

## ON METHODOLOGY OF CONCENTRATION DATA PROCESSING AT MATHEMATICAL MODELLING OF SUBSTITUTION ELEMENT DIFFUSION IN THE ZONE OF WELDED JOINT OF STEELS

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## K METODICE ZPRACOVÁNÍ KONCENTRAČNÍCH DAT PŘI MATEMATICKÉM MODELOVÁNÍ DIFÚZE SUBSTITUČNÍCH PRVKŮ V OBLASTI SVAROVÉHO SPOJE OCELÍ

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### Abstrakt

Příspěvek se zabývá metodikou zpracování původních výsledků měření redistribuce substitučních prvků (Cr, Si, Mo, Ni) ve svarovém spoji ocelí, tvořeném nízkolegovanou CrNiMoV ocelí a nízkolegovanou křemíkovou ocelí. Oceli, tvořící příslušný svarový spoj, jsou stejného strukturního typu, to znamená - obě mají feritickou strukturu. Měření bylo prováděno v teplotním intervalu 500 – 1000°C. Rozložení vybraných prvků kolmo přes svarové rozhraní se zjišťovalo pomocí energiově disperzní (ED) rtg. mikroanalýzy. Tato analýza se provedla bodově, podél tří úseček kolmo na svarové rozhraní. Celková délka těchto měřených úseků byla 180 μm a vzdálenost jednotlivých bodů se zvolila 3 μm. V jednom měřeném úseku se získal koncentrační soubor obsahující 61 hodnot koncentrací měřených prvků. Ukázalo se, že v průběhu difúzních ohřevů dochází k měřitelné redistribuci všech prvků. Redistribuce substitučních prvků má charakter vzájemné difúze.

Teoretickým základem je řešení 2. Fickova zákona jednorozměrové difúze s příslušnými okrajovými podmínkami. Parametry difúzní rovnice se určovaly metodou nelineární regrese. Tři soubory naměřených koncentračních dat vedly k výpočtu difúzních koeficientů příslušných substitučních prvků a dalších parametrů difúzní rovnice. Zpracování lze provádět různými způsoby a podrobit je podrobnému statistickému vyhodnocení. Ukázalo se, že vypočtené hodnoty difúzního koeficientu a jejich přesnost velmi záleží na zvolené metodě výpočtů, proto jednotlivé metody výpočtu byly vzájemně porovnány a byla vybrána nejlepší metoda, která je zatížena nejmenší chybou. Výsledky mají význam pro posouzení chemické i strukturní nehomogenity svaru a použitelnosti modelu molekulární difúze.

### Abstract

The paper deals with methodology of processing of original results from measurement of redistribution of substitution elements (Cr, Si, Mo, Ni) in welded joint of steels made from low-alloy steel CrNiMoV and low-alloy silicon steel. The steels forming the given welded joint are of same structural type, both of them have ferritic structure. The measurement was made in temperature interval 500 - 1000°C. Distribution of selected elements perpendicularly across welded boundary was determined with use of energy dispersive (ED) X-ray micro-analysis. This analysis was made in the individual points, along three line segments perpendicularly to the

welded boundary. Overall length of each line segment was approx. 180  $\mu\text{m}$  and distance between individual points was 3  $\mu\text{m}$ ; the centre of each line was the boundary of welded joint. In one measured segment there was obtained a concentration set containing 61 values of concentration of measured elements. It was established that during diffusion annealing there occurs measurable redistribution of all elements. Redistribution of substitution elements has character of mutual diffusion.

Solution of the 2<sup>nd</sup> Fick's law on one-dimensional diffusion with suitable boundary conditions was theoretical basis for evaluation of concentration profiles. Parameters of diffusion equation were determined by method of non-linear regression. Three sets of measured concentration data lead to calculation of diffusion coefficients of analysed substitution elements and other parameters of diffusion equation. Processing of data can be made by various manners and they can be subjected to a detailed statistical evaluation. It was established that calculated values of diffusion coefficient and their accuracy are very sensitive to selected calculation method, that's why individual calculation methods were mutually compared and the best method was chosen, i.e. the method with the smallest error. The results are important for evaluation of chemical and structural nonhomogeneity of welded joint and usability of the model of molecular diffusion.

**Keywords:** redistribution of substitution elements, diffusion, welded joint of steels

## 1. Introduction

Knowledge of redistribution of elements in welded joints of different steels has theoretical and practical meaning particularly for pipelines that are in the long run subjected to thermal loads, e.g. in power engineering. Numerous works oriented on interstitial and substitution elements [1-5] pay on a long-term basis attention to investigation of these phenomena.

Methodology leading to obtaining of relevant results consists of collection of necessary experimental data, theoretical solution of the problem, its evaluation and interpretation of results.

Experience gained from this methodology is demonstrated in the paper on redistribution of chromium.

## 2. Experiment

Measurement of chromium redistribution was made in a welded joint formed by low-alloy steel CrNiMoV (marked as P2) and low-alloy silicon steel (marked as V) in temperature interval 500 - 1000°C. During diffusion annealing the redistribution of all elements occurs. Redistribution of substitution elements has character of mutual diffusion.

Chemical composition of used steels is given in the Table 1.

Table 1 Chemical composition of steels of welded joints [weight %]

Steel	C	Mn	Si	P	S	Cr	Ni	Cu	Mo	V	Al	Fe
P2	0.16	0.48	0.28	0.009	0.010	2.20	1.29	0.06	0.59	0.100	0.01	rest
V	0.80	0.66	2.34	0.026	0.033	0.09	0.05	0.09	0.004	0.007	0.15	rest

Note: P2 – steel GOST 15Ch2NMFAA; V – steel 80CSi2,3 non-standard

Samples in the form of cylinders with diameter 12 mm and height 4 mm were made from the above steels. A polished metallographic section was made on top surface of each cylinder. The samples were on their ground and polished surfaces welded in diffusion pairs by electric shock under protective argon stream.

The welded diffusion pairs were then sealed into quartz tubes with titanium chips and annealed isothermally in electric resistance furnace in the interval from 500 to 1000°C with stepping of 50°C. The samples were after annealing taken out of quartz tubes, cut in half perpendicularly to the welded boundary and polished metallographic sections were made on cut surfaces. Afterwards the samples were processed by electro-spark cutting on the opposite side to the polished section and plan-parallelly with polished section to the height of approx. 4 mm. Polished sections were slightly etched by Nital in order to visualise microstructure in the area of welded joint. With use of light microscope Neophot 2 the areas suitable for micro-analysis were selected on etched surfaces. These areas, as well as position of the welded boundary were then marked by micro-punctures by micro-durometer Hannemann and the samples were repolished by diamond pastes with final granularity  $\leq 1\mu\text{m}$  in order to remove the etched layer. After cleaning of samples with ethyl alcohol the samples were inserted in the sample holder enabling orientation of the welded boundary marked by micro-punctures perpendicularly to the axis Y, along which distribution of selected elements was then determined perpendicularly through welded boundary by ED microanalysis. This analysis was made in the individual points, along three line segments perpendicularly to the welded boundary, which were distant mutually at least 30  $\mu\text{m}$ , from the distance of approx. 90  $\mu\text{m}$  from the welded boundary in the steel marked as V, up to the distance of approx. 90  $\mu\text{m}$  from the welded boundary in the steel marked as P2. Overall length of these measured segments is therefore 180  $\mu\text{m}$  and the distance of individual points was chosen to be 3 $\mu\text{m}$ . In one measured segment there was obtained a concentration set containing 61 values of concentrations of 8 measured elements - aluminium, silicon, titanium, chromium, manganese, iron, nickel and molybdenum, and for each sample there were obtained three such files (see Fig. 1).

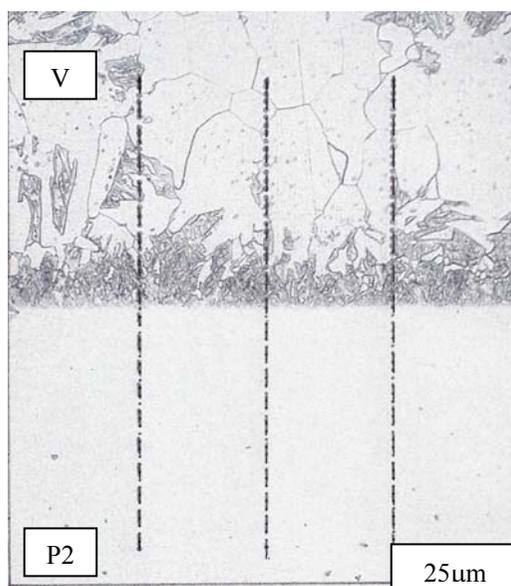


Fig.1 Structure of the welded joint P2/V (sample 4, 650°C / 80 h)

Working conditions for ED analysis were identical for all the samples: accelerating voltage of the primary electron beam  $U = 15$  kV, current of the primary electron beam  $i = 1$  nA, duration of collection (of measurement) of one spectre  $t = 50$  s, user program of the company KEVEX "Quantex VI", quantitative manner of evaluation of concentrations.

### 3. Theoretical basis

#### 3.1 Diffusion

Solution of diffusion in the system that is formed by two media (welded joint of steels P2/V – of structural type ferrite/ ferrite) is based the concept of one-dimensional diffusion for semi-infinite areas:  $(0 < x < \infty)$ ,  $(-\infty < x < 0)$ . The basis equation can be found in the Ref. [6], or with respect to analogy between diffusion and heat conduction also in Ref. [7].

$$c_1 = A_1 + B_1 \operatorname{erf} \frac{x}{2\sqrt{D_1 t}}, \quad x > 0 \quad (1)$$

$$c_2 = A_2 + B_2 \operatorname{erf} \frac{|x|}{2\sqrt{D_2 t}}, \quad x < 0 \quad (2)$$

where  $c_1$  is concentration in the area  $x > 0$ ,  $c_2$  is concentration in the area  $x < 0$ ,  $A_1$ ,  $B_1$ ,  $A_2$ ,  $B_2$  are constants, which are obtained after insertion of initial and boundary conditions,  $D_1$  is diffusion coefficient in the area  $x > 0$ ,  $D_2$  is diffusion coefficient in the area  $x < 0$ .

Diffusion of substitution elements in the welded joint of steels P2/V, of structural type ferrite/ferrite, is solved by the equations (1), (2) with the following initial and boundary conditions:

Initial conditions:

$$1.) \quad c_1 = c_0, \quad t \leq 0, \quad 0 < x < \infty \quad (3)$$

$$2.) \quad c_2 = d_0, \quad t \leq 0, \quad 0 > x > -\infty \quad (4)$$

Initial conditions assume constant concentrations of diffusing component, different in both diffusion domains (diffusion areas).

Boundary conditions:

$$3.) \quad \frac{c_2}{c_1} = 1, \quad x = 0, t > 0 \quad (5)$$

$$4.) \quad D_1 \frac{\partial c_1}{\partial x} = D_2 \frac{\partial c_2}{\partial x}, \quad x = 0, t > 0 \quad (6)$$

Boundary conditions (5), (6) are valid in the time  $t > 0$  on the boundary of both diffusion domains at  $x = 0$ . The boundary condition (5) assumes equality of concentrations on the boundary, the boundary condition (6) assumes equality of densities of diffusion flows on the

boundary. It is assumed that diffusivity in both areas is independent on concentration. If the equality  $D_1 = D_2$  is true, the concentration profile at the time  $t > 0$  at  $x = 0$  is continuous. The next calculation comprises this assumption.

Solution leads to the result that is valid for both parts of the welded joint - in the following form:

$$N_i(x,t) = N_1 + 0,5(N_2 - N_1) \operatorname{erfc}\left(\frac{x}{2\sqrt{D_i t}}\right). \quad (7)$$

This form is cited in the work [2], where the values  $N$ ,  $N_1$ ,  $N_2$  substitute generally expressed concentration by weight percents:  $N(x,t) \equiv c_1 \equiv c_2$ ,  $N_1 \equiv c_0$ ,  $N_2 \equiv d_0$ . The equation (7) satisfies the initial and boundary conditions. It can be easily proven that at big distance on both sides of the welded joint the following is valid:  $N(\infty, t) = N_1$ ,  $N(-\infty, t) = N_2$ , i.e. that these concentrations are therefore identical with initial concentrations at the time  $t = 0$ .

Table 2 Concentration of chromium in the steels P2, V and its diffusion coefficients

Sample No. (T[K], t[s])		$10^3 N_1$ [weight %]	$10^2 N_2$ [weight %]	$10^{15} D_C$ [ $\text{cm}^2/\text{s}$ ]
sample 3	mean	$222.8 \pm 2.3$	$7.6 \pm 2.5$	$6.7 \pm 1116.0$
(600°C, 383h)	mean*	$222.7 \pm 1.6$	$7.7 \pm 1.7$	$5.3 \pm 2.2$
sample 4	mean	$216.4 \pm 3.2$	$7.2 \pm 3.7$	$164.9 \pm 70.3$
(650°C, 80h)	mean*	$215.9 \pm 1.8$	$7.3 \pm 2.0$	$111.4 \pm 30.5$
sample 6	mean	$255.7 \pm 22.9$	$10.3 \pm 25.3$	$217.4 \pm 1274.7$
(700°C, 40h)	mean*	$256.4 \pm 15.5$	$6.8 \pm 17.5$	$1000.0 \pm 1330.0$
sample 7	mean	$215.9 \pm 3.5$	$5.3 \pm 3.9$	$401.4 \pm 213.0$
(750°C, 7h)	mean*	$215.9 \pm 2.6$	$5.3 \pm 3.0$	$395.3 \pm 161.0$
sample 8	mean	$218.1 \pm 2.5$	$7.4 \pm 2.7$	$114.1 \pm 204.6$
(800°C, 30h)	mean*	$218.1 \pm 1.5$	$7.4 \pm 1.6$	$101.8 \pm 23.8$
sample 9	mean	$214.9 \pm 2.6$	$3.5 \pm 2.8$	$2131.6 \pm 626.2$
(850°C, 16h)	mean*	$214.2 \pm 1.7$	$3.4 \pm 1.8$	$1590.6 \pm 298.0$
sample 10	mean	$222.5 \pm 2.0$	$8.7 \pm 2.4$	$3394.6 \pm 748.3$
(900°C, 8h)	mean*	$222.4 \pm 1.2$	$8.8 \pm 1.4$	$3016.7 \pm 413.0$
sample 11	mean	$220.4 \pm 1.8$	$4.9 \pm 2.0$	$14191.1 \pm 2363.3$
(950°C, 4h)	mean*	$219.7 \pm 1.1$	$5.1 \pm 1.2$	$10875.0 \pm 1130.0$
sample 12	mean	$216.8 \pm 1.8$	$5.6 \pm 2.0$	$16827.3 \pm 3190.0$
(1000°C, 2h)	mean*	$216.8 \pm 1.3$	$5.6 \pm 1.4$	$16881.0 \pm 2270.0$

**Note:** Mean – the value is determined as a mean from calculated values given in the table for the measured areas 1-3. Mean\* - the value calculated from the averaged

measured concentrations. The samples 1, 2 and 5 are described in detail in the Table 3.

#### 4. Evaluation of experimental data

##### 4.1 Optimisation program

A modified form of the equation (7) from the work [9] was used for evaluation of experimental data:

$$N_i(x,t) = N_1 + 0,5(N_2 - N_1) \operatorname{erfc} \left( \frac{x - x_0}{2\sqrt{D_i t}} \right) \quad (8)$$

From the measured values  $N_i(x,t)$  and  $x, t$  the free optimisation parameters  $N_1, N_2, D, x_0$  were evaluated by method of non-linear regression. The parameter  $x_0$  represents a correction of inaccuracy of deduction of (zero) position of the welded joint; from mathematical viewpoint it is a transformation of the coordinate  $x$ .

The attempt of evaluation of parameters from the equation (7) by the user program Polymath 5.1 [10] was unsuccessful. That's why there was developed a proprietary optimisation program of non-linear regression. The Levenberg–Marquardt's method, which uses an algorithm according to the Ref. [11], is the core of the program. The program was at first tested on simulated data with small scatter. When real experimental data with greater scatter were used, it was found that the pursued special function minimising sum of squares of deviations can have several local minimums. That's why the basic algorithm was applied only on limited part of multi-dimensional space (from the viewpoint of optimisation parameters). The limitation did not permit e.g. negative values of the parameters  $N_1, N_2, D$  and too big deviations of the pars  $N_1, N_2$  from the relevant chemical composition. It chose from the found local minimums the most suitable one, i.e. the one with the minimum residual sum of squares. In case of close magnitudes of these values it preferred a minimum with the smallest error of the value of diffusivity.

Scatters of real data cannot be attributed to a systematic error of the experiment, but rather to processes embedded already in steelmaking technology, which result in structural and chemical non-homogeneity in the area of the welded joint.

##### 4.2 Statistics of the model

The optimisation program comprises also statistical evaluation of results of the used model. Standard deviations of free optimisation parameters are determined by the radical from diagonal elements of co-variation matrix. Confidence is calculated as a multiple of the standard deviation of the quantile of Student's distribution for the confidence level 0.05. All other quantities are related to the dependent variable of the equation (8). Determination coefficient is calculated from the relation:

$$R^2 = 1 - \frac{\sum (N_i - N_i^*)^2}{\sum N_i^2 - \frac{(\sum N_i)^2}{n}} \quad (9)$$

Here  $N_i$  represents the experimental value,  $N_i^*$  represents the calculated value of dependent variable,  $n$  represents their number of the measured data.

Adjoint determination coefficient determines the relation:

$$R_{adj.}^2 = 1 - \frac{n-1}{k-1} (1 - R^2). \quad (10)$$

Here  $k$  is the number of optimised parameters.

Variance is determined by the relation:

$$V = \frac{1}{n} \sum (N_i - \bar{N}_i)^2. \quad (11)$$

Here  $\bar{N}_i$  is an arithmetic mean of the dependent variable.

Arithmetic mean:

$$\bar{N}_i = \frac{1}{n} \sum N_i. \quad (12)$$

Residual sum of squares:

$$Res = \sum (N_i - N_i^*)^2. \quad (13)$$

The program calculates apart from the standard deviation also a confidence interval for reliability  $\alpha = 0.05$ . That's why calculation of quantiles of Student's distribution is also implemented in it.

Statistical characteristics thus give a quantitative picture about accuracy of results, or of usability of the given model for real situation.

## 5. Results

Results of the ED analysis can be processed only in one manner, if only one data file is available. Three data files that were available can be evaluated in the following manner:

Optimisation:

- optimisation of each set separately and determination of an arithmetic mean of parameters  $N_1$ ,  $N_2$ ,  $D$  and of their errors,
- optimisation of an mean experimental concentrations from all areas (from three data sets),
- optimisation of a median of all experimental concentrations. This procedure is a certain form of robust regression; that is it does not exclude boundary points, but gives lesser weight to them,
- joint optimisation of all the data from all the files.

It is probably impossible to determine a single procedure for all cases. It is, however, possible to compare the results by the F-test [12], which can be made in the program Microsoft Excel [13]; in case of comparable standard deviation it is then possible to choose the model with higher determination coefficient.

The models with determination coefficient below the value of 0.8 or with the standard deviation greater than the value of the parameter are considered by the authors as unreliable and unstable.

The Table 3 gives basic data for the following examples of processing.

Table 3 Chromium concentration in the steels P2, V and its diffusion coefficients

Sample (T[K], t[s])		$10^2 N_1$ [wt %]	$10^2 N_2$ [wt %]	$10^{15} D_{Cr}$ [cm <sup>2</sup> /s]
sample 1 (500°C, 860h) (Fig. 3)	1 <sup>st</sup> area	245.2 ± 2.1	12.9 ± 2.4	4.2 ± 1.4
	2 <sup>nd</sup> area	244.6 ± 2.3	21.7 ± 2.6	1.9 ± 0.7
	3 <sup>rd</sup> area	237.2 ± 2.3	21.9 ± 2.6	1.3 ± 0.6
	mean	242.3 ± 2.3	18.8 ± 2.5	2.5 ± 0.9
	mean*	242.6 ± 1.4	18.8 ± 1.6	3.6 ± 0.7
sample 2 (550°C, 529h) (Figs. 4, 5)	1 <sup>st</sup> area	213.4 ± 1.6	4.2 ± 1.7	5.6 ± 1.6
	2 <sup>nd</sup> area	216.4 ± 2.0	5.4 ± 2.1	2.7 ± 1.1
	3 <sup>rd</sup> area	218.9 ± 1.5	5.1 ± 1.6	9.8 ± 2.7
	mean	216.2 ± 1.7	4.9 ± 1.8	6.0 ± 1.8
	mean*	216.1 ± 0.9	4.9 ± 1.0	5.6 ± 0.9
sample 5 (700°C, 49h) (Fig. 2)	1 <sup>st</sup> area	275.1 ± 26.7	4.0 ± 25.8	2375.3 ± 3370.0
	2 <sup>nd</sup> area	235.4 ± 21.1	6.0 ± 22.7	636.7 ± 1300.0
	3 <sup>rd</sup> area	257.5 ± 24.8	6.9 ± 26.1	853.3 ± 1710.0
	mean	256.0 ± 24.2	5.6 ± 24.9	1288.4 ± 2126.7
	mean*	252.9 ± 11.0	5.6 ± 11.5	1394.1 ± 1100.0

Fig. 2 corresponds to the sample No. 5 with big scatter of experimental data. Although the program calculates the concentration profile, the standard deviations are high. The model is unreliable and unstable.

Fig. 3 corresponds to the sample No. 1 with acceptable values of standard deviations. Majority of calculations fall into this situation.

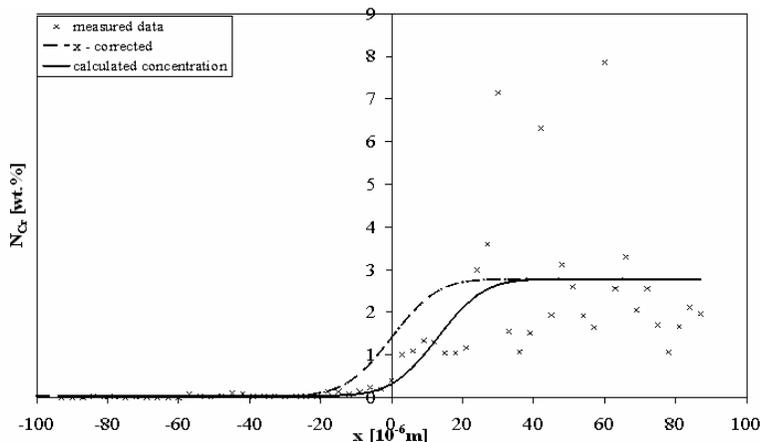


Fig.2 Chromium redistribution (sample 5, 1. area , 700°C, 49h)

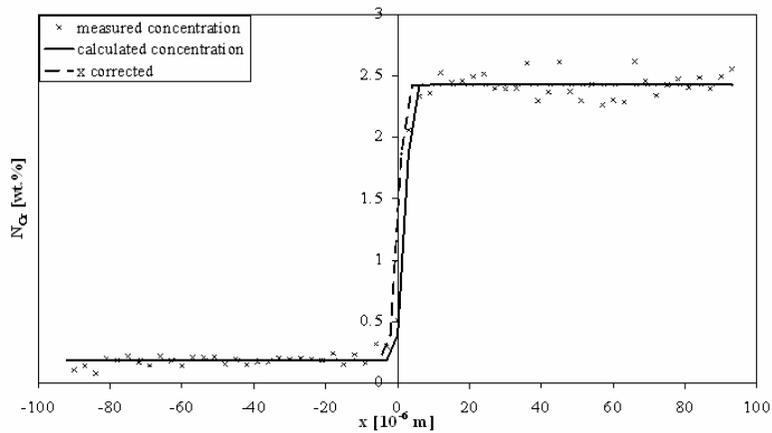
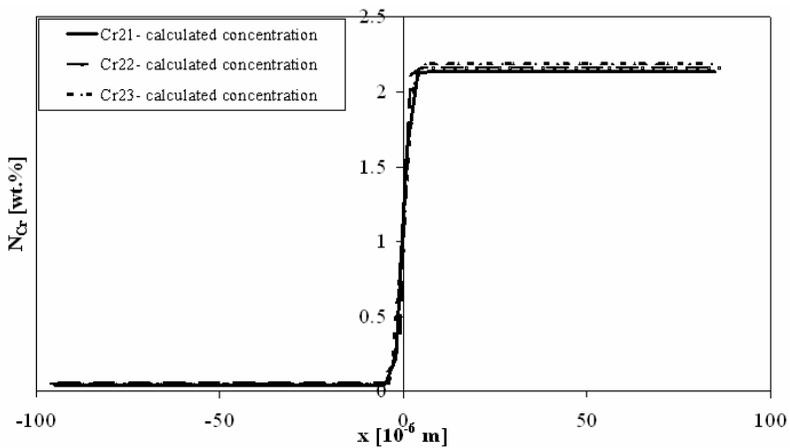


Fig.3 Chromium redistribution (sample 1, averaged concentration, 500°C, 860h)

Fig.4 Chromium redistribution in the 1<sup>st</sup>, 2<sup>nd</sup> and 3<sup>rd</sup> area of the sample 2 (550°C, 529 h)

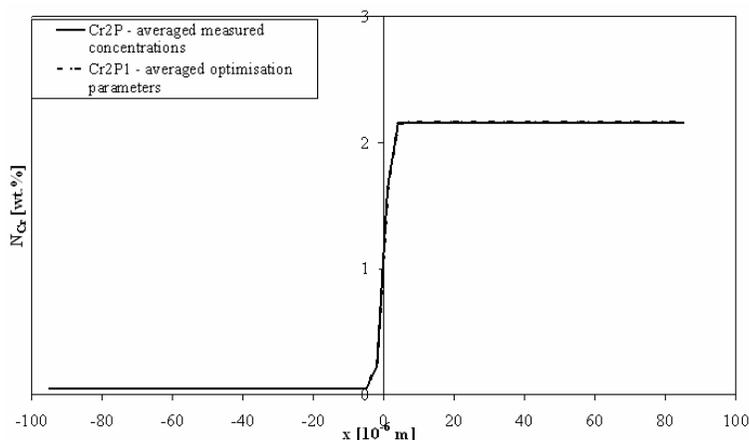


Fig.5 Comparison of two manners of evaluation of chromium redistribution – 2<sup>nd</sup> sample (550°C, 529 h)

The Figures 4 and 5 show processing of experimental data by methods a) and b). The curves in the Fig. 4 are the result of regression of three areas individually. The Figure 5 compares the curve Cr2P, obtained by regression of the mean of concentrations from all areas, with the curve Cr2P1, obtained from the means of optimisation parameters according to the Fig. 5 (mean in the Table 3). Both diagrams show comparatively small chemical and structural heterogeneity. This is confirmed also by the F-test for the files, corresponding to the file of the Fig. 5 with the values  $F \approx 1,019$  a  $F(\text{crit}) \approx 1,584$ . Comparison of determination coefficients 0.998 (Cr2P) and 0.992 (Cr2P1) bears evidence slightly in favour of the file Cr2P.

## 6. Conclusion

The paper presents original results of methodology for evaluation of experimental data at redistribution of elements in the welded joint. The methodology is illustrated by examples from chromium redistribution in steels with polycomponent system of elements. Considerations concerning methodology for evaluation ensued from the scatter of experimental data, which in the authors' opinion cannot be attributed to a systematic error of an analysis made by the ED method. It is also impossible to find comparison with other works. It is possible to express an opinion that the cause of scatter of experimental data can lie in the processes running concurrently with diffusion. Their basis arises from thermodynamic disequilibria, which were formed already by steelmaking technology. There can be running phase transformations, there can be created inter-metallic compounds, or some other physical-chemical process can occur. Formation of Laves phases in steels with comparatively high chromium contents was established in the works [14, 15], both experimentally and also by theoretical thermodynamic calculation.

Due to the fact that the processes mentioned above are not sufficiently quantified, statistic evaluation provides a measure for notion of chemical and structural non-homogeneity also from the viewpoint of time and temperature dependencies. Statistic evaluation can be viewed also as a measure of validity of the model of molecular diffusion for the given physical situation.

Adaptation of the Levenberg-Marquardt algorithm for solution of optimisation of parameters of diffusion equation is also original.

The results serve also as a stimulus for next theoretical and experimental investigation of these issues.

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