NUMERICAL MODELLING OF WELDING OF MARTENSITIC STEEL

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ABSTRACT

The mathematical model and computer simulation for prediction of mechanical properties and microstructure composition of steel welded joint was developed. Because of wide range of applicability and ease of use of finite volume method (FVM), this numerical method was suitable to create integrated computer program for simulation of transient temperature field, microstructure transformation and mechanical properties during welding of steel.
The computer simulation of mechanical properties and microstructure of welded joint is consisted of numerical calculation of transient temperature field in process of cooling, and of numerical calculation of hardness. The computer simulation of hardness of welded joint is based on both, CCT diagrams and the thermo-kinetic expressions using linear alignment with the actual chemical composition. Microstructure and hardness of welded joint has been predicted based on calculated characteristic time of cooling from 800 °C to 500 °C, ($t_{8/5}$). Results of steel welding were estimated by taking into account the process of reheating of workpiece during the welding. The established procedure was applied in computer simulation of martensitic steel welded joint.

Keywords: Mathematical modelling, computer simulation, welded joint, hardness distribution, microstructure composition

INTRODUCTION

Computer simulation of the welding can be done by considering the issues such as achievement of tolerable defects, desired mechanical properties distribution and required microstructure distribution. Many very useful software exist for the calculation of grain structure, porosity, hot tearing, and solid-state transformation. But, there are still questions on which answers should be given to satisfy all industry needs in mathematical modelling and simulation of welding [1, 2].

During the welding, many different physical processes, such as, melting, solidification, solid state phase transformation, evolution of microstructure, diffusion, heat conduction, and mechanical stressing and distortion are at once taking place inside metal [3-7]. Simulations of microstructural transformations can be based on the both, CCT diagrams

and thermo-kinetic expressions. The first approach is more consistent, but the second approach gives good results using the real chemical composition of the steel.

The input of the simulation is composed of the following categories: geometry, physical characteristics of the steel and, kinematic boundary conditions and thermal boundary conditions. It is necessary to establish the appropriate algorithm which describes heating and cooling processes and to involve appropriate input data in the model. Inverse heat transfer problems should be solved to determine thermal properties for welding material and filler material based on experimentally evaluated results [8].

Proposed numerical model of welding in this work is based on finite volume method (FVM). The finite volume method (FVM) has been established as a very efficient way of solving fluid flow and heat transfer problems. The key feature of the FVM approach is that the FVM is based on flux integration over the control volume surfaces. The method is implemented in a manner that ensures local flux conservation, regardless of the grid structure [9]. FVM is used as a simple and effective tool for the solution of a large range of problems in the analysis of welding processes [10-12].

COMPUTER MODELLING OF THERMAL PROCESSES

Numerical simulation of welding gives consideration to both, the melting and solidification processes.

Mathematical formulation of process of welding, i.e., melting, solidification and cooling is based on the following system of differential equations [4, 5, 13]:

- the Navier-Stokes equations

$$\begin{aligned}
&\mu\left(\frac{\partial^2 v_r}{\partial r^2}+\frac{1}{r}\frac{\partial v_r}{\partial r}+\frac{\partial^2 v_r}{\partial z^2}-\frac{v_r}{r^2}\right)-\frac{\partial p}{\partial r}+\rho g_r\beta\left(T-T_\infty\right)=\rho\frac{\mathrm{d}v_r}{\mathrm{d}t}\\
&\mu\left(\frac{\partial^2 v_z}{\partial r^2}+\frac{1}{r}\frac{\partial v_z}{\partial r}+\frac{\partial^2 v_z}{\partial z^2}\right)-\frac{\partial p}{\partial z}+\rho g_z\beta\left(T-T_\infty\right)=\rho\frac{\mathrm{d}v_z}{\mathrm{d}t}
\end{aligned} \tag{1}$$

- the continuity equation

$$\frac{\partial v_r}{\partial r}+\frac{v_r}{r}+\frac{\partial v_z}{\partial z}=0 \tag{2}$$

- the Fourier's heat conduction equation including the convection term

$$\frac{\lambda}{r}\frac{\partial T}{\partial r}+\frac{\partial}{\partial r}\left(\lambda\frac{\partial T}{\partial r}\right)+\frac{\partial}{\partial z}\left(\lambda\frac{\partial T}{\partial z}\right)=\rho c_{\mathrm{ef}}\left(\frac{\partial T}{\partial t}+v_r\frac{\partial T}{\partial r}+v_z\frac{\partial T}{\partial r}\right) \tag{3}$$

Characteristic boundary condition for the top face is:

$$-\lambda \left.\frac{\delta T}{\delta n}\right|_{s} = \alpha_{ef}\left(T_s - T_a\right) + q_{source} \tag{4}$$

and for the other faces

$$-\lambda \left.\frac{\delta T}{\delta n}\right|_{s} = \alpha\left(T_s - T_a\right) \tag{5}$$

where T_s/K is surface temperature, T_a/K is air temperature, q_s/Wm^{-3} is volumetric density of heat source, α/Wm^{-2}K^{-1} is heat transfer coefficient of air, α_{ef}/Wm^{-2}K^{-1} is effective heat transfer coefficient by which convection and radiation are taken into account and q_{source}/Wm^{-2} is arc source heat flux.

where T/K is the temperature, t/s is the time, $\rho = \rho(T)$/kgm^{-3} is the density, λ/Wm^{-1}K^{-1} is the thermal conductivity coefficient, T_s/K is surface temperature, T_a/K is air temperature, α/Wm^{-2}K^{-1} is heat transfer coefficient, v_r, v_z/ms^{-1} are the r- and z-component of velocity, respectively, $\mu(T)$/Nsm^{-2} is dynamical viscosity coefficient, $c_{ef} = c + L/(T_\beta - T_\alpha)$/Jkg^{-1}K^{-1} is the effective specific heat of a mushy zone, L/Jkg^{-1} is the latent heat of solidification, c/Jkg^{-1}K^{-1} is the specific heat, p/Nm^{-2} is the pressure, g_r, g_z/ms^{-2} are the r- and z-component of gravitational acceleration, respectively, β/K^{-1} is the volume coefficient of thermal expansion, r, z/m are the coordinates of the vector of the considered node's position, T_∞/K is the reference temperature $T_\infty = T_{in}$, r/m is the radius.

In this model it was presumed that convection term has no relevant role and that liquid metal flow could be neglected after melting.

Quantity of growth of solidified part of welded joint was predicted by calculation of solidification rate in control volume (Fig. 1).

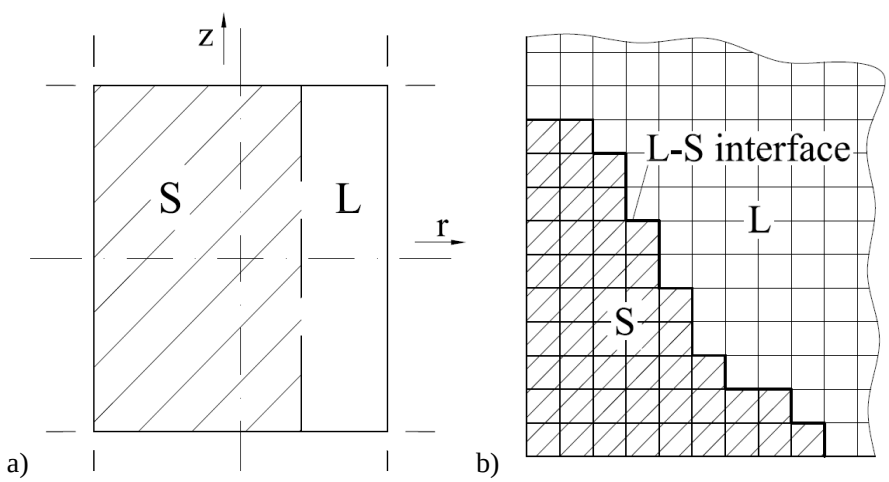

Fig. 1 Liquid-solid interface, a) control volume, b) welding joint [14].

Increment of melted or solidified part, f_i in control volume can be calculated by:

$$f_i = \frac{m_i}{m_{vol}} = \frac{c_m (T_1 - T_2)}{L} \tag{6}$$

where m_i/kg is mass quantity increase of solidified part in control volume, m_{vol}/kg is mass quantity of control volume, c_m/Jkg^{-1}K^{-1} is heat capacity of liquid and solid mixture, T_1/K is the temperature at the beginning and T_2/K is the temperature at the end of time step Δt. In proposed model it was presumed that convection term has no relevant role and that liquid metal flow could be neglected after pouring [15]. Equations 1 to 3 were found out using the finite volume method. Physical properties included in equations 1 to 6 should be defined [9]. Accuracy of the heat transfer prediction directly influences to the accuracy of both, calculations of phase transformation kinetics and calculations of mechanical properties of steel. Involved variables in model should be additionally adjusted.

Quantity of growth of solidified part of casting was predicted by calculation of solidification rate in control volume. When $\Sigma f_i = 1$, the mass of solidified part of casting will grow up for mass of control volume.

The temperature field change in an isotropic rigid body with coefficient of heat conductivity, λ/Wm^{-1}K^{-1}, density, ρ/kgm^{-3} and specific heat capacity, c/Jkg^{-1}K^{-1} can be described by Fourier's law of heat conduction:

It is assumed that the arc has a Gaussian distribution on the top face of the workpiece:

$$Q = q_0 \int_0^{\infty} e^{-\frac{d}{r_0^2} r^2} \, 2\pi r dr \tag{7}$$

where Q/W is the total heat input into the workpiece, r_0/m is the radius of the heat input distribution, d is the exponential factor and q_0/Wm^{-2} is the volumetric energy generation rate [10].

Solution of equation 1 can be found out using the finite volume method [9, 11, 12]. If the total volume is divided in N number of control volumes, discretization system has N linear algebraic equations, with N unknown temperatures of control volumes. Time of cooling from T_a to specific temperature in particular point is determined as sum of time steps, and in this way, the diagram of cooling curve in every grid-point of a specimen is possible to find out [10].

Accuracy of the heat transfer prediction directly influences to the accuracy of both, calculations of solidification kinetics, phase transformation kinetics and calculations of mechanical properties of steel. If the variables ρ and c were accepted, variable λ and specially variable α must be estimated, i.e., calibrated according to variables ρ and c [10]. Total heat conductivity coefficients of steel at some temperature T should be calculated in accordance to composition and distribution of microstructure. Heat transfer coefficients of air are given in Table 1 [10].

Table 1 Calibrated values of heat transfer coefficient of air

Temperature, *T*/°C	20	100	200	400	600	800	1000
Heat transfer coefficient, *α*/Wm^{-2}K^{-1}	12	15	21	33	50	84	113

MATHEMATICAL MODELING OF MICROSTRUCTURE COMPOSITION AND HARDNESS

Microstructure composition after the welding depends on chemical composition of steel and nature of cooling process. Kinetics of transformations was calculated by Avrami's isothermal equation. Transformed part of microstructure, x can be calculated by:

$$x = 1 - \exp(-k \cdot t^n) \tag{8}$$

where k and n are kinetic parameters.

For purpose of numerical analysis by computer, it is convenient when kinetics of austenite decomposition is defined in an incremental form of Avrami's isothermal equation. By differentiating the Avrami's equation it follows that:

$$\frac{dx}{dt} = \exp(-kt^n) nkt^{n-1} \tag{9}$$

and by extracting the time component from equation 9 it follows that:

$$\frac{dx}{dt} = nk^{\frac{1}{n}} \left(\ln \frac{1}{1-x} \right)^{1-\frac{1}{n}} (1-x) \tag{10}$$

Equation 10 can be written in an incremental form and the volume fraction Δx of austenite transformed in the time interval Δt_i at temperature T_i can be calculated as follows:

$$\Delta x_{(m)} = nk^{\frac{1}{n}} \left(\ln \frac{1}{1-x_{(m-1)}} \right)^{1-\frac{1}{n}} \left(1-x_{(m-1)}\right) \Delta t_{(m)} \tag{11}$$

In accordance to the Scheil's additivity rule, characteristic microstructure transformation is completed when transformed part of microstructure, $\Sigma\Delta x$ is equal to one [16, 17]:

$$\sum_{m=1}^{M} nk^{\frac{1}{n}}\left(\ln\frac{1}{1-x_{(m-1)}}\right)^{1-\frac{1}{n}}\left(1-x_{(m-1)}\right)\Delta t_{(m)}=1 \tag{12}$$

The non-isothermal transformation kinetics can be described as the sum of a series of the small isothermal transformations. The temperature range of cooling is divided into a series of small finite steps. Maintaining the time interval, Δt_i to sufficiently short times permits the assumption that the conditions are isothermal over each time step. It was assumed that each time step produces such a transformation as occurs in the isothermal condition of transformation at the same temperature and microstructure composition. Kinetic parameters k and n from equation 11 can be determined inversely by using data of time of isothermal transformation, t_T:

$$k=\frac{\ln(1-x)}{t_T^n} \tag{13}$$

Characteristic time of isothermal transformation could be calculated by kinetic equations based on chemical composition of steel or could be found out by using IT diagram of steel with standard chemical composition [17]. The IT diagram should be additionally adjusted based on actual chemical composition or based on Jominy test results for applied steel [18].

The martensitic transformation relation is based on the following expression [19]:

$$x_M=\left(1-x_F-x_P-x_B\right)\left(1-\exp\left(-0.011\left(M_S-T\right)\right)\right) \tag{14}$$

Increment of martensite is equal to:

$$\Delta x_M=x_M\left(T_{m+1}\right)-x_M\left(T_m\right) \tag{15}$$

Between critical temperatures of austenite decomposition and hardenability properties, regression relations are established [20]:

$$A_3=862-0.04\left(\mathrm{HRC}_{\max.}-20\right)^2-\frac{6E_d}{\mathrm{HRC}_{\max}-20} \tag{16a}$$

$$B_s=586-0.02\left(\mathrm{HRC}_{\max}-20\right)^2-\frac{30.6E_d}{\mathrm{HRC}_{\max}-20} \tag{16b}$$

$$M_s=502-0.09\left(\mathrm{HRC}_{\max}-20\right)^2-\frac{9E_d}{\mathrm{HRC}_{\max}-20} \tag{16c}$$

$$M_{\mathrm{f}} = 502 - 0.2\left(\mathrm{HRC}_{\max} - 20\right)^2 - \frac{9E_{\mathrm{d}}}{\mathrm{HRC}_{\max} - 20} \tag{16d}$$

It was accepted that equilibrium temperature of eutectoid transformation A_1 is equal to 721 °C.

Simulation of as welded hardness at different welding joint points is estimated by the conversion of the calculated equivalent cooling time, $t_{8/5\mathrm{e}}$ to the hardness. This conversion is provided using the relationship between the equivalent cooling time $t_{8/5\mathrm{e}}$ and distance from the quenched end of the Jominy test specimen, E_{d}, i.e. by the using the diagram of cooling time $t_{8/5}$ versus distance from the quenched end of the Jominy test specimen [21].

$$E_{\mathrm{d}} = f\left(t_{8/5\mathrm{e}}\right) \tag{17}$$

Hardness $\mathrm{HRC_q}$ was predicted by using the Jominy curve diagram:

$$\mathrm{HRC_q} = f\left(E_{\mathrm{d}}\right) \tag{18}$$

In the developed computer simulation of welding, the hardness at different points of steel plate is estimated by the conversion of the calculated cooling time $t_{8/5}$ to the hardness and microstructure composition by using CCT diagram and thermo-kinetic equation [10, 22].

Since steel plate is repeatedly heated during the welding processes, influence of reheating of workpiece during welding on microstructure transformation should be taken into account. The reference value of hardness of welded steel plate can be estimated based on hardness at the start of welding, $\mathrm{HRC_{start}}$, by [10, 23, 24]:

$$\mathrm{HRC} = \frac{\mathrm{HRC}_{\mathrm{start}} - \mathrm{HRC}_{\min}}{K} + \mathrm{HRC}_{\min} \tag{19}$$

where $\mathrm{HRC_{min}}$ is the material constant with known physical meaning, K is the coefficient or ratio between reference hardness at the start of welding, $(\mathrm{HRC_{start}} - \mathrm{HRC_{min}})$ and reference welded hardness, $(\mathrm{HRC} - \mathrm{HRC_{min}})$. Factor K is equal to:

$$K = \exp\left[AB\left(\frac{T_{\mathrm{tr}}}{a}\right)^{n_1}\right] \tag{20}$$

where T_{tr}/K is the reference value of reheating temperature, while A, B, a and n_1 are the material constants, that are established by regression analysis of hardness of quenched and tempered steel. The algorithm for prediction of hardness of welded steel given by equations 19 and 20 was established by regression analysis [25]. Since the duration of processes of annealing or tempering at some temperature T_{p} is equal to Δt, temperature T_{tr} can be expressed by the following equation:

$$T_{\mathrm{tr}} = \frac{T_{\mathrm{p}}(C + a \ln \Delta t)}{C} \tag{21}$$

where a is a constant. Constant C depends on chemical composition and has the same meaning as constant C in Hollomon-Jaffe expression.

APPLICATION

The developed method for prediction of hardness and microstructure distribution was applied in computer simulation of welded joints of steels with different hardenabilities. Welded joints were made of normalized steels, EN 52CrMoV4 and EN X15Cr13. Joint design is shown in Fig. 2. Welding rate was 30 cm/min and heat input was 4.8 kJ/cm. It was accepted that chemical composition of filler metal was the same as was of the base metal. Steel joints are tempered after welding at 380 °C for one hour. Computer simulation of hardness and microstructure distribution of the welded joints were done using the computer software BS Thermal, module BS-Welding.

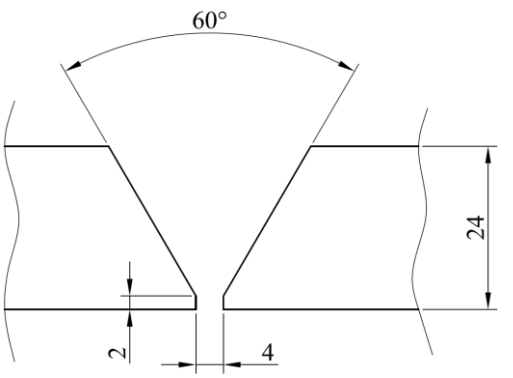

Fig. 2 Joint design.

WELDING JOINT MADE OF STEEL EN 52CRMOV4

The distribution of hardness and microstructure of the welding joint made of steel EN 52CrMoV4 are shown in Fig. 3.

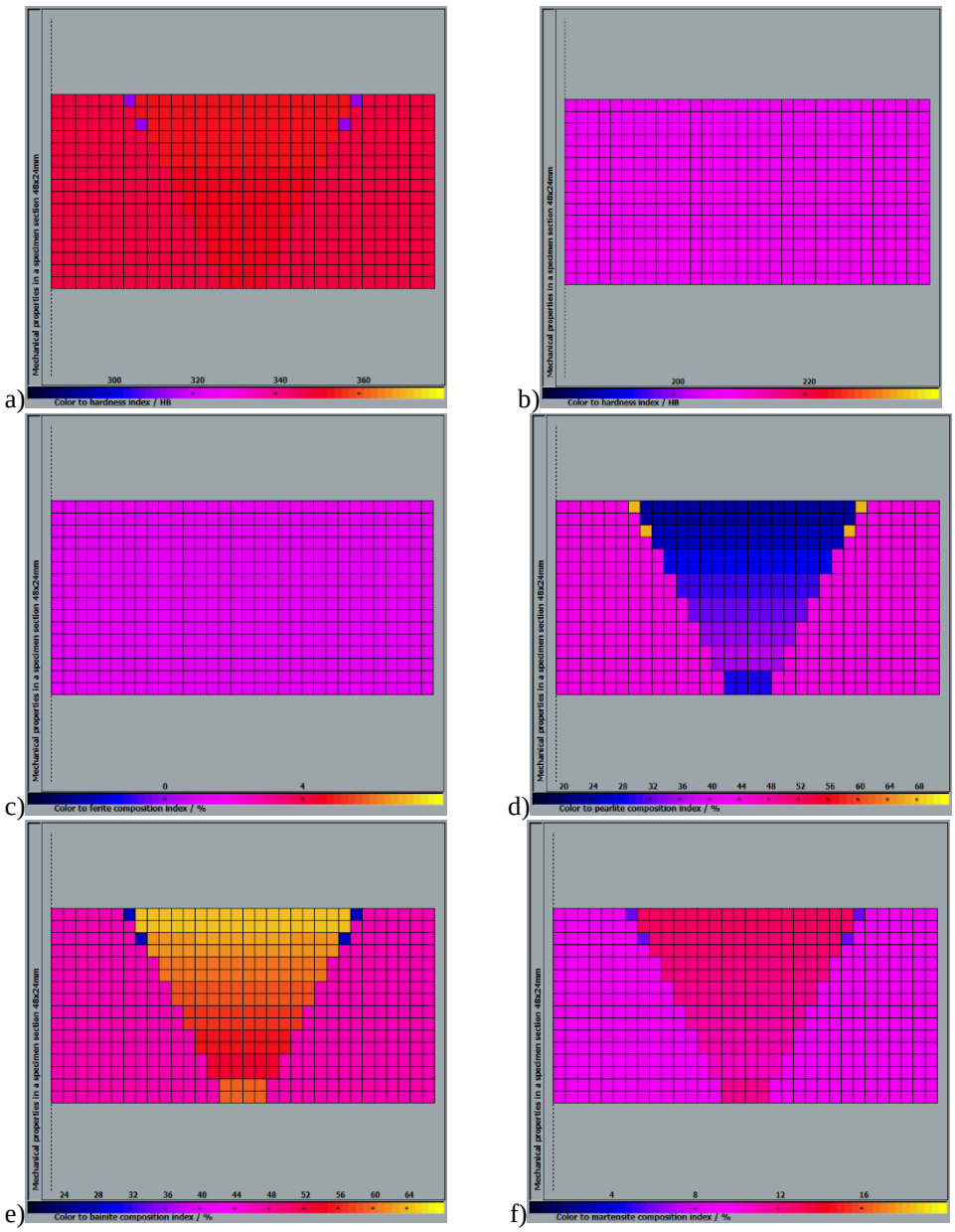

Fig. 3 Distribution of hardness and microstructure of welded joint of steel EN 52CrMoV4, a) hardness as-welding, b) hardness after tempering, c) ferrite, d) pearlite, e) bainite, f) martensite.

WELDING JOINT MADE OF STEEL EN X15CR13

The distribution of hardness and microstructure of the welding joint made of steel EN X15Cr13 are shown in Fig. 4.

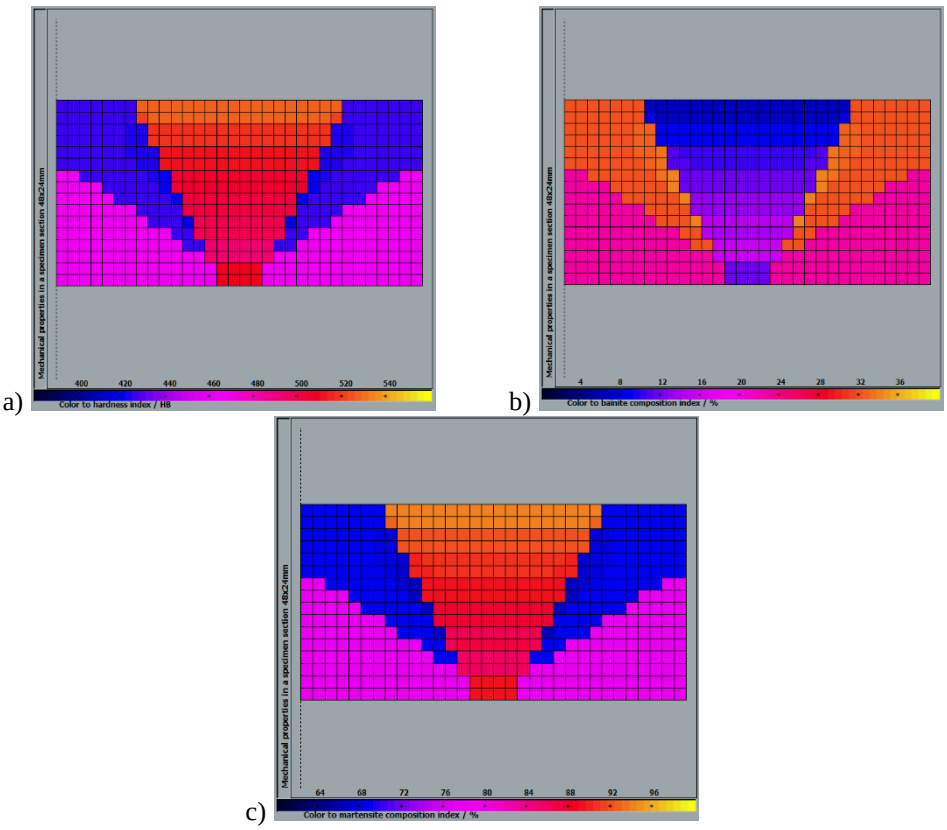

Fig. 4. Distribution of hardness and microstructure of welded joint of steel EN X15Cr13, a) hardness as-welding, b) ferrite+cementite, c) martensite [26]

CONCLUSIONS

The mathematical model of steel welding has been developed to predict the hardness and microstructure distribution in welded joint. The model is based on the finite volume method. The numerical simulation of welding is consisted of numerical simulation of transient temperature field of cooling process, numerical simulation of mechanical properties and microstructure transformation in solid state.

Input material data involved in mathematical model of welding, i.e., density and specific heat capacity of steel, heat transfer coefficient and heat conductivity coefficient were

accepted from literature. Moreover, heat transfer and heat conductivity coefficients are additionally calibrated.

Hardness and microstructure composition in specimen points were calculated by the conversion of calculated time of cooling from 800 to 500 °C, $t_{8/5}$ to hardness and microstructure composition using the CCT diagram and thermo-kinetic expressions. Hardness of steel wildings was estimated by taking into account the process of reheating of workpiece during the welding. Also, influence of tempering on welding joints properties was studied.

A developed mathematical model has been applied in computer simulation of welding of steel plates. It can be concluded, that hardness and microstructure composition in welded steel can be successfully calculated by proposed method.

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