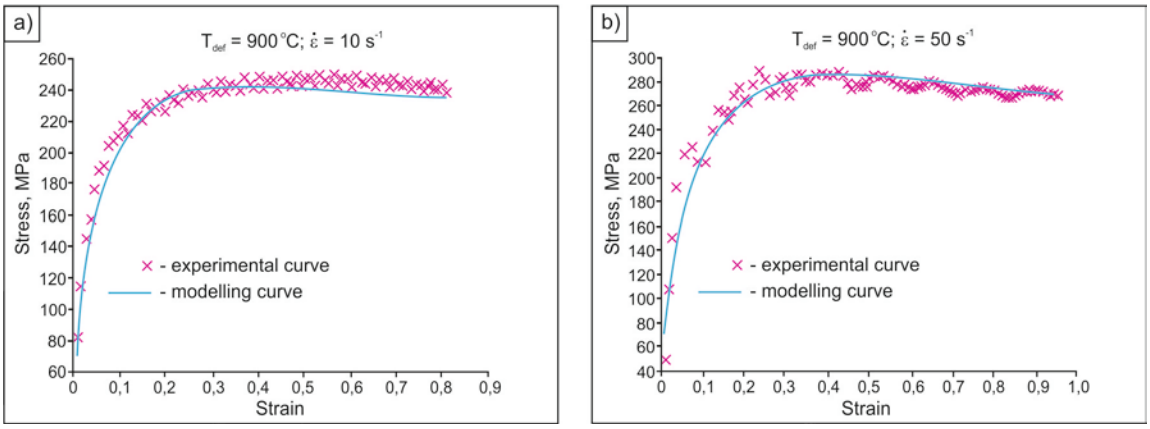

***Fig*.1**. *Comparison of modelling and experimental flow curves of the A steel hot compressed at the temperature of 900°C with the rates of: a) 10 s^{-1}, b) 50 s^{-1}*

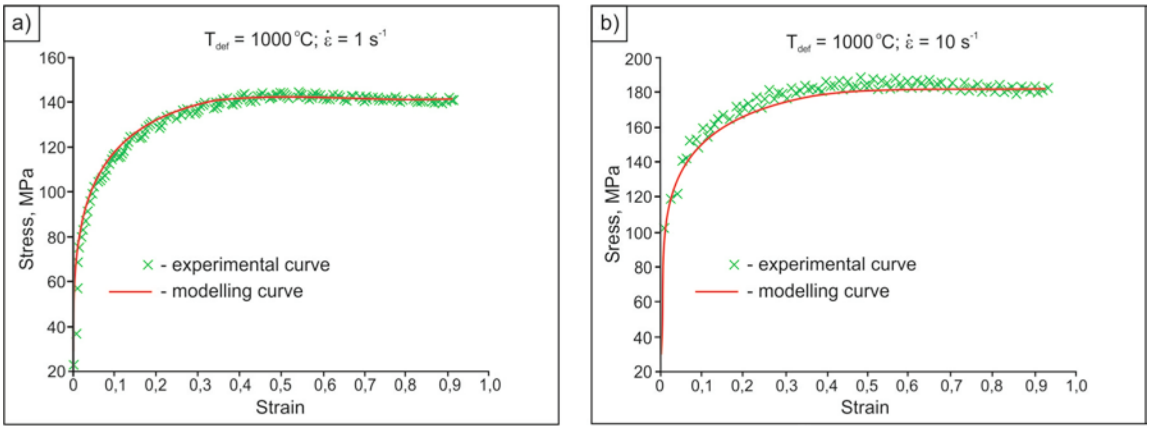

***Fig*.2**. *Comparison of modelling and experimental flow curves of the B steel hot compressed at the temperature of 1000°C with the rates of: a) 1 s^{-1}, b) 10 s^{-1}*

Table 2: Optimal coefficients of the rheological model obtained as a results of Simplex optimization concerning the investigated microalloyed steels

<table>
<tr><td rowspan="3">Steel No.</td><td colspan="4">Rheology – σ_0</td><td colspan="2" rowspan="3">Activation energy Q, kJ/mol</td><td rowspan="3">Goal function Φ</td></tr>
<tr><td colspan="4">Coefficients</td></tr>
<tr><td colspan="2">A_o</td><td>n_o</td><td>α_o</td></tr>
<tr><td>A</td><td colspan="2">$1.30 \cdot 10^{12}$</td><td>0.4897</td><td>2451.33</td><td colspan="2">382.4</td><td>0.0412</td></tr>
<tr><td>B</td><td colspan="2">$3.54 \cdot 10^{13}$</td><td>0.4532</td><td>1787.08</td><td colspan="2">397.9</td><td>0.0375</td></tr>
<tr><td rowspan="3">Steel No.</td><td colspan="7">Rheology – strain hardening and dynamic recovery</td></tr>
<tr><td colspan="7">Coefficients</td></tr>
<tr><td colspan="2">A_{sse}</td><td>n_{sse}</td><td>α_{sse}</td><td colspan="2">q_1</td><td>q_2</td></tr>
<tr><td>A</td><td colspan="2">$1.34 \cdot 10^{17}$</td><td>4.9712</td><td>0.0048</td><td colspan="2">0.0004</td><td>$0.0504 \cdot 10^{-2}$</td></tr>
<tr><td>B</td><td colspan="2">$6.56 \cdot 10^{18}$</td><td>5.9643</td><td>0.0035</td><td colspan="2">0.0213</td><td>$0.0428 \cdot 10^{-2}$</td></tr>
<tr><td rowspan="3">Steel No.</td><td colspan="7">Rheology – strain hardening and dynamic recrystallization</td></tr>
<tr><td colspan="7">Coefficients</td></tr>
<tr><td>A_{ss}</td><td>n_{ss}</td><td>α_{ss}</td><td>C_c</td><td>N_c</td><td>C_x</td><td>N_x</td></tr>
<tr><td>A</td><td>$2.33 \cdot 10^{12}$</td><td>0.3385</td><td>0.1679</td><td>$1.0 \cdot 10^{-8}$</td><td>$1.2 \cdot 10^{-8}$</td><td>0.00017</td><td>0.284</td></tr>
<tr><td>B</td><td>$1.12 \cdot 10^{13}$</td><td>0.6129</td><td>0.0920</td><td>$6.5 \cdot 10^{-8}$</td><td>$1.0 \cdot 10^{-8}$</td><td>0.00010</td><td>0.289</td></tr>
</table>

An analysis of the shape of curves obtained in the compression test allows to state that in the studied range of hot deformation parameters the decrease in strain hardening, both in case of the A and B steel, was caused by the process of continuous dynamic recrystallization. This is also confirmed by the results of evaluating the activation energy of the plastic deformation process of the examined steels. Activation energy of plastic deformation of the A steel, determined with the use of equation (1), is equal to Q = 382 $kJ \cdot mol^{-1}$, while activation energy of plastic deformation process of the B steel is equal to Q = 398 $kJ \cdot mol^{-1}$, wherin values of constants in this equation for the stress corresponding with ε_m deformations are equal: $A = 3.43 \cdot 10^{15}$, $\alpha = 0.00628$, $n = 6.93$ and $A = 7.42 \cdot 10^{15}$, $\alpha = 0.00649$, $n = 7.17$ – for the A and B steel, respectively. Similar values of activation energy of plastic strain process for microalloyed steels have been achieved in the works [24-27]. The obtained values of activation energy for investigated steels is substantially higher than the activation energy of self-diffusion, i.e. when the processes which control the course of plastic deformation are dislocation climbing and form subgrains. This means that the process of plastic deformation of the studied steels is controlled by dynamic recrystallization.

4. Conclusions

Rheological model assumed in the study, proposed by C.M. Sellars, describing the yield stress of investigated steels with microadditions as a function of strain, strain rate and temperature, proved to be the proper and effective tool for appropriate adjustment of the course of experimental and theoretical σ-ε flow curves, determined in plastometric hot compression tests.

Regardless of chemical constitution of steel, assumed $\sigma_p = f(\varepsilon, \dot{\varepsilon}, T)$ type function correctly took into account the impact of the process of dynamic recrystallization on yield stress during high-temperature plastic strain.

In the procedure for identification of yield stresses, determined basing on axisymmetrical hot-compression test, the method of inverse analysis appeared to be significantly useful, eliminating practically the majority of disturbances arising from the mechanical test, such as: non-uniformity of deformation, strain rate and temperature of sample, friction phenomenon at the die – deformed metal contact and heat exchange from the sample holder and surrounding, etc. The best matching accuracy of analyzed curves was determined in the work by minimum value of the goal function, which represented simultaneously the best performance of applied inverse solution of finite element method. It has been found that the best matching accuracy of analyzed σ-ε curves was obtained for constructional steel containing 0.28% C and microadditions of Nb, Ti and V (Fig. 2). Minimum value of the goal function $\Phi = 0.0375$ was obtained in the entire range of examined conditions of high temperature deformation.

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