Analysis of Various Aspects in Metals Creation with Given Microheterogeneity Degree

A. Anikeev(✉), I. Chumanov, and V. Sedukhin

South Ural State University, 76. Lenin Avenue, Chelyabinsk 454080, Russia
anikeevan@susu.ru

Abstract. Automation of technological processes is one of the priority areas of industrial development. Areas in particular in need of automation and computerization are directions with not yet standardized process of obtaining, in particular, the direction of creating materials with a gradient of properties. The article discusses various aspects of the metals creation with given microheterogeneity degree, obtained by introducing dispersed particles into the melt. When creating such materials, it is important to take into account many aspects: the conditions for the dispersed particles separation from supersaturated solution, the particles interaction level with metal, the feed rate to the melt, distribution control, the particles number in the melt volume, the microheterogeneity influence on the properties' level, and other aspects. The article analyzes modern approaches for solving each aspect, proposes the methodology for calculating the crystallization rate and particle distribution when fed into the metal during centrifugal casting. Based on the developed methodology, computer model was built allowing to predict the particles distribution depending on many factors.

Keywords: Dispersed particles · Cast alloys · Wetting · Injection rate · Microheterogeneity · Distribution density

1 Introduction

Given the finiteness of natural resources and the new challenges posed by the technology development, the materials creation with given properties level, while reducing cost is the most important task of our time. One of the solutions to this problem can be economically alloyed met-als with given microheterogeneity degree. Microheterogeneity can be obtained by introducing carbides, oxides, or nitrides dispersed particles (or isolating them from supersaturated solution) and their predetermined distribution in the volumes that are most affected. The low cost of the resulting material is due to the fact that the main material (matrix) volume can consist of carbon steel, inexpensive steel, and a high level of mechanical characteristics in surface volumes is achieved by creating microheterogeneity.

When creating materials with given microheterogeneity degree, scientists face various problems:

© The Author(s), under exclusive license to Springer Nature Switzerland AG 2023
A. A. Radionov and V. R. Gasiyarov (Eds.): RusAutoCon 2022, LNEE 986, pp. 147–156, 2023.
https://doi.org/10.1007/978-3-031-22311-2_15

1. the difference in the microparticles densities and the melt (uncontrolled uneven distribution);
2. microparticles interaction with metal (wetting level);
3. predicting the micro-particles distribution by the melt volume;
4. the microheterogeneity effect on properties level.

For controlled particles sedimentation in the melt by specific gravity, some researchers have proposed the method of introducing dispersed particles into the melt when casting on centrifugal casting machine.

The essence of the method: when pouring metal material into the centrifugal caster, solid refractory fine disperse particles of different densities are continuously fed into the metal jet, during the entire time of casting.

If the density of refractory disperse particles immersed in the melt differs from the density of the melt, then the force acting on the particle is not balanced by their own centrifugal force and gravity. Therefore, conditions arise for the particles to move to one side or the other, i.e., to the inner or outer surface of the blank to be formed. When the particle comes in contact with the crystallization front it is pressed by the melt to the crystallization front and no longer floats, but is captured by the growing dendrites. As a result surface hardening occurs.

To harden the outer surface of the tubular billet, refractory dispersed particles with a density higher than that of the melt are used. In this case the centrifugal force prevails over the Archimedean force, and the particle in the melt moves from the rotation axis to the crystallization front. It is pressed by the melt to the crystallization front, does not float, and is captured by the growing dendrites. As a result, the outer surface of the tube billet is hardened.

For the hardening of the inner surface of the tube billet refractory dispersed particles with a density less than the density of the melt are fed. In this case the value of the Archimedean force prevails over the centrifugal force and the particle in the melt moves to the rotation axis, floats to the free surface of the melt and is captured by the growing dendrites. This results in solidification of the inner surface of the tube billet.

For simultaneous hardening of the outer and inner surface of the tubular billet, particles of different densities (above and below the density of the melt) are simultaneously fed into the mixtures. When entering the mold, the particles are separated under the action of centrifugal forces and Archimedean floating force, and the inner and outer surfaces of the tubular billet are simultaneously hardened. By changing various casting parameters (workpiece size, volume and the supplied particles dispersion, crystallization rate, etc.), it is possible to obtain material with a given microheterogeneity degree [1, 2]. Khan's work [3] on the topic of "pushing" particles into the melt stream. Khan claims that such parameter as the melt jet's speed has special effect on refractory particles, since the low flow rate does not allow the particles to move to the calculated destination and can "get stuck" in the filling channel or intermediate tank. Here, the author operates with two main parameters of the interaction be-tween particles and the melt: the particles wettability and the free energy amount, which are directly dependent on each other. Next, based on these parameters, the influence of the flow velocity and the friction forces between the particles and the flow are calculated. Khan displays the jet's (flow) critical velocity parameter. The jet's speed is critical if, after passing through the certain calculated mileage of the casting channel with given cross section, the particles fraction ratio remaining in the channel due to crystallizing metal at the channel walls to the fraction of particles passing through the channel or to the total number of particles is certain number that satisfies the technological conditions and does not interfere further casting process due to the cross section reduction of the flow channel. In his research course, Khan derived formula for the critical flow velocity, which is directly proportional to the transported particle's radius, the acceleration of gravity, the difference in density between the particles substances and the carrier fluid, as well as the surface tension, expressed in terms of the sum of the fluid wetting angle and the correction distance, and vice versa proportional to the inverse wetting angle.

The short conclusion is the fact that the smaller the particle in size and density, the lower the speed necessary to maintain its buoyancy and prevent sedimentation, which is the critical flow rate. This formulation is quite plausible, because the author used the elementary laws of hydro-dynamics and the bodies's buoyancy physics. In addition, the experiment was carried out with properties scaling of the introduced particles and the liquid melt body, transferred into the ordinary water image and microscopic size polymer balls, but for clear comparison, additional aluminum and steel balls similar to polymer sizes were used [3].

To study the wetting dispersed metal particles parameters, leading research laboratories apply the still drop techniques and capillary technique. The distinctive feature in the second method is the high accuracy corresponding to real conditions. In this technique, the particles under investigation and the metal wetting them are heated in separate chambers, and the liquid metal is deposit-ed on particles substrate. This technique has already shown impressive results in number of studies, proving its accuracy [4]. The topic of the wettability was raised again by Catalina [5], supplementing Khan results with an additional unaccounted mathematical apparatus. Catalina's work was aimed to study the interaction dynamics of powder microparticles with moving fluid flow, as the result of which the model was developed for the dynamic dispersed particles inter-action with the melt body.

The author identified 3 states of interfacial interaction between the liquid and dispersed particles during crystallization: direct capture of dispersed particles during the passage through the crystallization front, particles ejection by the crystallization front, dispersed particles gradual complete absorption with their simultaneous ejection by the crystallization front, which subsequently forms the material's gradient structure.

The author experiments with three systems: aluminum (matrix) - zirconium oxide (inclusions), succinonitrile (succinic acid, matrix) - polystyrene (inclusions), biphenyl (preservative, matrix) - glass chips (inclusions). This work essence is to build such mathematical model of the dispersed particles behavior, which could give fairly accurate prediction of the dispersed particles distribution at given flow velocity, the crystallization front velocity, expressed in determining their ab-sorption / pushing potential / gradient distribution over the workpiece's body. The result of Cat-alina's work is more precise in relation to the Khan's work, and also creates more accurate description of particles interaction when exposed to the crystallization front. The particles interaction dynamic model with the melt proposed by Catalina is aimed to determine the value of the matrix buoyancy / absorption force based on information about the flow velocity.

The author claims that his model is valid only at speed range close to subcritical [5]. There are several mathematical models for prediction of the particles distribution by volume, in the world at the moment. Most of them are based on the steady state assumption: models describing the criteria for dropping particles by a growing crystallization front [6], models calculating the critical particle absorption rates by growing dendrites crystals [7].

2 Computer Modeling

Some models attempt to describe the system dynamic state [8] or to determine the criterion for capturing non-metallic inclusions by the solidification front during centrifugal metal casting [9]. Some researchers use existing models not to predict the introduced particles distribution, but to more efficiently remove existing oxide particles from the metal and increase its properties [10, 11].

Based on existing models, the article's authors developed mathematical and computer model of the particles distribution over the metal volume during centrifugal casting. The model takes into account various parameters: casting temperature, workpiece size, volume fraction and dispersion of particles, crystallization rate and others. The computer model was developed on the"Ansys" basis and allows predicting the dispersed particles input distribution in real conditions with a high degree of accuracy (Fig. 1, 2).

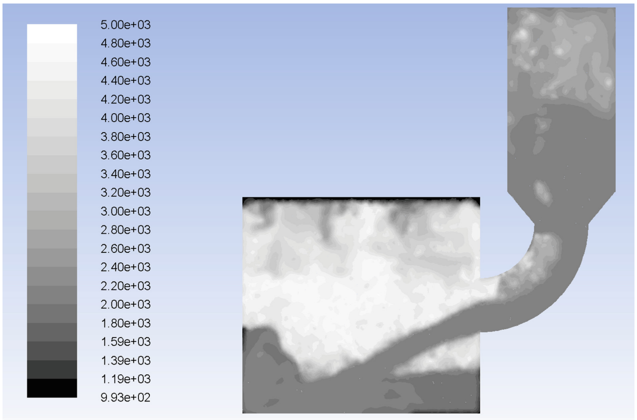

Fig. 1. Modeling the temperature fields dis-tribution during casting.

In designing the model, the following constraints were accepted:

1. The model describes some fixed volume of continuous medium without surrounding atmosphere and walls of working units and auxiliary devices;
2. Gravitational, centrifugal, centripetal forces, the force of surface tension in air, and thermodynamic interaction act on the melt for aggregate transformation;
3. Gravitational, centrifugal, centripetal, Archimedean forces act on particles except surface tension forces, thermodynamic interaction;

4. The behavior of particles in the volume of a metallic melt is described without taking into account the melt wetting phenomenon;
5. Values of density, viscosity, heat capacity of media, initial temperature values of boundary conditions, temperature of particles are assumed constant instead of polynomial dependencies
6. Disperse particles are combined into packages of 5–108 pieces each without reference to their geometric size.

The capabilities of the model are quite broad: it makes it possible to predict the movement of particles and trace the movement of each packet of particles at any moment of crystallization (Fig. 2, 3), and to present the results as a three-dimensional image (Fig. 4).

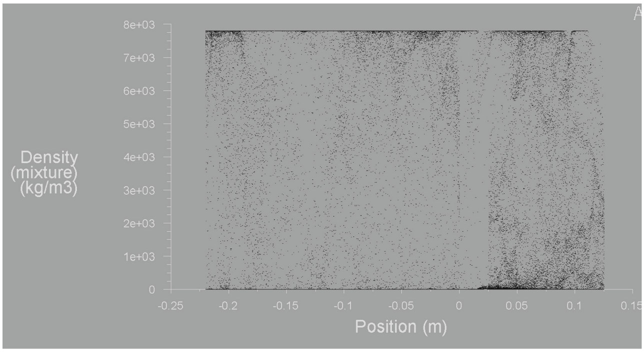

Fig. 2. Diagram of the distribution of all particles along the horizontal axis.

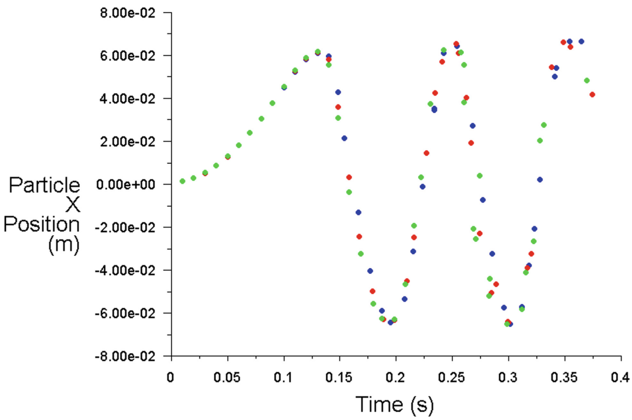

Fig. 3. Distribution diagrams of individual particle packets.

The introduced particles have significant effect on the metal properties. This is achieved by in-creasing the crystallization rate, particles incorporation into the crystal lattice and the “reinforcement” effect. The particles influence degree on the mechanical properties is determined by several factors: the metal chemical composition, the introduced particles type and dispersion, and the density of particles distribution in the crystallized metal volume [12].

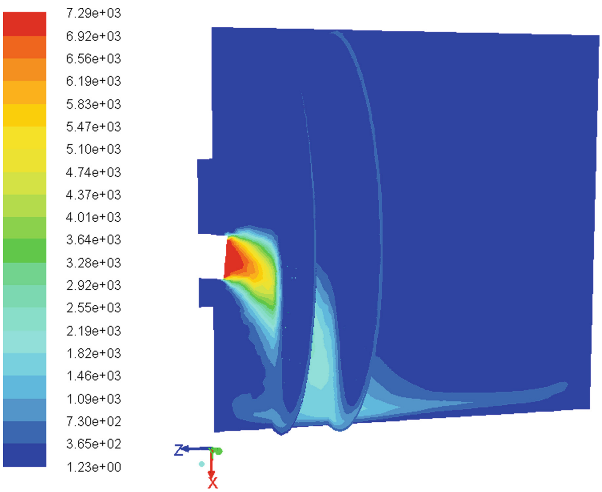

Fig. 4. Volume modeling of metal crystallization and particle distribution.

3 Experimental Results

The authors performed several simulation iterations with different parameters, as well as experimental melts of the metal. After the experiments, the obtained blanks were cut and prepared for metallographic studies. The metal samples were examined in the cast state without heat treatment and examined on an «Axio Observe»d microscope and a «JEOL» electron microscope in several sections along the length of the billet. Particular attention was paid to counting the number of particles per unit area (Fig. 5, 6).

The results of the experimental castings were compared with the results of mathematical and computer modeling (Fig. 7). Distribution curves at experimental castings.

Obtained, the results of computer simulation have differences from the results of experimental melting. The estimated deviation of the results is not more than 15%. In Fig. 6, the distribution lines on the curves show waviness with some increase or decrease in concentration. This phenomenon is observed due to rotation of the mold. When hitting the mold, the melt jet and the particles it contains succumb to a helical movement, which creates a twisting effect in the formation of the crystallizing layer. The absence of such a phenomenon in computer modeling can be explained by the insufficient number of introduced coefficients responsible for the thermal conductivity of the phases, the speed of the crystallization front, as well as the effect of the phases wetting each other.

Microhardness studies were carried out to confirm the uneven distribution of particles over the cross-section of the obtained blanks. Microhardness of samples was investigated by means of a stationary hardness meter according to the Micro-Vickers method. The load and holding time used were 4.9 N and 60 s, respectively. The ratio of this microhardness to the macro-hardness given by Rockwell C was 0.01. The measurement was performed in 10 iterations at 200 μm intervals from the inner edge to the outer edge of each specimen. The measurement results are presented in Table 1.

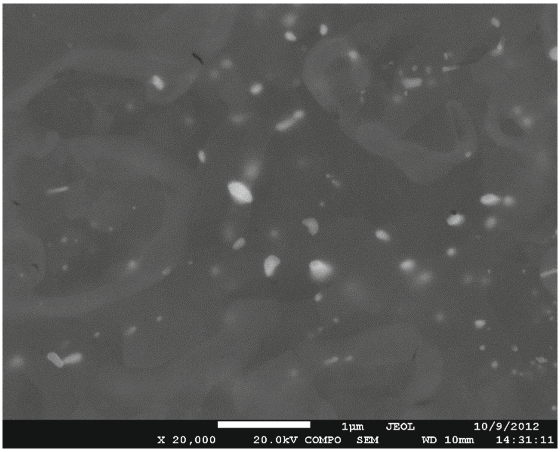

Fig. 5. Microstructure of experimental workpieces: tungsten carbides in the metal, x 20000.

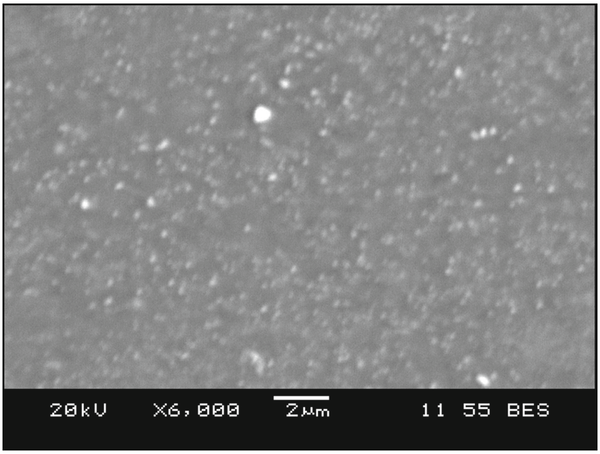

Fig. 6. Microstructure of experimental workpieces: tungsten carbides in the metal, x 6000.

According to the data obtained, it can be noted that hardness and microhardness have maximum values at the outer edge, gradually decreasing to the inner edge. Introduction of dispersed WC particles increases values of these indicators. The maximum microhardness values are reached, respectively, at high concentrations of refractory particles.

Conducting a heat treatment reduces the hardness on a given corrosion-resistant steel, while reducing the hardness gradient over the volume of the castings. This is due to the alignment of the structure obtained by centrifugal casting.

For the experimental materials obtained, mechanical properties were tested in different sections from edge to center: impact toughness, ultimate strength, hardness, wear resistance. Thus, the introduction of 3.6% of tungsten carbide dispersed particles allows to increase the mechanical properties of low carbon steel, to increase the tensile strength by 36–38%, impact strength by 23–26% and wear resistance by 29–34%. According to the data obtained, diagrams were plotted, some of them are shown in the Fig. 8.

This approach feature is that when using different class steel (for example, stainless steels), the introduction effect will be different [13–20].

Thus, the article analyzes various aspects of creating metals with given microheterogeneity de-gree obtained by introducing dispersed particles into the melt, and modern approaches to solving each of the aspects. The computer model has been developed that has great application possibilities for materials with given microheterogeneity degree. This materials' class is one of the most promising, since it allows to significantly increase properties only in given volumes, reducing the scarce alloying elements consumption.

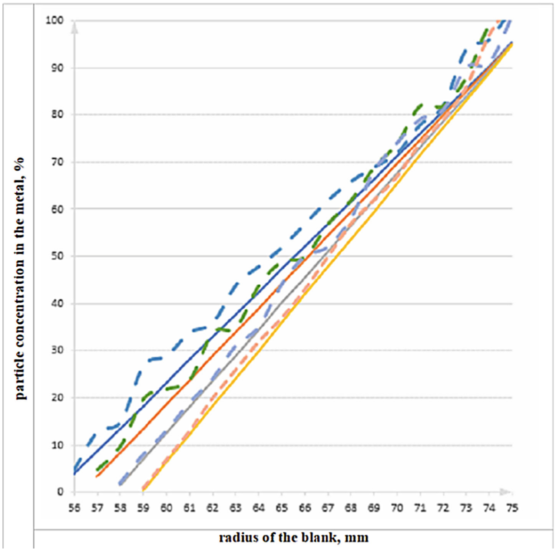

Fig. 7. Distribution diagram of WC carbides when simulating in the CFD-complex Ansys Fluent: 1, 2, 3, 4 - tungsten carbide particle distribution lines at different simulation iterations; 1', 2', 3', 4' - tungsten carbide particle.

Table 1. Results of microhardness measurements from inner edge (1) to outer edge (10), HV.

№	Sample Label					
	Reference	WC, 1 wt%	WC, 2 wt%	WC, 1 wt% after heat treatment	WC, 2 wt% after heat treatment	Reference after heat treatment
1	147.1	169.1	185.9	153.5	155.9	160
2	150.8	170.7	183.2	155.1	162.5	161.7
3	153.2	171.1	192.3	156	165.9	161.2
4	158.1	171.9	189.5	157.4	164.8	163.6
5	164	172.3	186.2	157	163.6	165.3
6	167.9	173.5	189.9	160.6	163.4	163.2
7	168.3	172.3	191.5	161	162.9	165.9
8	173.5	179.5	189.4	161	167.9	169.6
9	175.9	181.7	187.1	165.8	164.9	169.6
10	184.7	183.9	197.2	165.9	168.9	171.5

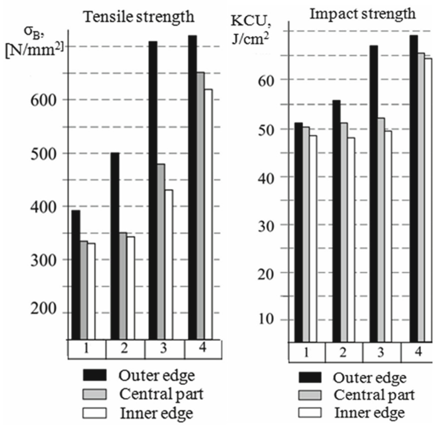

Fig. 8. Change diagrams of tensile strength and impact toughness of samples billets from steel AISI 1020.

References

1. Al-Mangour, B., Grzesiak, D.: Selective laser melting of TiC reinforced 316L stainless steel matrix nanocomposites: influence of starting TiC particle size and volume content. Mater. Des. **104**, 141–151 (2016)
2. Anikeev, A., Seduhin, V., Sergeev, D.: Increase in wear resistance by introduction of titanium carbide dispersed particles. Mater. Sci. Forum **843**, 269–273 (2016)
3. Han, Q., Hunt, D.: Particle pushing: critical flow rate required to put particles into motion. J. Cryst. Growth **152**(3), 221–227 (1995)

4. Chumanov, I., Anikeev, A.: Fabrication of functionally graded materials by introducing wolframium carbide dispersed particles during centrifugal casting and examination of FGM's structure. Procedia Engineering **2**, 816–820 (2015)
5. Catalina, A., Mukherjee, S., Stefanedcu, D.: A dynamic model for the interaction between a solid particle and an advancing solid/liquid interface. Metall. Mater. Trans. A **31**(10), 2559–2568 (2000)
6. Kiviö, M., Holappa, L., Louhenkilpi, S.: Studies on interfacial phenomena in titanium carbide/liquid steel systems for development of functionally graded material. Metall. Mater. Trans. B **47**, 2114–2122 (2016)
7. Kiviö, M., Holappa, M., Yoshikawa, T.: Interfacial phenomena in Fe-TiC systems and the effect of Cr and Ni. High Temp. Mater. Processes **31**(4–5), 645–656 (2012)
8. Li, H., Li, P., Chen, W.: Effect of WC and Co on the microstructure and properties of TiC steel-bonded carbide. Mater. Sci. Forum **898**, 1468–1477 (2017)
9. Martinez, E., Peaslee, D., Lekakh, S.: Calcium wire ladle treatment to improve cleanliness of centrifugally cast steel. Trans. American Foundry Society **119**, 513–520 (2011)
10. Sobczak, N., Nowak, R., Radziwill, W.: Experimental complex for investigations of high-temperature behaviour of molten metals in contact with refractory materials. Mater. Sci. Eng. A **495**(1–2), 43–49 (2008)
11. Türker, M., Çapan, L.: Effect of inclusions on mechanical properties of Nb stabilized austenitic stainless steels (316Nb) with centrifugal and sand casting techniques. Matériaux et Techniques **105**(3), 2017035 (2017)
12. Wang, Q., Zhang, L.: Detection of non-metallic inclusions in centrifugal continuous casting steel billets. Metall. Mater. Trans. B **47**(3), 1594–1612 (2016)
13. Wang, Q., Zhang, L.: Determination for the entrapment criterion of non-metallic inclusions by the solidification front during steel centrifugal continuous casting. Metall. and Mater. Trans. B. **47**(3), 1933–1949 (2016)
14. Watanabe, Y., Sato, H.: Review fabrication of functionally graded materials under a centrifugal force, in book "nanocomposites with unique properties and applications in medicine and industry". InTech., pp. 372–378 (2011)
15. Wilde, G., Perepezko, H.: Experimental study of particle incorporation during dendritic solidification. Mater. Sci. Eng. A **283**(1–2), 25–37 (2000)
16. Klimova, M., Shaysultanov, D., Semenyuk, A., Zherebtsov, S., Stepanov, N.: Effect of carbon on recrystallised microstructures and properties of cocrfemnni-type high-entropy alloys. J. Alloy. Compd. **851**, 156839 (2021)
17. Peng, J., et al.: The predicted rate-dependent deformation behaviour and multistage strain hardening in a model heterostructured body-centered cubic high entropy alloy. Int. J. Plast **145**, 103073 (2021)
18. Semenyuk, A., Klimova, M., Zherebtsov, S., Stepanov, N.: Effect of interstitial elements on the cryogenic mechanical behavior of fcc high entropy alloys. Mater. Sci. Forum **1016**, 1386–1391 (2021)
19. Yurchenko, N., Panina, E., Zherebtsov, S., Stepanov, N.: Design and characterization of eutectic refractory high entropy alloys. Materialia **16**, 101057 (2021)
20. Zherebtsov, S.N., Mikhailets, S.N., Zabegailo, I.V., Rogachev, E.A.: Use of a developed production process of centrifugal electroslag casting for manufacturing a reducer. Chem. Pet. Eng. **52**(11–12), 859–862 (2017)