https://doi.org/10.37434/tpwj2021.01.09

MATHEMATICAL MODELS OF THE DEPENDENCE OF MECHANICAL PROPERTIES ON CHEMICAL COMPOSITION OF STEELS FOR ESW

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The paper deals with the possibility of constructing mathematical models of the dependence of mechanical properties of silicon-manganese steels designed for ESW, which have high brittle fracture resistance in the HAZ, as well as of the overheated zone, on chemical composition. Data on mechanical properties of these steels were obtained as a result of studying the influence of additional alloying (microalloying) of silicon-manganese steel by manganese, chromium, vanadium, boron, cerium and zirconium, on overheating resistance at electroslag welding. The method of multiple linear regression was used for construction of mathematical models. Mathematical models were constructed for the following set of base metal mechanical properties: impact toughness for temperatures of (+20, –40, –60, –70 °C), yield limit, ultimate strength, relative elongation and reduction in area. For overheated zone at electroslag welding mathematical models were constructed for impact toughness (*KCU* and *KCV*) for temperatures of +20, –60, –70 °C. Initial validation of the constructed models was performed. 9 Ref., 12 Tables, 2 Figures.

Keywords: silicon-manganese steels, chemical composition, microalloying, mechanical properties, mathematical models, electroslag welding

Investigations conducted at PWI of the influence of chemical composition on the mechanical properties of silicon-manganese steels produced by the method of induction remelting and designed for electroslag welding (ESW), which have a high brittle fracture resistance [1], provided experimental data on the composition and mechanical properties of the base material (Tables 1, 2) and overheated zone (of the HAZ) (Table 3) for 55 experimental melts of low-alloy steels. This information was used to plot the mathematical models for prediction of the mechanical properties of base metal and overheated zone metal at ESW, depending on the chemical composition of steels. Derived models can find effective use at development of new silicon-manganese steels for determination of optimum alloying with the purpose of obtaining the specified mechanical properties and required level of brittle fracture resistance in the HAZ of welded joints produced with ESW application.

General information on construction of regression models. The mathematical models by the available experimental data on mechanical properties and chemical composition of the experimental steels were constructed with application of the method of multiple linear regression, which is designed for modeling the dependence between one dependent variable and several independent variables [2, 3]. Such a relation can be theoretically described by a linear dependence of the following form:

$$Y = b_1x_1 + b_2x_2 + ... + b_kx_k + u,$$

where Y is the dependent variable — regressand; U is the random component of the model; x_k are the independent variables — regressors.

The coefficients of the model of multiple linear regression are found by the least-squares method.

The least-squares method [4] allows finding such values of the coefficients, for which the sum of squares of deviations will be minimal. The following system of normal equations is solved to determine the coefficients:

$$\begin{cases} nb_0 + b_1\sum x_1 + \ldots b_p\sum x_p = \sum y \\ b_0\sum x_1 + b_1\sum x_1^2 + \ldots b_p\sum x_1x_p = \sum x_1y \\ \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \\ b_0\sum x_p + b_1\sum x_1x_p + \ldots b_p\sum x_px_p = \sum x_py \end{cases}.$$

Solution of the system can be derived, for instance, by Cramer's method:

$$b_0 = \frac{\Delta b_0}{\Delta}, \quad b_1 = \frac{\Delta b_1}{\Delta}, \ \ldots, \ b_p = \frac{\Delta b_p}{\Delta}.$$

System determinant is written as follows:

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Table 1. Chemical composition of experimental steels, wt.%

No.	Alloying system	Experimental melt number	C	Mn	Si	S	P	Cr	Ni	V	Al	Ce	B	Zr
1	Mn–Si–Al	20	0.069	1.550	0.530	0.031	0.012	0.150	0.630	–	0.100	0.050	–	–
2	Mn–Si–Ce–Al	25	0.065	1.550	0.770	0.021	0.012	0.200	0.100	–	0.130	0.033	–	–
3	Mn–Si–Al–B	26	0.060	1.350	0.600	0.024	0.012	0.160	0.300	–	0.200	–	0.006	–
4	Mn–Si–Al–B	33	0.091	1.580	0.650	0.021	0.013	0.170	0.140	–	0.330	–	0.005	–
5	Mn–Si–Al	37	0.038	2.350	0.320	0.028	0.040	–	–	–	0.200	–	–	–
6	Mn–Si–Ce–Al	38	0.065	2.300	0.190	0.018	0.012	0.290	0.200	–	0.067	0.075	–	–
7	Mn–Si–Al–Ce–B	82	0.120	2.700	0.500	–	–	–	–	–	0.100	0.065	0.008	–
8	Mn–Si–Ce–Al–Cr–Ni	99	0.080	0.315	–	–	1.000	1.100	–	0.110	0.290	–	–	–
9	Mn–Si–Al–Ce–B	100	0.062	1.860	0.280	0.021	0.012	0.450	0.350	–	0.110	0.029	0.005	–
10	Mn–Si–Al–Ce–Zr–B	133	0.053	2.300	0.520	0.017	0.009	0.080	0.100	–	0.185	0.024	0.004	0.017
11	Mn–Si–Ce–Al–Zr–V–P–Cr	152	0.076	1.260	0.038	0.068	0.009	1.450	0.320	0.035	0.070	0.069	0.003	0.015
12	Mn–Si–Al–Ce–Zr–B–V	153	0.082	1.950	0.580	0.012	0.110	0.320	0.185	0.275	0.160	0.140	0.022	0.200
13	Mn–Si–Al–Ce–Zr–B	156	0.069	2.400	0.550	0.018	0.009	0.060	0.180	–	0.240	0.093	0.003	0.040
14	Mn–Si–Ce–Al–Zr–V–P–Cr	157	0.056	1.600	0.400	0.002	0.009	1.400	0.130	0.032	0.100	0.064	0.004	0.035
15	Mn–Si–Al–Ce–Zr–B–V	163	0.072	1.500	0.500	0.020	0.012	0.080	0.180	0.210	0.140	0.004	0.003	0.075
16	Mn–Si–Al–Ce–Zr	164	0.058	2.400	0.550	0.083	0.015	0.090	0.165	–	0.125	0.100	–	0.086
17	Mn–Si–Al–Ce–B–V	165	0.058	2.500	0.560	0.020	0.013	0.095	0.110	0.200	0.089	0.090	0.005	–
18	Mn–Si–Al–Ce–Zr–B–V	167	0.073	2.350	0.820	0.019	0.018	0.083	0.100	0.130	0.190	0.090	0.004	0.100
19	Mn–Si–Ce–Al–Zr–B–Cr	177	0.068	2.250	0.630	0.014	0.011	2.850	0.100	–	0.220	0.100	0.003	0.045
20	Mn–Si–Ce–Al–Zr–V–P–Cr	203	0.051	1.600	0.050	0.018	0.011	1.500	0.100	0.022	0.110	0.066	0.004	0.020
21	Mn–Si–Ce–Al–Cr	205	0.080	1.280	0.690	0.015	0.010	2.700	0.100	–	0.290	0.072	–	–
22	Mn–Si–Ai–Ce–B	206	0.045	1.280	0.210	0.008	0.013	0.500	–	–	0.038	0.040	0.003	–
23	Mn–Si–Al–Ce–B–V	207	0.052	1.600	0.820	0.016	0.013	0.190	–	0.210	0.075	0.110	0.006	–
24	Mn–Si	410	0.120	1.900	0.380	–	–	–	–	–	–	–	–	–
25	Mn–Si	411	0.130	1.180	0.140	–	–	–	–	–	–	–	–	–
26	Mn–Si	412	0.100	1.400	0.430	–	–	–	–	–	–	–	–	–
27	Mn–Si	413	0.120	2.600	0.570	–	–	–	–	–	–	–	–	–
28	Mn–Si–Al–Ce–V	432	0.080	1.300	0.440	–	–	–	0.100	0.200	0.100	0.160	–	–
29	Mn–Si–Ce–Al–Zr–Cr	433	0.085	1.400	0.800	–	–	2.200	–	–	0.065	0.018	–	0.060
30	Mn–Si–Ce–Al–V–Cr	434	0.085	1.350	0.650	–	–	2.400	0.075	0.051	0.045	0.040	–	–
31	Mn–Si–Ce–Al–Zr–B–Cr	435	0.080	1.420	0.680	–	–	2.350	0.080	–	0.150	0.130	0.004	0.023
32	Mn–Si–Ce–Al–Zr–V–P–Cr	436	0.080	2.100	0.550	–	–	2.600	0.070	0.010	0.185	0.075	0.008	0.020
33	Mn–Si–Ce–Al–Zr–V–B–Cr	437	0.083	2.000	0.490	–	–	2.300	0.070	0.190	0.110	0.085	0.006	–

Table 1 (cont.)

34	Mn–Si–Ce–Al–Zr–V–Cr	438	0.115	2.500	0.670	–	–	2.900	0.100	0.275	0.115	0.080	–	0.040
35	Mn–Si–Al–Ce–V	458	0.080	1.100	0.220	–	–	0.450	0.085	0.010	0.160	0.035	–	–
36	Mn–Si–Al–Ce–Zr–V	459	0.090	2.350	0.760	–	–	0.080	0.140	0.050	0.087	0.150	–	0.017
37	Mn–Si–Ce–Al–Zr–V–Cr	460	0.070	1.700	0.600	–	–	2.600	0.130	0.155	0.095	0.300	–	0.030
38	Mn–Si–Ce–Al–Zr–Cr	505	0.075	1.850	0.770	–	–	1.720	0.170	–	0.130	0.200	–	0.030
39	Mn–Si–Ce–Al–Zr–V–Cr	506	0.080	1.900	0.490	–	–	1.750	–	0.180	0.080	0.110	–	0.010
40	Mn–Si–Ce–Al–Zr–V–B–Cr	507	0.100	1.850	0.680	–	–	1.400	–	0.032	0.070	0.080	0.004	–
41	Mn–Si–Ce–Al–Mo	530	0.050	1.900	0.030	0.030	0.011	0.044	0.070	–	0.068	0.060	–	–
42	Mn–Si–Ce–Al	531	0.065	2.050	0.600	0.014	0.015	0.053	0.110	–	0.063	0.085	–	–
43	Mn–Si	597	0.200	1.100	0.240	–	–	0.140	–	–	–	–	–	–
44	Mn–Si	598	0.190	1.000	0.120	–	–	0.160	–	–	–	–	–	–
45	Mn–Si–Ce–Al–Cr	718	0.090	2.300	0.450	–	–	1.100	–	–	0.040	–	–	–
46	Mn–Si–Ce–Al–Cr	727	0.080	1.200	0.500	–	–	0.650	0.120	–	0.085	–	–	–
47	Mn–Si–Ce–B	728	0.080	2.050	0.600	–	–	0.240	0.090	–	0.042	0.009	0.005	–
48	Mn–Si–Ce–Al–Cr	881	0.063	1.600	0.630	–	–	0.440	0.190	–	0.048	–	–	–
49	Mn–Si–Ce–B	882	0.080	1.750	0.640	–	–	0.160	0.100	–	0.033	0.029	0.006	–
50	Mn–Si–Ce–Al	883	0.065	1.650	0.680	–	–	0.100	0.165	–	0.050	0.085	–	–
51	Mn–Si–Ce–B	894	0.075	1.600	0.650	–	–	0.165	0.145	–	0.032	0.040	0.005	–
52	Mn–Si–Ce–Al	895	0.089	2.250	0.250	–	–	0.080	–	–	0.034	–	–	–
53	Mn–Si–Ce–B	896	0.070	1.230	0.540	–	–	0.040	–	–	0.010	0.046	0.003	–
54	Mn–Si–Ce	127-2	0.120	2.800	0.300	–	–	–	–	–	–	0.060	–	–

Table 2. Mechanical properties of experimental steels (base metal)

No.	Alloying system	Melt number	σ_y, MPa	σ_t, MPa	δ, %	ξ, %	Impact toughness (*KCU*), J/cm^2			
							+20 °C	–40 °C	–60 °C	–70 °C
1	Mn–Si–Al	20	314	444	32.8	65.4	131.5	92.5	89.0	73.5
2	Mn–Si–Ce–Al	25	298	434	34.5	75.0	35.0	343.0	298.0	270.5
3	Mn–Si–Al–B	26	302	447	27.8	75.1	–	44.0	31.0	–
4	Mn–Si–Al–B	33	258	404	36.6	75.0	172.0	130.0	114.5	90.0
5	Mn–Si–Al	37	258	430	39.3	60.9	116.0	37.0	47.5	53.5
6	Mn–Si–Ce–Al	38	270	411	38.5	78.2	236.0	147.0	159.5	140.5
7	Mn–Si–Al–Ce–B	82	441	561	27.3	71.6	–	132.5	125.0	116.0
8	Mn–Si–Ce–Al–Cr–Ni	99	413	523	30.0	71.5	237.0	147.5	121.5	117.0
9	Mn–Si–Al–Ce–B	100	284	410	36.2	79.0	225.5	116.0	156.0	75.0
10	Mn–Si–Al–Ce–Zr–B	133	378	498	31.8	78.2	298.0	184.5	211.5	208.5
11	Mn–Si–Ce–Al–Zr–V–P–Cr	152	488	616	24.2	66.0	220.0	192.0	70.0	11.0
12	Mn–Si–Al–Ce–Zr–B–V	153	760	820	18.6	55.6	–	–	5.5	6.5
13	Mn–Si–Al–Ce–Zr–B	156	417	544	31.3	73.3	150.0	72.0	–	147.0
14	Mn–Si–Ce–Al–Zr–V–P–Cr	157	394	484	28.5	66.9	–	196.0	8.0	7.0
15	Mn–Si–Al–Ce–Zr–B–V	163	378	519	26.9	75.0	202.0	8.0	4.5	4.5
16	Mn–Si–Al–Ce–Zr	164	503	592	18.8	51.0	68.0	9.5	6.0	6.0
17	Mn–Si–Al–Ce–B–V	165	419	535	24.2	66.0	75.0	14.5	–	9.0
18	Mn–Si–Al–Ce–Zr–B–V	167	407	566	–	–	–	16.0	6.0	–
19	Mn–Si–Ce–Al–Zr–B–Cr	177	399	517	18.8	66.0	–	6.0	4.5	–
20	Mn–Si–Ce–Al–Zr–V–P–Cr	203	259	394	–	–	212.0	189.5	167.0	43.0

Table 2 (cont.)

21	Mn–Si–Ce–Al–Cr	205	389	495	27.2	75.0	97.5	29.0	10.5	6.0
22	Mn–Si–Ai–Ce–B	206	268	415	36.5	73.5	246.7	97.0	8.0	5.5
23	Mn–Si–Al–Ce–B–V	207	340	478	32.9	75.0	218.5	112.5	73.5	5.5
24	Mn–Si	410	380	516	32.0	70.8	350.5	196.5	105.0	–
25	Mn–Si	411	303	460	30.8	69.5	197.5	15.0	6.500	–
26	Mn–Si	412	336	432	28.8	70.7	353.0	–	179.5	10.5
27	Mn–Si	413	403	536	28.5	72.1	214.5	–	144.0	162.0
28	Mn–Si–Al–Ce–V	432	293	447	34.2	77.4	325.0	256.0	244.0	252.5
29	Mn–Si–Ce–Al–Zr–Cr	433	376	570	30.0	70.2	–	58.5	7.5	–
30	Mn–Si–Ce–Al–V–Cr	434	424	590	28.5	70.2	121.0	25.0	–	–
31	Mn–Si–Ce–Al–Zr–B–Cr	435	304	425	24.7	44.9	250.0	119.0	2.5	–
32	Mn–Si–Ce–Al–Zr–V–P–Cr	436	633	690	20.0	67.5	63.5	7.0	–	–
33	Mn–Si–Ce–Al–Zr–V–B–Cr	437	507	625	23.8	75.0	5.0	3.5	–	–
34	Mn–Si–Ce–Al–Zr–V–Cr	438	607	714	21.1	66.0	5.5	4.0	–	–
35	Mn–Si–Al–Ce–V	458	602	684	22.8	70.7	3.0	3.0	–	–
36	Mn–Si–Al–Ce–Zr–V	459	455	572	21. 5	62.7	75.0	32.0	–	–
37	Mn–Si–Ce–Al–Zr–V–Cr	460	454	577	27.2	70.5	141.0	15.0	–	–
38	Mn–Si–Ce–Al–Zr–Cr	505	752	669	12.8	37.2	58.5	29.5	–	–
39	Mn–Si–Ce–Al–Zr–V–Cr	506	735	832	18.5	-	34.0	7.0	–	–
40	Mn–Si–Ce–Al–Zr–V–B–Cr	507	401	575	29.5	75.0	75.0	44.5	–	–
41	Mn–Si–Ce–Al–Mo	530	298	443	33.7	77.5	350.0	324.0	–	254.0
42	Mn–Si–Ce–Al	531	323	500	34.9	75.0	295.5	243.0	–	200.0
43	Mn–Si	597	400	487	31.0	68.5	136.0	–	–	–
44	Mn–Si	598	390	492	31.0	38.5	142.5	–	–	–
45	Mn–Si–Ce–Al–Cr	718	386	561	26.2	73.3	–	142.5	126.0	108.5
46	Mn–Si–Ce–Al–Cr	727	245	406	39.2	79.8	–	101.5	–	12.9
47	Mn–Si–Ce–B	728	288	431	36.8	80.5	–	188.2	183.3	33.2
48	Mn–Si–Ce–Al–Cr	881	318	469	–	–	–	274.0	–	224.5
49	Mn–Si–Ce–B	882	385	517	28.7	64.9	–	195.0	–	204.0
50	Mn–Si–Ce–Al	883	–	–	–	–	–	269.5	133.0	98.0
51	Mn–Si–Ce–B	894	318	493	30.7	68.9	–	297.5	–	184.5
52	Mn–Si–Ce–Al	895	319	491	30.3	66.0	–	223.0	–	191.0
53	Mn–Si–Ce–B	896	305	488	26.9	64.9	–	268.0	–	242.5
54	Mn–Si–Ce	127-2	500	637	25.0	69.8	–	131.0	100.0	108.5
53	Mn–Si–Ce–B	896	305	488	26.9	64.9	0.0	268.0	0.0	242.5
54	Mn–Si–Ce	127-2	500	637	25.0	69.8	0.0	131.0	100.0	108.5

Table 3. Mechanical properties of overheated zone

No.	Alloying system	Melt number	Impact toughness (*KCU*), J/cm^2			Impact toughness (*KCV*), J/cm^2		
			+20 °C	–40 °C	–70 °C	+20 °C	–40 °C	–70 °C
1	Mn–Si–Al	20	–	–	142.0	53.5	11.0	–
2	Mn–Si–Ce–Al	25	165.5	–	–	206.0	118.5	41.0
3	Mn–Si–Al–B	26	183.0	–	99.0	–	–	90.5
4	Mn–Si–Al–B	33	191.5	–	–	111.0	73.5	17.5
5	Mn–Si–Al	37	134.5	–	–	81.0	52.5	29.5
6	Mn–Si–Ce–Al	38	187.5	–	–	56.5	66.0	22.5
7	Mn–Si–Al–Ce–B	82	–	121.0	–	108.5	108.5	68.5
8	Mn–Si–Ce–Al–Cr–Ni	99	–	–	–	128.0	116.5	109.5
9	Mn–Si–Al–Ce–B	100	106.5	–	83.5	62.5	66.0	32.5
10	Mn–Si–Al–Ce–Zr–B	133	–	–	–	160.5	148.5	6.5
11	Mn–Si–Ce–Al–Zr–V–P–Cr	152	–	127.5	–	6.0	–	4.0
12	Mn–Si–Al–Ce–Zr–B–V	153	–	8.0	–	405.0	–	4.0
13	Mn–Si–Al–Ce–Zr–B	156	–	167.0	–	5.0	–	5.5
14	Mn–Si–Ce–Al–Zr–V–P–Cr	157	–	19.5	–	5.0	–	4.0
15	Mn–Si–Al–Ce–Zr–B–V	163	–	6.0	–	–	–	4.0
16	Mn–Si–Al–Ce–Zr	164	–	5.0	–	4.5	–	4.0
17	Mn–Si–Al–Ce–B–V	165	–	63.5	–	–	14.5	–

Table 3 (cont.)

18	Mn–Si–Al–Ce–Zr–B–V	167	–	–	–	4.0	–	–
19	Mn–Si–Ce–Al–Zr–B–Cr	177	–	–	–	4.0	–	–
20	Mn–Si–Ce–Al–Zr–V–P–Cr	203	–	49.5	–	17.0	–	6.0
21	Mn–Si–Ce–Al–Cr	205	–	9.5	–	7.0	–	6.0
22	Mn–Si–Ai–Ce–B	206	–	–	–	104.5	7.5	7.0
23	Mn–Si–Al–Ce–B–V	207	–	–	–	7.5	–	4.0
24	Mn–Si	410	266.0	237.5	133.0	103.0	12.5	–
25	Mn–Si	411	172.5	100.5	72.5	–	–	–
26	Mn–Si	412	308.0	232.0	–	185.0	10.5	–
27	Mn–Si	413	152.0	66.5	56.0	35.0	–	–
28	Mn–Si–Al–Ce–V	432	18.5	3.5	–	4.5	–	–
29	Mn–Si–Ce–Al–Zr–Cr	433	82.0	4.5	–	4.5	–	–
30	Mn–Si–Ce–Al–V–Cr	434	28.5	6.0	–	5.0	–	–
31	Mn–Si–Ce–Al–Zr–B–Cr	435	36.0	5.5	–	3.5	–	–
32	Mn–Si–Ce–Al–Zr–V–P–Cr	436	53.5	13.0	–	15.0	–	–
33	Mn–Si–Ce–Al–Zr–V–B–Cr	437	28.0	5.0	–	5.0	–	–
34	Mn–Si–Ce–Al–Zr–V–Cr	438	2.0	3.5	–	3.0	–	–
35	Mn–Si–Al–Ce–V	458	5.0	5.0	–	3.0	–	–
36	Mn–Si–Al–Ce–Zr–V	459	26.5	4.5	–	7.0	–	–
37	Mn–Si–Ce–Al–Zr–V–Cr	460	11.0	3.0	–	4.0	–	–
38	Mn–Si–Ce–Al–Zr–Cr	505	3.0	3.0	–	3.5	–	–
39	Mn–Si–Ce–Al–Zr–V–Cr	506	13.0	4.5	–	9.5	–	–
40	Mn–Si–Ce–Al–Zr–V–B–Cr	507	–	46.0	–	20.5	–	–
41	Mn–Si–Ce–Al–Mo	530	–	–	–	216.5	171.0	103.5
42	Mn–Si–Ce–Al	531	–	–	149.0	170.0	46.0	9.5
43	Mn–Si	597	150.5	106.5	59.5	17.5	–	–
44	Mn–Si	598	157.5	72.5	67.0	25.0	–	–
45	Mn–Si–Ce–Al–Cr	718	–	–	–	108.5	73.5	60.0
46	Mn–Si–Ce–Al–Cr	727	–	–	–	–	11.5	16.5
47	Mn–Si–Ce–B	728	–	203.5	194.0	–	–	187.0
48	Mn–Si–Ce–Al–Cr	881	–	–	–	95.0	207.5	9.5
49	Mn–Si–Ce–B	882	–	–	–	156.0	–	143.5
50	Mn–Si–Ce–Al	883	–	–	201.5	105.0	6.0	–
51	Mn–Si–Ce–B	894	–	–	–	208.0	22.0	8.5
52	Mn–Si–Ce–Al	895	–	–	–	108.5	-	165.5
53	Mn–Si–Ce–B	896	–	–	–	103.5	52.0	76.5
54	Mn–Si–Ce	127-2	–	103.5	–	96.5	74.5	75.0

$$\Delta = \begin{vmatrix} n & \sum x_1 \ldots & \sum x_p \\ \sum x_1 & \sum x_1^2 \ldots & \sum x_1 x_p \\ \ldots & \ldots \ldots & \ldots \\ \sum x_p & \sum x_1 x_p \ldots & \sum x_p x_p \end{vmatrix}.$$

The data of observations and coefficients of multiple regression equation can be presented in the form of the following matrices:

$$Y = \begin{pmatrix} y_1 \\ y_2 \\ \ldots \\ y_n \end{pmatrix}, X = \begin{pmatrix} 1 & x_{11} & x_{12} & \ldots & x_{1m} \\ 1 & x_{21} & x_{22} & \ldots & x_{2m} \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ 1 & x_{n1} & x_{n2} & \ldots & x_{nm} \end{pmatrix},$$

$$b = \begin{pmatrix} b_0 \\ b_1 \\ \ldots \\ b_m \end{pmatrix}, \quad e = \begin{pmatrix} e_1 \\ e_2 \\ \ldots \\ e_n \end{pmatrix}.$$

The formula of the coefficients of multiple linear regression in the matrix form is as follows:

$$b = (X^T X)^{-1} X^T Y,$$

where X^T is the matrix which is transposed to matrix X; $(X^T X)^{-1}$ is the matrix inverted to matrix $X^T X$.

Solving this equation, we obtain column-matrix b, the elements of which are exactly the coefficients of the equation of multiple linear regression.

An important index of the constructed model quality is the coefficient of determination or approximation confidence value which determines the level of prediction accuracy. This index is a statistical measure, consistency which allows establishing the extent to which the regression equation corresponds to the real data.

The coefficient of determination R^2 is the square of the correlation coefficient (Pearson coefficient) [5, 6]:

$$R = \frac{\sum \left(x_i - \overline{x}\right)\left(y_i - \overline{y}\right)}{\sqrt{\sum \left(x_i - \overline{x}\right)^2 \sum \left(y_i - \overline{y}\right)^2}},$$

where x_i is the value of variable X; y_1 is the value of variable Y; $\overline{x}$ is the arithmetic mean for variable X; $\overline{y}$ is the arithmetic mean for variable Y.

The coefficient of determination varies in the range from 0 to 1. If it is equal to zero, it means that the connection between the regression model variables is absent, and simple mean value may just as well used instead of it for evaluation of the initial variable value. Contrarily, if the coefficient of determination is equal to 1, it corresponds to an ideal model, when all the points of observation are located exactly on the regression line, i.e. the sum of squares of their deviation is equal to 0.

In practice, if the coefficient of determination is close to a unity, it shows that the model works well (has a high significance), and if it is close to zero, it means that the input variable poorly determines the behaviour of the output variable, i.e., there is no linear dependence between them. Evidently, such a model will have a low efficiency.

Depending on the level of the coefficient of determination, the models are usually divided into three groups:

- at $0.8 < R^2 < 1$ we obtain a model of good quality;
- at $0.5 < R^2 < 0.8$ — the model will be of acceptable quality;

at $0 > R^2 < 0.5$ – its quality will be poor.

Also at construction of a regression model, it is possible to assess the influence (contribution) of each predictor variable on the values of a dependent variable, and in some cases to essentially reduce the number of independent variables.

An important parameter at testing the statistic hypothesis is p-value [7–9]. The p-value is usually equal to the probability of a random quantity with this distribution taking a value, which is not smaller than the actual value of test statistics, and which is expressed by a number from 0 to 1. It should be determined whether the obtained experimental result is random. A result with p-value equal to the level of significance or below it, is considered significant. This is usually denoted as follows: $p \leq 0.05$.

In the case of a regression model, such a method as stepwise regression is quite well-established. Stepwise regression is a method to construct a model by adding or removing predictor variables. There are several approaches to performance of stepwise regression: forward step regression and backward step regression. At forward step regression the equations first contain no predictors. Then they are added one by one. In backward step regression first all the predictors are included into the regression equation, and then they are removed from the equation in turn.

Construction of mathematical models «composition-properties» for experimental samples of base material of steels and overheated zone at ESW. We will show construction of mathematical models of the dependence of mechanical properties on the composition of base material of the studied steels, as well as for the overheated zone at ESW of the studied steels after high-temperature tempering in the case of a model of *KCU* impact toughness at the temperature of –40 °C.

We will perform the following actions: First, we remove from experimental data for 55 experimental melts those, for which KCU_{-40} values are absent: 598, 153, 597, 412, 413.

When a matrix for 49 experimental steels was used (Table 4), a regression model of a poor quality was obtained, as the values of the coefficient of determination were below 0.5, namely $R^2 = 0.44$.

Having analyzed the diagram of comparison of the experimental and predicted data, we remove another 12 melts (Nos 458, 438, 165, 411, 37, 206, 33, 156, 410, 432, 881, 25), as the predicted (calculated) KCU_{-40} values for these experimental melts differ markedly from the general trend. We will obtain a matrix from 37 variants of steels (Table 5, Figure 1). And the regression model of a good quality was constructed exactly on this matrix ($R^2 = 0.84$):

$$KCU_{-40} = 556.89 - 2726.72\ C + 2788.66\ B - 375.29\ Al + 134.424\ Ce - 45.61\ Cr - 28.27\ Mn - 219.65\ Ni + 45.25\ P - 1790.66\ S - 97.17\ Si - 616.70\ V - 345.55\ Zr.$$

For a reduced model with a smaller number of independent variables (chemical elements) we will remove those elements which do not have any significant influence on impact toughness value at the tem-

Table 4. Correspondence of experimental melt number to melt number in the matrix

Melt number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Experimental melt number	458	437	438	177	436	506	163	164	165	411	460	167	434	205	505

Melt number	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
Experimental melt number	459	37	26	507	433	156	20	206	727	207	100	435	33	127-2	82

Melt number	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45
Experimental melt number	718	38	99	133	728	203	152	882	157	410	895	531	432	896	883

Melt number	46	47	48	49
Experimental melt number	881	894	530	25

Table 5. Correspondence of experimental melt number to melt number

Melt number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Experimental melt number	437	177	436	506	163	164	460	167	434	205	505	459	26	507	433

Melt number	16	17	18	19	20	21	22	23	24	25	25	27	28	29	30
Experimental melt number	156	20	727	207	100	435	127-2	82	718	38	99	133	728	203	882

Melt number	31	32	33	34	35	36	37
Experimental melt number	157	895	531	896	883	894	530

Table 6. Correspondence of experimental melt number to melt number

Melt number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Experimental melt number	177	436	506	164	460	434	505	459	507	433	156	20	207	100	127

Melt number	16	17	18	19	20	21	22	23	24	25	25	27	28
Experimental melt number	82	718	38	99	133	728	203	882	157	895	531	896	530

perature of –40 °C. At forward direction of stepwise regression a good model was obtained ($R^2 = 0.81$):

KCU_{-40} = 549.75 – 302.65 Al – 3101.87 Cr – – 44.03 Cr – 193.84 Ni – 2639.73 S – 117.84 Si – – 569,92 V.

In this model the following independent variables are removed: Mn, P, Ce, B, Zr. Figure 1 shows the results.

Once can see from Figure 1 that some calculated KCU_{-40} values for steels Nos 437, 163, 167, 205, 26, 727, 435, 883, 894 by the constructed model differ essentially from the specified line, so we remove them from the matrix of experimental values (correspondence of experimental melts and melt numbers from Figure 1, are given in Table 6).

We obtain a matrix from 28 observations (experimental steels), and construct a regression model with coefficient of determination $R^2 = 0.91$:

KCU_{-40} = 568.53 – 2732.83 C – 28.39 Mn – – 119.04 Si – 1638.39 S + 38.66 P – 47.68 Cr – – 205.94 Ni – 619.31 V – 382.65 Al + 75.81 Ce + + 2442.99 B – 439.62 Zr.

We can also reduce the number of chemical elements (we remove P, Ce, B, Zr) which are used in the model, considering that p-value ≤ 0.05 for these elements. As a result, we obtain the following regression model:

KCU_{-40} = 584.09 – 326.71 Al – 2647.62 Cr – – 53.90 Cr – 32.83 Mn – 192.39 Ni – 2099.09 Si – – 132.66 Si – 542.62 V and coefficient of determination $R^2 = 0.91$.

Calculation shows that in this case there are several KCU_{-40} values which differ markedly from the general line. We remove them: melts Nos 177, 506, 436, 164, 460.

We derive the following model:

KCU_{-40} = 573.52 – 362.89 Al – 2020.46 Cr – – 64.01 Cr – 56.39 Mn – 276.03 Ni – 117.59 Si – 108.44 Si – 662.79 V.

The coefficient of determination is $R^2 = 0.90$ that points to a good quality of the model.

Comparison of experimental and calculated KCU_{-40} values is given in Figure 2.

Thus, processing the entire amount of experimental data for 55 experimental melts of steels designed for ESW (Table 1) resulted in construction of a mathematical models «Chemical composition – Mechanical properties» (impact toughness, yield limit, ultimate strength, relative elongation and reduction in area) based on application of the method of multiple (multifactorial) regression.

All the plotted models are characterized by a high value of the coefficient of determination ($R^2 > 0.8$) that defines a sufficient level of prediction accuracy.

The method of stepwise regression was used to create a reduced mathematical model, and p-value was applied to reduce the number of independent variables.

In the derived regression models such elements as Mn, Cr, Zr have the greatest impact on the mechanical properties of base material (steel), designed for ESW. Si, P, Al, V, Ce have less influence on the mechanical

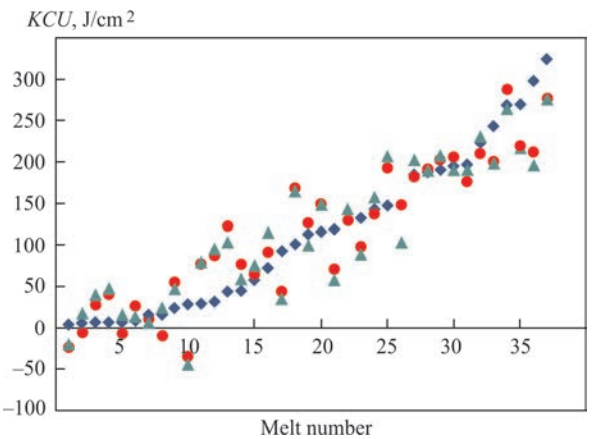

Figure 1. Comparison of experimental (♦) and calculated KCU_{-40} values for 37 experimental melts ($R^2 = 0.84$), taking into account all the independent parameters (●) and for a reduced number of independent parameters (▲) ($R^2 = 0.81$)

Table 7. Chemical composition of steels for testing

Steel	C	Mn	Si	S	P	Cr	Ni	V	Al	Ce	B	Zr	Mo	Cu
09KhG2SYuCh	0.09	2.00	0.45	0.01	0.015	1	0	0	0.05	0.004	0	0	–	–
10Kh2GNM	0.10	1.10	0.33	0.022	0.023	2.15	0.52	0	0.052	0	0	0	–	–
10Kh2GNMA-A	0.10	0.96	0.27	0.007	0.006	2.09	0.2	0	0.005	0	0	0	–	–
12KhM	0.12	0.55	0.30	0.018	0.016	0.5	0.25	0	0.055	0	0	0	0.5	0.2
10KhG2MCh	0.10	2.10	0.30	0.018	0.016	1.2	0.15	0	0.055	0.018	0	0	–	–
10Kh2GM	0.10	0.93	0.30	0.018	0.016	2.3	0.66	0	0.055	0	0	0	–	–

properties. Ni, S and B have practically no impact in the plotted models.

For the overheated zone at ESW, such chemical elements (by increase of the degree of impact) as P, C, Mn, S, Cr, Ni, V, B have the greatest influence on the metal mechanical properties, while the impact of Si, Ce and Zr elements is small, judging from the regression models.

Testing the constructed mathematical models. Developed models (regression equations) for determination of mechanical properties of steels designed for ESW, were tested on 6 steel grades (Table 7), for which the respective experimental data are available [7–9].

For the overheated zone (of the HAZ, after tempering, without normalizing) a comparison was performed with experimental data of the calculation results by the complete and reduced models for KCV_{+20}, KCV_{-60}, KCU_{-60}, KCU_{-70}.

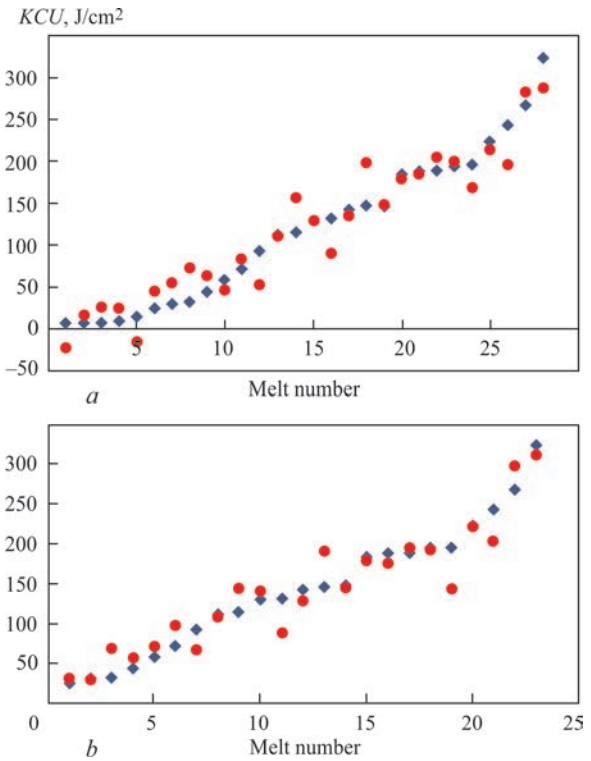

Figure 2. Comparison of experimental (♦) and calculated (●) KCU_{-40} values: *a* — for 28 experimental steels and full number of independent parameters (R^2 = 0.91); *b* — for 23 experimental steels and reduced number of independent parameters (R^2 = 0.90)

The constructed models for prediction of KCV_{-60}, KCU_{-60}, KCU_{-70} yield quite adequate values, compared to experimental data. The models for KCV_{+20} give considerably underestimated values (Table 8).

For the base metal (after normalizing or hardening and tempering), a comparison of experimental data and results of calculation by the complete and reduced models was performed for KCU_{-40}, KCU_{-60}, yield limit σ_y, ultimate strength σ_t, relative elongation δ and reduction in area ψ.

The models for prediction of KCU_{-40} yield adequate values, models for KCU_{-60} in some cases give underestimated, but rather close values, compared to experimental data (Table 9). The models for yield limit σ_y, ultimate strength σ_t, and reduction in area ψ yield adequate values, and models for relative elongation δ give somewhat overestimated values.

In order to improve (increase the accuracy) of the models, the procedure of construction of the regression models was repeated, based on an expanded scope of experimental data from 55 experimental melts of low-alloy steels up to 61 steel by complimenting the experimental data [7–9]. It allowed to noticeably improve the calculated and experimental data (Tables 10–12), for impact toughness *KCV* (at –70 °C) in the overheated zone, for impact tough-

Table 8. Overheated zone (HAZ, after tempering, without normalizing)

Steel	KCV_{+20}[1], J/cm^2		KCV_{-60}[2], J/cm^2	
	Model	Exp.	Model	Exp.
09KhG2SYuCh	111	–	79	–
10Kh2GNM	61	142–161	36	12–21
10Kh2GNMA-A	79	181–209	82	16–102
12KhM	197	–	1	–
10KhG2MCh	73	–	87	102–137
10Kh2GM	54	–	10	44–60
09KhG2SYuCh	95	87–163	20	13–25
10Kh2GNM	141	100–120	106	–
10Kh2GNMA-A	94	86–90	27	–
12KhM	111	–	171	–
10KhG2MCh	118	–	–53	–
10Kh2GM	137	–	109	–

Notes. [1]Models give underestimated values and require optimizing. [2]Models yield adequate values.

Table 9. Base metal (after normalizing or hardening and tempering)

Steel	KCU_{-40}[1], J/cm²			KCU_{-60}[2], J/cm²		
	Model	Red. model	Exp.	Model	Red. model	Exp.
09KhG2SYuCh	120.31	133.71	–	117.05	115.88	84–188
10Kh2GNM	139.17	124.78	94–192	131.98	87.64	100–107
10Kh2GNMA-A	97.30	155.57	155–163	94.73	89.11	117–142
12KhM	341.69	356.50	–	93.09	128.16	–
10KhG2MCh	104.88	113.12	–	120.27	110.97	–
10Kh2GM	155.01	130.20	–	144.46	83.95	–
	σ_y[2], MPa			σ_t[3], MPa		
Steel	Model	Red. model	Exp.	Model	Red. model	Exp.
09KhG2SYuCh	341.01	347.55	360–395	490.04	492.99	560–600
10Kh2GNM	469.92	458.26	460–503	585.36	570.97	565–610
10Kh2GNMA-A	433.56	433.90	460–503	576.89	581.01	565–610
12KhM	318.00	323.13	318	491.00	491.00	491
10KhG2MCh	459.32	455.76	467–550	591.47	588.24	662–689
10Kh2GM	470.30	448.05	437–487	588.90	569.29	578–604
Steel	δ[4]. %			ψ[3]. %		
	Model	Red. model	Exp.	Model	Red. model	Exp.
09KhG2SYuCh	30.13	30.79	22–28	71.255	70.64	49–80
10Kh2GNM	24.46	23.68	15–20	64.080	66.62	55–67
10Kh2GNMA-A	23.60	23.85	15–20	64.494	65.57	55–67
12KhM	23.00	26.73	23	67.599	69.82	–
10KhG2MCh	25.04	26.44	20–26	68.368	68.49	–
10Kh2GM	25.38	23.24	21–26.6	64.067	66.41	–

Note. [1]Models give individual underestimated values and require optimizing. [2]Models give close values. [3]Models yield adequate values. [4]Models yield close but somewhat overestimated values and require optimizing.

ness *KCU* (at –40 °C) of the base metal and for relative elongation δ (base metal).

Thus, the most rational way to improve the constructed models consists in expanding the experimental data base.

We give the final form of the mathematical models, taking into account their optimization.

Impact toughness (KCV and *KCU*) *for the overheated zone* (*of the HAZ after tempering without normalizing):*

$$KCV_{+20} = 181.00 - 819.95\,C + 4.88\,Mn + 83.96\,Si + 173.93\,P - 605.91\,S - 20.15\,Cr - 199.17\,V - 364.01\,Al - 520.19\,Ce + 3931.41\,B - 430.55\,Zr + 248.89\,Mo;$$

$$KCV_{-60} = 2.52 + 132.21\,C + 14.62\,Mn - 70.94\,Si + 953.25\,S + 81.4186\,P + 50.21\,Cr - 205.99\,Ni - 541.64\,V + 74.96\,Al + 544.33\,Ce + 11371.4\,B + 4090.56\,Zr;$$

$$KCU_{-60} = 23.47 + 364.76\,C + 17.48\,Mn - 11.36\,Si + 912.35\,S + 1047.04\,P - 2.91\,Cr +$$

Table 10. Comparison of model results for KCV_{-70} for overheated zone (HAZ, after tempering, without normalizing)

Steel	First variant[1]		Improved variant[2]	
	Model	Exp.	Model	Exp.
09KhG2SYuCh	520	13–25	20	13–25
10Kh2GNM	829	–	106	–
10Kh2GNMA-A	1167	–	27	–
12KhM	350	–	171	–
10KhG2MCh	521	–	–53	–
10Kh2GM	802	–	109	–

Notes. [1]Models yield underestimated values and require optimizing. [2]Models yield adequate values.

Table 11. Comparison of model results for KCU_{-40} for base metal (after normalizing or hardening and tempering)

Steel	First variant[1]			Improved variant[2]		
	Model	Red. model	Exp.	Model	Red. Model	Exp.
09KhG2SYuCh	130	147	–	120.31	133.71	–
10Kh2GNM	0	–29	94–192	139.17	124.78	94–192
10Kh2GNMA-A	82	96	155–163	97.30	155.57	155–163
12KhM	64	144	–	341.69	356.50	–
10KhG2MCh	63	80	–	104.88	113.12	–
10Kh2GM	0	–65	–	155.01	130.20	–

Notes. [1]Models yield underestimated values and require optimizing. [2]Models yield adequate values, but require optimizing in some cases.

Table 12. Comparison of model results for relative elongation δ for base metal (after normalizing or hardening and tempering)

Steel	First variant[1]			Improved variant[2]		
	Model	Red. model	Exp.	Model	Red. Model	Exp.
09KhG2SYuCh	28	33	22–28	30.13	30.79	22–28
10Kh2GNM	28	31	15–20	24.46	23.68	15–20
10Kh2GNMA-A	29	31	15–20	23.60	23.85	15–20
12KhM	34	34	23	23.00	26.73	23
10KhG2MCh	26	33	20–26	25.04	26.44	20–26
10Kh2GM	29	30	21–26.6	25.38	23.24	21–26.6
Notes. [1]Models yield underestimated values and require optimizing. [2]Models yield adequate values.						

+ 77.23 Ni – 131.98 V – 244.51 Al – 147.71 Ce + + 254.12 B – 610.58 Zr;

KCU_{-70} = 258.07 – 665.22 C – 89.57 Mn + + 226.31 Si – 6870.75 S + 8430.52 P – 95.4137 Cr + + 319.41 Ni – 1259.5 Al + 18087.1 B.

Base metal after normalizing or hardening and tempering:

1. Yield limit:

σ_y = 127.77 + 982.92 C + 74.1854 Mn – – 50.5011 Si + 1075.06 S + 202.153 P + 62.2906 Cr + 62.5862 Ni + 28.1904 V – 304.692 Al + 147.574 Ce + + 8400.33 B + 933.64 Zr – 76.7431 Mo + 161.927 Cu.

2. Ultimate strength:

σ_t = 376.487 + 197.733 B36 + 74.597 C36 – – 80.1669 Si – 51.6227 S + 170.066 P + 58.1997 Cr + + 52.2038 Ni – 62.8523 V – 414.44 Al + 330.174 Ce + + 5461.85 B + 991.499 Zr – 130.434 Mo + 589.374 Cu.

3. Relative elongation:

δ = 38.5232 – 46.8034 B36 –2.12612 C36 – – 0.0489085 Si – 75.0961 S – 4.93551 P – 4.2477 Cr + + 5.78539 Ni + 7.0119 V + 16.5739 Al + 23.3941 Ce – – 278.698 B – 64.3938 Zr – 26.2339 Mo + 27.954 Cu.

4. Reduction in area:

ψ = 77.5019 – 87.8572 B36 + 2.24134 C36 – – 7.31298 Si – 86.2487 S – 11.5188 P – 1.78764 Cr – – 0.778479 Ni + 39.5843 V + 33.1262 Al – – 38.0401 Ce + 110.365 B – 129.132 Zr + 5.208 Mo.

Conclusions

1. Proceeding from earlier results of experimental studies we constructed mathematical models of the dependence of mechanical properties of silicon-manganese steels, designed for electroslag welding and characterized by high brittle fracture resistance in the HAZ, as well as of the overheated zones, on the chemical composition of these steels.

2. The mathematical models were constructed with application of the method of multiple linear regression. Mathematical models were constructed for a set of mechanical properties of base metal: impact toughness for temperatures of (+20, –40, –60, –70 °C), yield limit, ultimate strength, relative elongation and reduction in area. For the overheated zone at electroslag welding mathematical models were constructed for impact toughness (*KCU* and *KCV*) for temperatures of +20, –60, –70 °C.

3. Initial validation of the constructed models was performed. Its results showed that the constructed models for the overheated zone (of the HAZ, after tempering, without normalizing) and for the base metal (after normalizing or hardening and tempering), mostly give quite adequate values, compared to experimental data, but, in some cases, they essentially underestimate or overestimate the mechanical property values. It is shown that the most rational way to improve the constructed models consists in expanding the experimental data base.

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Received 10.12.2020