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Modelling of Distribution of Ultradisperse Particles of Titanium, Tungsten and Zirconium Carbide During Centrifugal Casting

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Abstract: Traditionally, an increase in the mechanical properties of used steels and alloys in ferrous metallurgy is achieved by introducing a significant amount of alloying elements into the metal or alloy. Analysis of the cost market for alloying elements has shown that prices for ferroalloys are increasing every year. An alternative to using expensive alloying elements can be heterophase dispersed-reinforced steels with an unexpressed layer interface. The principal method of creating bulk-gradient metallic materials is dispersion hardening. And one of the effective methods of dispersed hardening is the introduction of particles during centrifugal casting. Although this technology is already known, it has not been studied much, both theoretically and experimentally. This work, which was carried out for grant AP23485709, funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan, is devoted to constructing a computer model of the crystallization process of 12X18H10T steel during centrifugal casting with the introduction of reinforcing particles of titanium, tungsten, and zirconium carbides into it and studying the dynamics of the distribution of dispersed particles under the influence of a gravitational field after the solidification process metal. In the course of this work, a computer model of the distribution of dispersed particles over the cross-section of cylindrical castings obtained by centrifugal casting was developed in order to obtain heterophase steels with a gradient of properties. This model makes it possible to predict the distribution of up to 40 billion particles simultaneously at each moment of casting on a horizontal casting machine. The results of the work indicate that the proposed technology of centrifugal casting with the introduction of dispersed particles during casting makes it possible to obtain research and experimental samples of heterophase steels with a gradient of properties.

Keywords: Process modeling, Ultradisperse particles, Crystallizing melt, Centrifugal casting

Introduction

Increasing the mechanical properties of used steels and alloys in ferrous metallurgy is achieved by introducing a significant number of alloying elements into the metal (base iron) or alloy. Currently, the existing vintage compositions are more than enough to solve most of the current industry challenges. An analysis of the cost market for alloying elements has shown that prices for ferroalloys (alloying compositions) are increasing every year.

An alternative to using expensive alloying elements can be heterophase dispersed-reinforced steels with an unexpressed layer interface, obtained by injecting ultrafine particles into a crystallizing melt in order to obtain gradient mechanical characteristics (Babkin & Trunova, 2021). Such steels are representatives of modern materials, since the technology of their creation implements a mechanism for rational design and providing the necessary properties only to those volumes that are affected by precisely those properties that are required of a given volume.

For this reason, it is a very urgent task to develop a technology for producing metals that meet the specific needs of the existing industry and at the same time have a relatively low cost, achieved by using a small number of correctly selected ultrafine powders, placing them on the work surface or in other volumes of the product that needs specific properties. Such materials are called gradient materials, i.e. materials whose functional properties systematically vary in volume or in one of the dimensional parameters of a particle, film, or bulk sample (Panin et.al., 1985; Kozlov et.al., 2003). The principal method of creating bulk-gradient metallic materials is dispersion hardening. And one of the effective methods of dispersed hardening is the introduction of particles during centrifugal casting (Chumanov et.al., 2012).

The essence of this method is as follows: when pouring metal material onto a centrifugal casting machine, solid refractory fine particles of various densities are continuously fed to the metal stream during the entire casting procedure. Although this technology is already known, it has not been studied much, both theoretically and experimentally. Therefore, research aimed at expanding theoretical and technological knowledge in the field of dispersed hardening during centrifugal casting is relevant.

The purpose of this work is to build a computer model of the crystallization process of 12X18H10T steel during centrifugal casting with the introduction of reinforcing titanium carbide (TiC) particles into it and to study the dynamics of the distribution of dispersed particles under the influence of a gravitational field after the metal solidification process is completed.

Method

When creating a geometric model, the key aspect is to ensure that all physical processes can be reproduced at the required scale. At the same time, it is important to determine the functions of each plane of the model in advance and make sure to provide all the necessary planes that will limit the movement of substances or serve as their sources or sinks. Grid modeling was used to construct a geometric model of the metal casting scheme in a rotating mold. As you know, the process of grid modeling is the division of a geometric model into the simplest elements of a much smaller size relative to the entire geometric model. The computational grid used in computer modeling is shown in Figure 1. The elementary element of this grid is the tetrahedron, since its shape is the best option for generating grids for bodies of rotation.

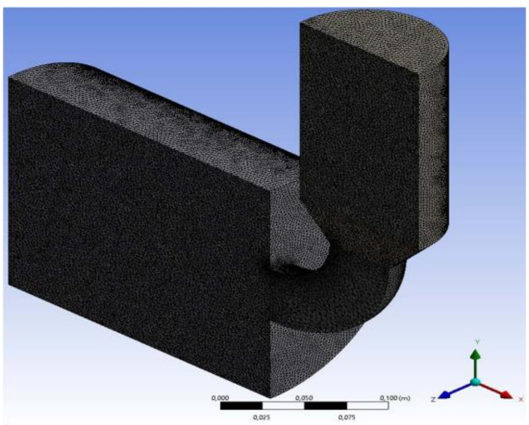


Figure 1. General view of the computational model and grid

During the simulation, Ansys Fluent 16.0 was chosen as the physical pre-processor. Setting up the physical impact model:

1. General environment settings. The solver type is based on the principle of measuring the pressure of the medium (pressure-based). The reason is the fact that the crystallization-melting model is performed exclusively in this type of solver, according to information from the official reference material of the complex. The solution time is continuous (transient). This will allow us to capture a picture of the events of the casting process at different time intervals. The modeling took into account the condition of the influence of the gravitational attraction of the Earth, expressed by the magnitude of the acceleration of gravity g.
2. Active physical phenomena and their mathematical models. A multiphase system. Category – elementary volume of liquid. The proposed model describes the behavior of a certain volume of liquid in a confined space. An example is the transfer of water from one tank to another through a connecting channel.

The model considers the interaction of two liquid phases: air and steel melt. The interphase interaction is described by the surface tension equation, where the coefficient of surface tension between liquid steel and air is assumed to be 1.5 N/m. The basic principle of operation of the constructed volumetric fluid model is to control the state of the unit cell. Mathematically, there is a fractional function C, which represents the result of integrating the characteristic functions of a liquid in a volume. The C values can range from 0 to 1, indicating the degree to which the cell is filled with liquid. If the grid cell is completely filled with liquid, then the C value for this cell is 1, otherwise it is 0.

The substances used and their physical properties. Figure 2 shows the distribution scheme of materials in the model. The material characteristics (physical properties) involved in our physical model were taken from the relevant reference books. During the simulation, 6 iterations of the simulation were carried out with different thicknesses of the workpiece being poured: from 20 mm to 40 mm thick. 1% of particles were added to each of the 12X18H10T blanks.

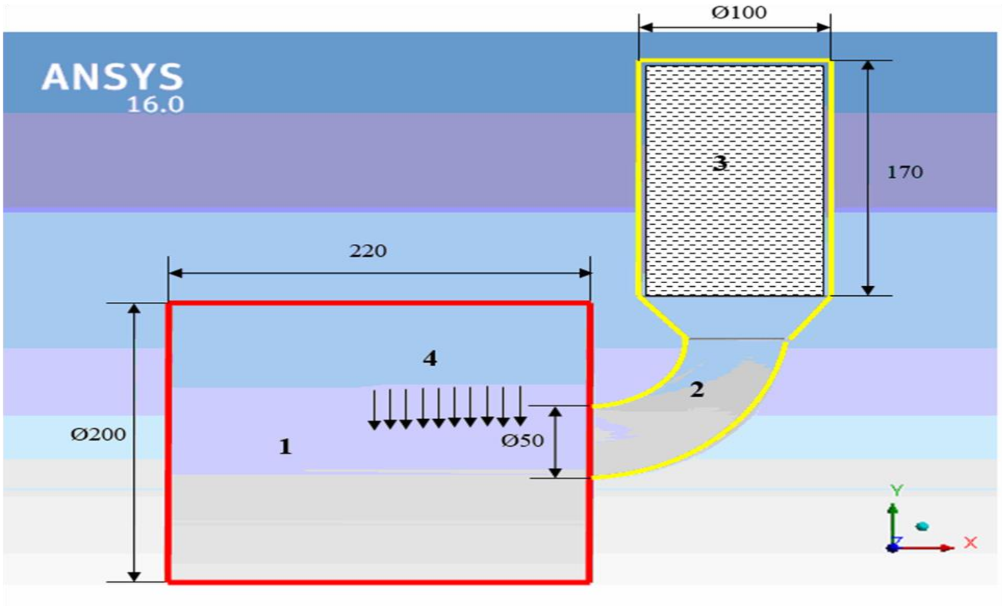


Figure 2. Diagram of the casting model with basic dimensions in millimeters: 1 – rotating mold: wall material – steel 20, wall temperature – 1000 K, rotation speed ~ 600 rpm; 2 – sock: wall material – fireclay brick, wall temperature – 2000 K; 3 – cylindrical ladle with steel melt: wall material - fireclay brick, wall temperature - 2000 K; 4 – injectors of dispersed carbides

Results and Discussion

As a result of the simulation, arrays of data necessary for analysis were obtained. All the simulation results are presented graphically below (Fig. 3-8).

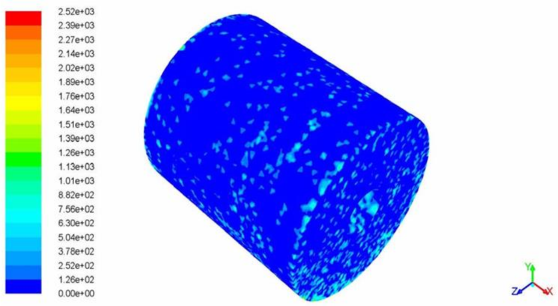


Figure 3. General picture of the distribution of TiC particles after 2.5 seconds of the start of casting (the gradient describes the accumulation of dispersed particles, depending on their density)

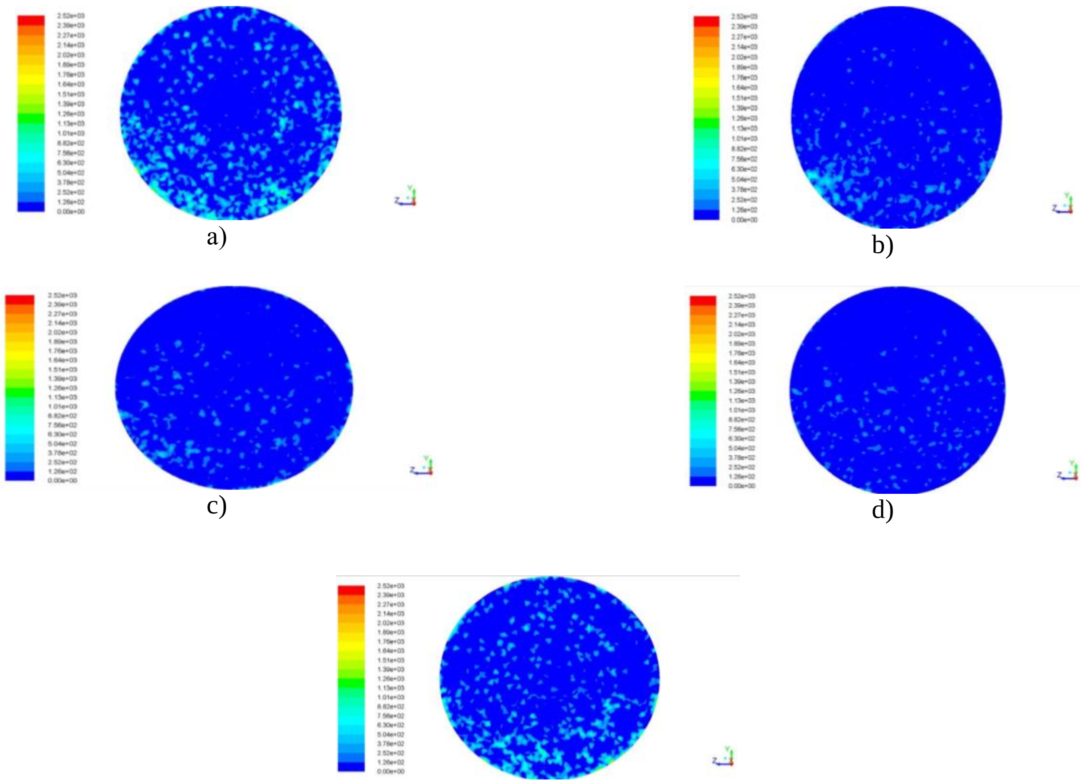


Figure 4. Distribution of TiC particles in the mold cross section: a – 0 mm (first end) from the mold beginning; b – 5 mm (boundary of the end crust) from the mold beginning; c – 110 mm (middle) from the mold beginning; d – 215 mm (boundary of the crust of the rear end) from the mold beginning; e – 220 mm (rear end) from the mold beginning

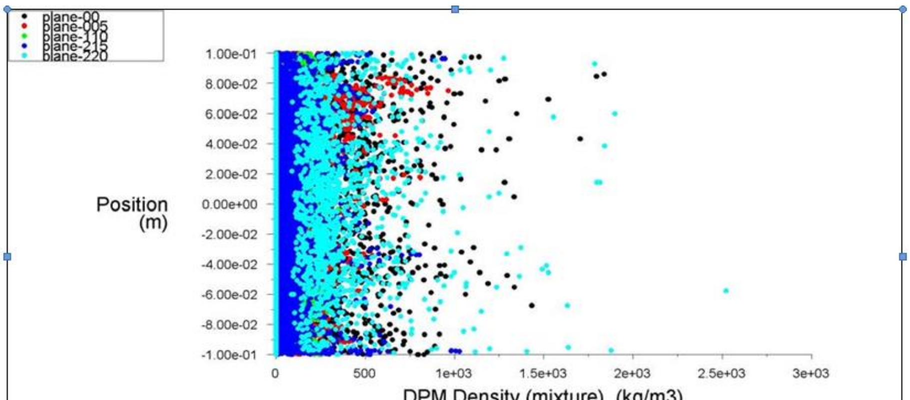


Figure 5. Graphical representation of the particle distribution along the Z axis based on density estimation (colors correspond to the cross-section, according to the legend)

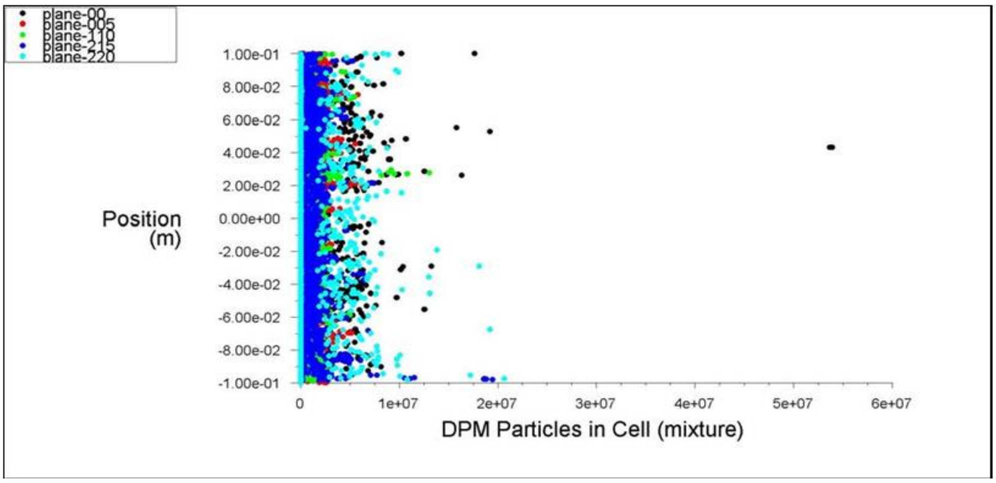


Figure 6. Graphical representation of the distribution of TiC particles along the Z axis based on an estimate of the number of particles in an elementary cell of the computational grid

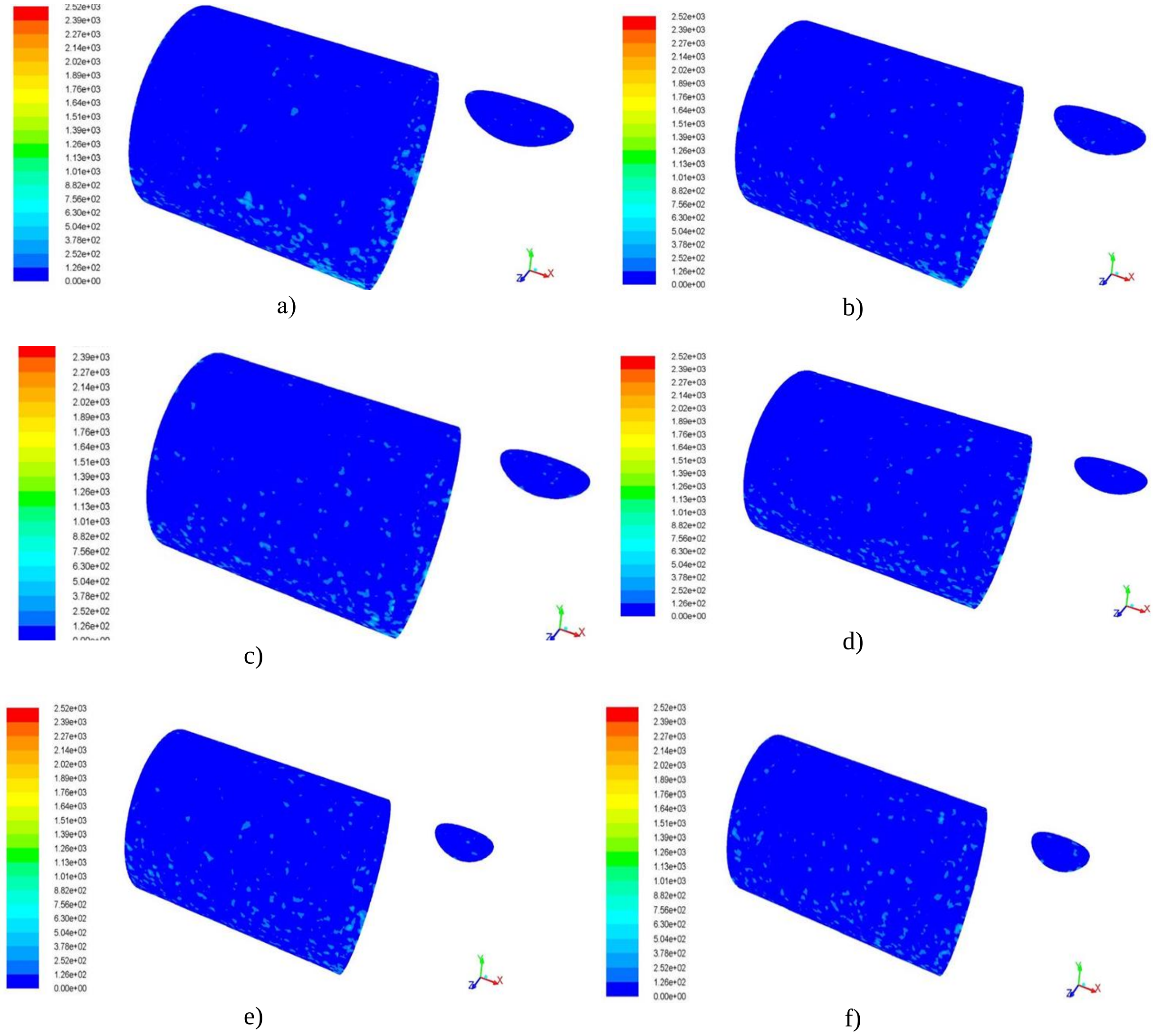
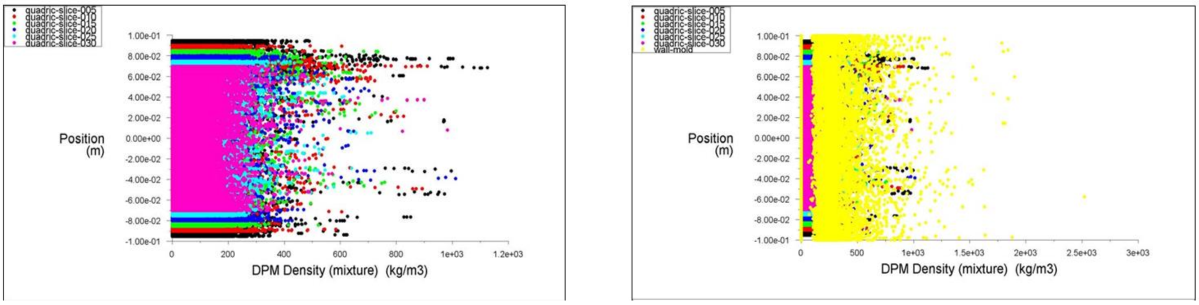


Figure 7. Distribution of dispersed particles over cylindrical concentric sections of the mold: a – 5 mm from the crust; b – 10 mm from the crust; c – 15 mm from the crust; d – 20 mm from the crust; e – 25 mm from the crust; f – 30 mm from the crust



a) b)

Figure 8. Graph of the distribution of dispersed particles along concentric cylindrical sections along the Z axis, estimated by density: a – layers without the outer crust; b – layers with the outer crust

An analysis of the computer simulation results showed the following:

1) regardless of the particle density and the size of the billet being cast, when particles are fed to the jet, particles crystallize on the billet outside being formed during the first moments of casting.
2) after crystallization of the cortical zone with a thickness of 5 mm, the conditions of heat dissipation change and for particles with a density less than the density of metal (in our case, titanium carbide), conditions are created for movement into the inner layers of the workpiece.
3) with an increase in thickness to 40 mm, the distribution of titanium carbide particles is more pronounced: the surface layers are saturated, a relatively small number of particles in 1/2 of the workpiece radius, and the inner layers are saturated.
4) the distribution of carbides is uneven not only in the thickness of the workpieces, but also in length: in all iterations, there is an increased content at the ends of the castings in the surface layers, which is associated with the hydrodynamics of filling the bath. The increased concentration drops sharply to a stable level after only 5 mm from the end. This fact must be taken into account when carrying out experimental castings: in case of confirmation of the distribution on experimental samples, it is necessary to provide for stripping the ends to a depth of up to 5 mm.

Conclusion

A computer model of the distribution of dispersed particles over the cross section of cylindrical castings obtained by centrifugal casting was developed in order to obtain heterophase steels with a gradient of properties. This model makes it possible to predict the distribution of up to 40 billion particles simultaneously at each moment of casting on a horizontal casting machine. The results of the work indicate that the proposed technology of centrifugal casting with the introduction of dispersed particles during casting makes it possible to obtain research and experimental samples of heterophase steels with a gradient of properties.

Scientific Ethics Declaration

* The authors declares that the scientific ethical and legal responsibility of this article published in EPSTEM journal belongs to the authors.

Conflict of Interest

* The authors declare that they have no conflicts of interest

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