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Optimization of Vibration Treatment and Modification Parameters for 40CrNi3MoV Steel Based on Mathematical Modeling

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Abstract. The targeted control of the structure and properties of high-strength alloy steels remains one of the key challenges in modern metallurgy. This study investigates the effect of solidification temperature, vibration treatment time, and the content of the complex modifier INSTEEL-7 on the hardness of 40CrNi3MoV steel. To substantiate the temperature parameters of the process, the modeling of phase transformations was performed using the Thermo-Calc software package. Experimental studies were carried out based on a multifactorial experimental design according to V.P. Malyshev's method, involving 25 experimental melts. Based on the experimental results, partial quadratic dependencies were obtained, and a generalized mathematical model was developed to describe the influence of technological factors on Vickers hardness (HV5). It was established that the steel hardness varies within the range of 356-492 HV depending on the combination of process parameters. The rational range of technological regimes was determined: a solidification temperature of 1520-1540 °C, a vibration treatment time of approximately 30 s, and an INSTEEL-7 modifier content of about 0.03 wt.%. The calculated hardness value (~487 HV) demonstrates good agreement with the experimental data, which confirms the adequacy of the developed model. The proposed approach enables the prediction of steel hardness without conducting additional full-scale experiments and can be used to optimize the technological casting parameters of high-strength alloy steels.

Keywords: 40CrNi3MoV steel; thermodynamic modeling; mathematical design of experiments; vibration treatment; modification; hardness prediction

Introduction

Increasing the operational reliability and durability of heavily loaded machine parts is one of the key tasks in modern mechanical engineering. Various approaches are used to solve this problem, including the application of protective coatings [1] and the optimization of modes for restoring worn surfaces by hardfacing [2]. However, the most fundamental way to ensure high mechanical properties of products is the directional formation of an optimal macro- and microstructure of the metal at the stage of its solidification.

High-strength alloy steels, including 40CrNi3MoV, are widely used for manufacturing critical components of heavy-duty equipment [3,4]. Their operational reliability is determined by the microstructure formed during solidification, where the phase composition, the degree of structural heterogeneity, and the characteristics of non-metallic inclusions play a key role in determining hardness, wear resistance, and fracture resistance.

An effective method for controlling the structure is a complex physicochemical treatment of the melt. The application of low-frequency vibration during the solidification process leads to the destruction of the dendritic structure, the intensification of convective flows, and the formation of a fine-grained structure, which is accompanied by a decrease in macrosegregation and an improvement in mechanical properties [5,6]. An additional effect is provided by melt modification: calcium- and barium-containing additives (INSTEEL) promote the formation of dispersed globular oxysulfide inclusions, reducing the stress concentration in the metal matrix [7,8]. It has been established that such modifiers ensure the refining of the melt and the stabilization of inclusions in alloy steels [9-11].

The most promising approach is the combined application of physical and chemical treatments, which provides a synergistic effect manifested in the refinement of the microstructure and the enhancement of mechanical properties [12,13]. Furthermore, structure formation is determined by the combined influence of technological factors, including temperature, treatment duration, and modifier content.

Optimizing these processes solely through empirical methods requires a substantial number of experiments and fails to fully account for the mutual influence of factors [14]. Therefore, the role of mathematical modeling becomes increasingly important. Thermodynamic calculations in software packages such as Thermo-Calc, which are based on Gibbs free energy minimization, enable the prediction of phase equilibria and the parameters of phase transformations [15,16]. The application of the CALPHAD approach allows for the determination of liquidus and solidus temperatures, as well as the phase composition of the alloy at the design stage, thereby justifying the variation range of the temperature factor during experimental design [17].

To quantitatively assess the impact of technological parameters, methods of mathematical design of experiments are applied. The probabilistic-deterministic method based on V.P. Malyshev's methodology significantly reduces the required volume of research while preserving modeling accuracy. This approach relies on constructing regression dependencies and utilizing M.M. Protodyakonov's generalized function to combine the partial dependencies of factors [18,19], and it has proven highly effective in optimizing metallurgical processes [20,21].

Despite the availability of studies on thermodynamic modeling, vibration treatment, and the use of modifiers, the comprehensive optimization of processing parameters for 40CrNi3MoV steel using a combined approach of thermodynamic calculations and mathematical design of experiments remains insufficiently explored.

The aim of this study is to establish the rational processing parameters for 40CrNi3MoV steel under vibration treatment and INSTEEL-7 modification, based on the combined application of thermodynamic modeling (Thermo-Calc) and Malyshev's method of mathematical design of experiments.

2. Research methods

The object of this study is the high-strength alloy steel 40CrNi3MoV, which belongs to the class of medium-carbon complex-alloy steels containing Cr, Ni, Mo, and V. This combination of elements provides high strength, hardenability, and wear resistance, determining the application of this steel in the manufacturing of critical components for mining, metallurgical, and power equipment [3,4].The operational properties of the steel are dictated by the conditions of structure formation during solidification; therefore, the effectiveness of the technological treatments was evaluated based on the changes in the mechanical characteristics of the cast metal. Vickers hardness (HV5), which is a sensitive indicator of structural and phase transformations, was selected as the primary response. The hardness measurements (Y_{exp}) were performed in accordance with standard procedures [22].To substantiate the temperature parameters of the experiment, solidification modeling was conducted using the Thermo-Calc software package (version 2025b, TCFE13 database), which is based on the CALPHAD method and the principle of Gibbs free energy minimization [15]. The analysis of the phase composition enabled the determination of the liquidus and solidus temperatures, as well as the solidification range of the steel [17]. Based on the obtained data, a temperature variation range of 1480-1560 °C was established and implemented in the experimental design matrix.

Experimental studies were conducted under laboratory conditions using a complex physicochemical treatment on the solidifying melt, which included low-frequency vibration and modification. The complex modifier INSTEEL-7, containing Ca, Ba, rare earth elements, and Ti, was used as a modifying additive, ensuring melt refining and control over the morphology of non-metallic inclusions [7,8].During the experiment, three technological parameters were varied: solidification temperature (X_1), vibration treatment time (X_2), and INSTEEL-7 modifier content (X_3). The experiment was implemented according to a five-level matrix (25 trials), which enabled the determination of the factors' influence on the response-Vickers hardness (Y_{exp}).To quantitatively evaluate the influence of these factors, the probabilistic-deterministic method of mathematical design of experiments according to V.P. Malyshev's methodology was applied. This method allows for a significant reduction in the volume of research while maintaining the reliability of the results [18-20]. To ensure the orthogonality of the design, dummy factors (X_4, X_5) were introduced into the model. The levels of factor variation are presented in Table 1.

Based on the experimental data, partial dependencies of the response on the varied factors were established, and a generalized mathematical model was developed, enabling the prediction of the hardness of 40CrNi3MoV steel under various combinations of technological parameters.

Table 1. Levels of variation for the technological factors.

Factors		Factor levels				
		1	2	3	4	5
X_1	Solidification temperature, °C	1480	1500	1520	1540	1560
X_2	Vibration treatment time, s	0	15	30	45	60
X_3	INSTEEL-7 modifier content, wt.%	0	0,05	0,03	0,02	0,01
X_4	Dummy factor	1	2	3	4	5
X_5	Dummy factor	1	2	3	4	5

Substantiation of the Process Temperature Parameters Based on Modeling

In this study, thermodynamic modeling was utilized to substantiate the temperature parameters of the experiment and was not considered as an independent object of research.

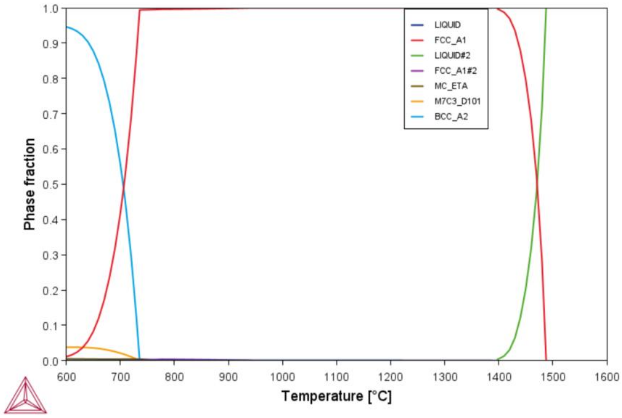

Fig.1 - Calculation of the phase composition of 40CrNi3MoV steel (Thermo-Calc, TCFE13).

The phase composition calculations were performed using the CALPHAD method [15,16], which enabled the determination of the phase transformation temperatures and the solidification behavior of 40CrNi3MoV steel. Figure 1 presents the dependence of the phase composition on temperature. It was established that the liquidus temperature is ~1500 °C, and the completion of solidification (solidus) occurs in the range of ~1420-1440 °C. In the range between the specified temperatures, the system is in the two-phase Liquid + FCC_A1 region, corresponding to the formation of an austenitic dendritic structure.

The technological treatment in this study was applied within the liquid–solid state interval (Liquid + FCC_A1), as vibration treatment is most effective during the nucleation and growth stages of dendrites while maintaining melt mobility. In the fully solidified state, the effect of vibration on structure formation is insignificant; therefore, the temperature range below the solidus was not considered.

Based on the modeling results, a temperature range of 1480-1560 °C was established for use in the experiment. The upper limit corresponds to the superheated liquid state, ensuring high melt fluidity and the active interaction of modifying elements. As the temperature decreases to 1540-1500 °C, the system transitions to the onset of solidification region, where primary austenitic dendrites are formed and the maximum effect of vibration treatment is realized due to the intensification of mass transfer [5,12].

Thus, the selected temperature interval covers the region of solidification nucleation and development, excluding the completely solidified state. The established limits of 1480-1560 °C were adopted as the variation range for the temperature parameter X_1 in the mathematical design of the experiment.

3. Results and discussion

The experimental study of the influence of technological factors on the hardness of 40CrNi3MoV steel was performed based on a multifactorial design of experiments according to V.P. Malyshev's methodology. The varied factors were the melt solidification temperature (X_1), vibration treatment time (X_2), and INSTEEL-7 modifier content (X_3).Each factor was varied at five levels, which enabled the formulation of the experimental design and the execution of 25 experimental melts corresponding to different parameter combinations. Vickers hardness (HV5) was considered as the response. The experimental results are presented in Table 2.

Table 2. Multifactorial experimental matrix and experimental hardness values of 40CrNi3MoV steel.

Trial No.	Temperature, °C	Vibration time, s	INSTEEL-7, wt.%	X4	X5	Experimental result (Y_{exp}), Hardness HV5
1	1480	0	0	1	1	356
2	1480	30	0.03	3	3	402
3	1480	15	0.05	2	2	372
4	1480	60	0.01	5	5	360
5	1480	45	0.02	4	4	386
6	1500	0	0.03	2	5	489
7	1500	30	0.05	5	4	492
8	1500	15	0.01	4	1	488
9	1500	60	0.02	1	3	472
10	1500	45	0	3	2	468
11	1520	0	0.05	4	3	422

Continuation of Table 2

Trial No.	Temperature, °C	Vibration time, s	INSTEEL-7, wt.%	X4	X5	Experimental result (Y_{exp}), Hardness HV5
12	1520	30	0.01	1	2	430
13	1520	15	0.02	3	5	445
14	1520	60	0	2	4	410
15	1520	45	0.03	5	1	440
16	1540	0	0.01	3	4	386
17	1540	30	0.02	2	1	455
18	1540	15	0	5	3	402
19	1540	60	0.03	4	2	462
20	1540	45	0.05	1	5	458
21	1560	0	0.02	5	2	465
22	1560	30	0	4	5	457
23	1560	15	0.03	1	4	474
24	1560	60	0.05	3	1	443
25	1560	45	0.01	2	3	464

An analysis of the obtained data shows that the hardness values vary over a wide range depending on the combination of technological factors. The minimum values correspond to lower solidification temperatures and the absence of an effective modifying treatment, whereas the maximum values are achieved with a rational combination of temperature, vibration time, and modifier content. The obtained hardness range confirms the significant influence of the investigated parameters on the structure formation and mechanical properties of 40CrNi3MoV steel.

To identify the partial regularities of the influence of each factor on hardness, the average response values for the variation levels were calculated. This approach enabled the transition from the matrix of individual experiments to generalized dependencies characterizing the influence of solidification temperature, vibration treatment time, and modifier content on the steel hardness. The average response values according to the factor levels are presented in Table 3.

Table 3. Average hardness values of 40CrNi3MoV steel according to the levels of the varied factors.

Temperature, °C		Vibration time, s		INSTEEL-7 modifier, wt.%	
X_1	$Y_{1\ avg}$	X_2	$Y_{2\ avg}$	X_3	$Y_{3\ avg}$
1480	375	0	404	0	419
1500	429	15	436	0.01	425
1520	481	30	447	0.02	444
1540	465	45	445	0.03	453
1560	460	60	429	0.05	447

The obtained average values were used to construct partial approximating dependencies. It was established that the solidification temperature has a decisive influence on the hardness formation, while vibration treatment and modification additionally intensify the processes of crystal nucleation and growth. Based on the experimental data, partial quadratic dependencies were constructed, describing the influence of each investigated factor on the steel hardness. For the temperature factor, the following dependence was obtained:

$$Y_1 = -0.0334X_1^2 + 102.54X_1 - 78240 \quad (1)$$

The coefficient of determination (R^2):

$$R^2 = 0.9563$$

The approximation is characterized by a high coefficient of determination ($R^2 = 0.9563$), which indicates good agreement between the model and the experimental data. The dependence exhibits an extremal character, pointing to the existence of an optimal solidification temperature range.

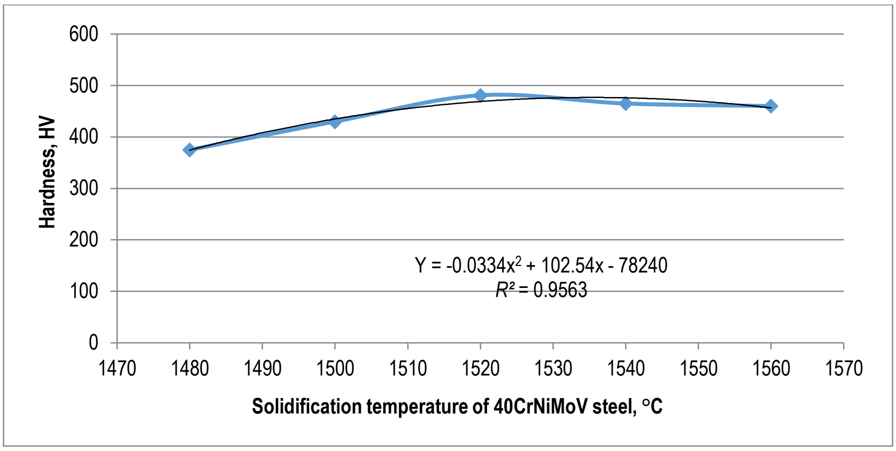

Fig.2 - Dependence of the hardness of 40CrNi3MoV steel on the solidification temperature.

For the vibration treatment time factor, the following dependence was obtained:

$$Y_2 = -0.0346X_2^2 + 2.4695X_2 + 404.83 \quad (2)$$

$$R^2 = 0.995$$

The value of the coefficient of determination ($R^2 = 0.995$) indicates a very high accuracy of the approximation. The presence of a pronounced maximum confirms the existence of a rational vibration treatment duration, at which the greatest structural impact on the melt is achieved.

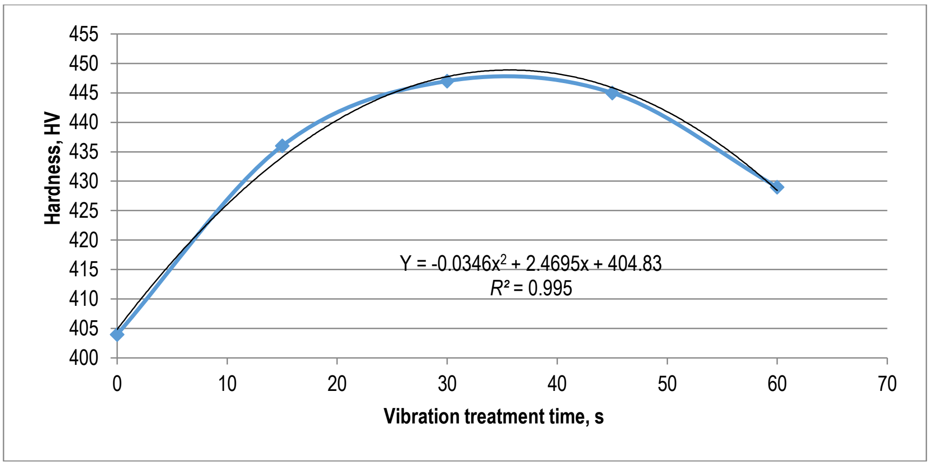

Fig.3 - Effect of vibration treatment time on the hardness of 40CrNi3MoV steel.

For the modifier content factor, the following dependence was obtained:

$$Y_3 = -23969X_3^2 + 1849X_3 + 415.62 \quad (3)$$

$$R^2 = 0.9186$$

The value of the coefficient of determination ($R^2 = 0.9186$) confirms the high adequacy of the model. The parabolic character of the dependence points to the existence of an optimal modifier content, beyond which the effectiveness of the treatment decreases.

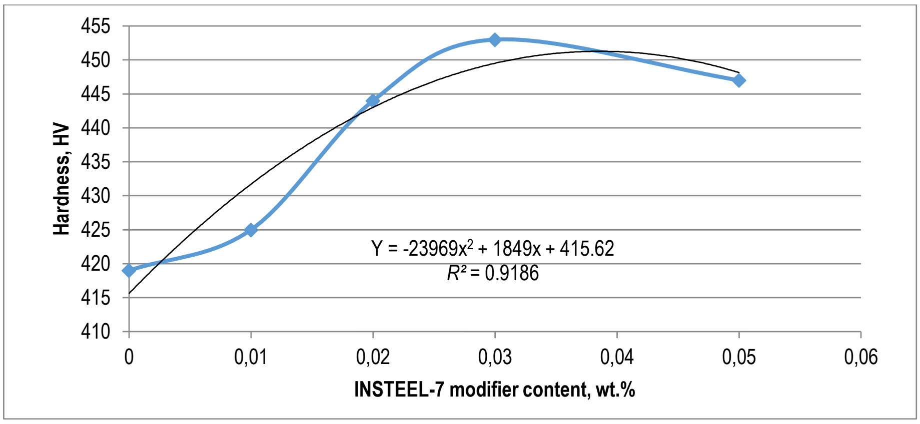

Fig.4 - Dependence of the hardness of 40CrNi3MoV steel on the INSTEEL-7 modifier content.

In general, the obtained dependencies exhibit an extremal character, which indicates the existence of rational values for all the investigated factors at which the maximum hardness of the metal is achieved. The high values of the coefficient of determination confirm the correctness of the approximation and allow the obtained functions to be used for further mathematical modeling.

The decrease in hardness after exceeding the optimal vibration treatment time may be associated with excessive mechanical action on the melt during the final stages of solidification. Prolonged vibration can disturb the stable formation of the solidifying structure and promote gas entrainment, which may lead to the formation of pores and reduce the structural homogeneity of the steel. Similarly, an excessive amount of INSTEEL-7 modifier may decrease the efficiency of modification due to possible coarsening or agglomeration of non-metallic inclusions, reducing their role as effective crystallization centres [23].

For an integral description of the influence of all factors on the steel hardness, the generalized Protodyakonov function was used, allowing the combination of partial dependencies into a single mathematical model:

$$Y = \frac{Y_1 Y_2 Y_3}{Y_{avg}^{m-1}} \tag{4}$$

where Y is the predicted hardness value;

Y_1, Y_2, Y_3 are the partial functions of the factors;

Y_{avg} is the average response value;

m is the number of factors.

In the case under consideration, m = 3 and Y_{avg} = 435.92. Substituting these values yields the final expression of the model, which is applicable for calculating the steel hardness under various combinations of technological parameters within the investigated range.

$$m=3$$

$$Y_{avg} = 435.92$$

Substituting these values, we obtain the final expression of the model:

$$Y = \frac{Y_1 Y_2 Y_3}{(435.92)^2}$$

$$(435.92)^2 = 190026.25$$

$$Y = (1/190026.25) \times (-0.0334X_1^2 + 102.54X_1 - 78240) \times (-0.0346X_2^2 + 2.4695X_2 + 404.83) \times (-23969X_3^2 + 1849X_3 + 415.62)$$

To determine the rational process parameters, an analytical search for the maximums of the partial functions was performed. Since the dependencies are quadratic functions with a negative coefficient for the squared variable, the maximum is determined by the coordinate of the parabola's vertex:

$$X_{opt} = -\frac{b}{2a} \quad (5)$$

The optimum solidification temperature, determined by the vertex coordinate, is:

$$X_{opt} = -\frac{102.54}{2(-0.0334)} \approx 1535 \text{ °C}$$

which practically corresponds to the experimental level of 1520-1540 °C.

For the optimum vibration treatment time, we obtain:

$$X_{opt} = -\frac{2.4695}{2(-0.0346)} \approx 35\ s$$

Consequently, the optimal vibration treatment duration is approximately 35 s, which practically coincides with the experimental level of 30 s.

For the optimum modifier content, the vertex coordinate is:

$$X_{opt} = -\frac{1849}{2(-23969)} \approx 0.03\ wt.\%$$

The calculation shows that the optimal solidification temperature is approximately 1535 °C, which corresponds to the experimentally established range of 1520-1540 °C. The optimal vibration treatment duration is around 35 s, which agrees with the level of 30 s adopted in the experiment. The optimal modifier content is approximately 0.03 wt.%.

Thus, the rational range of the technological process parameters can be defined as follows:

- solidification temperature: 1520-1540 °C;
- vibration treatment time: approximately 30 s;
- INSTEEL-7 modifier content: approximately 0.03 wt.%.

To verify the adequacy of the developed mathematical model, the rational factor values were substituted: a temperature of 1540 °C, a vibration time of 30 s, and a modifier content of 0.03 wt.%. The calculated hardness value was approximately 487 HV, which is in good agreement with the experimental data.

This confirms the correctness of the constructed model and the possibility of its use for predicting the properties of 40CrNi3MoV steel under varying technological parameters.

Conclusions

1. It was established that the complex physicochemical treatment, including vibration treatment of the melt and modification with the INSTEEL-7 additive, provides a significant change in the structure and hardness of 40CrNi3MoV steel. The hardness variation range was 356-492 HV, which confirms the high sensitivity of the material to the variation of technological parameters.

2. It was determined that the solidification temperature is the dominant factor in the formation of the steel's properties, while vibration treatment and modification perform an intensifying function, affecting the processes of crystal nucleation and growth.

3. Quadratic dependencies of hardness on solidification temperature, vibration treatment time, and modifier content were established. The high values of the coefficient of determination (R^2 = 0.9563-0.995) confirm the adequacy of the approximation and the reliability of the experimental data.

4. A generalized mathematical model based on the Protodyakonov function was developed, allowing the prediction of the steel hardness within the specified parameter range. The calculated value (~487 HV) is in agreement with the experimental data, which confirms the correctness of the model.

5. The rational range of technological regimes ensuring maximum hardness values was established: a temperature of 1520-1540 °C, a vibration treatment time of approximately 30 s, and an INSTEEL-7 modifier content of approximately 0.03 wt.%. The proposed approach allows for a reduction in the volume of experimental research and can be used in the optimization of high-strength steel casting processes.

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