# ON THE ISSUE OF ALLOY CRYSTALLIZATION DURING CASTING INTO METAL MOLDS

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#### Abstract

The modern scientific and technological revolution, along with social progress, has ensured tremendous scales of production development in our country. When obtaining many machine parts, instruments, and structures, cast blanks are the most cost-effective option, and in the case of particularly complex parts or when using alloys that cannot be processed by pressure, casting technology becomes the only possible method. At the same time, a significant number of specific defects occur in castings; surface roughness and dimensional accuracy often do not meet the requirements set for products; the properties of alloys in their cast state are generally lower than those in their deformed state. Therefore, the problem of further improving the quality of cast blanks has become critically important today. To address this issue, a specialist must understand the mechanisms of casting processes and be able to control them.

The article discusses the physical and mechanical processes that occur during the pouring of molten metal into a metal mold. Various scenarios of premature formation of heterogeneous nucleation sites are considered. The features of nucleus formation on the solid surface of the mold are described depending on its geometric characteristics. Additionally, physical models of crystallization of heterogeneous nuclei are presented, describing the mechanism of appearance of a widespread defect in castings in the form of shrinkage cavities.

Keywords: casting, crystallization, shrinkage.

### I. Introduction

Casting in metal molds is a common method for producing castings. At the same time, modern trends in market development dictate the need for constant improvement in the operational and quality characteristics of manufactured products. Traditionally, enhancing the operational properties of components made from metallic alloys is achieved by increasing the chemical and physical homogeneity of the metal and minimizing defects of various scales, the majority of which arise during the formation of blanks—ingots and castings. Currently, defects in the internal structure of ingots and castings are often associated solely with the thermal processes of solidification. However, there is evidence that both thermal and mechanical processes significantly influence the

formation of alloy structures and the occurrence of defects [1].

The primary cause of defects in cast blanks and parts is the phase transition of the alloy from a liquid to a solid state, which is accompanied by a series of physicochemical phenomena, including shrinkage—reduction in volume during solidification. Due to shrinkage, mechanical movement of the alloy occurs during the formation of blanks to compensate for the shrinkage of the already solidified part of the metal. Insufficient feeding of the ingots and castings at this moment leads to the formation of defects such as shrinkage cavities, dents, and porosity.

This article investigates the patterns of alloy mechanics during the crystallization period. Understanding these patterns provides the opportunity to develop and optimize new and existing casting technologies.

### II. The main part

When pouring the melt into the mold cavity, it comes into contact with the metallic surface, which determines the formation of a solid shell. This moment is crucial in terms of the formation of crystallization nuclei, which can negatively affect the strength of the resulting casting. The further cooling process depends on several factors, including the superheat of the melt relative to the crystallization temperature, the physicochemical properties of the mold, the flow rate, and the mechanical characteristics of the gating system and the mold cavity [2].

The degree of superheat is the main factor influencing the subsequent cooling and solidification process of the melt. Depending on the level of superheat, there are three possible pouring scenarios: without superheat, with slight superheat, and with significant superheat [3], [4].

In the first scenario of pouring without superheat (Figure 1a), the contact of the metallic mold surface with the melt immediately leads to the formation of a shell, over which a new shell is subsequently formed when the following streams of melt reach the surface of the mold.

When pouring the melt with slight superheat (Figure 1b), a solid shell will also form at the point of contact between the melt and the metallic surface of the mold. However, the subsequent flow of the melt will deliver a heat transfer that slows the growth of the shell near the gate and impedes the solidification process at the initial stage. Once the heat supply ends, solidification will continue similarly to the first case.

In the case of pouring the melt with significant superheat (Figure 1c), a solid shell will form upon contact with the metallic surface of the mold, just like in the first two cases. However, the heat flow from the incoming stream of overheated alloy will melt the formed shell, leading to solidification occurring some distance away from the gate, following the mechanism of the second case. At some distance from the gate, the further solidification process will proceed similarly to the case of slight superheat.



**Figure 1:** Diagram of the interaction between the metal and the mold during the filling of the channel when pouring the melt: a) without superheat; b) with slight superheat; c) with significant superheat

In the areas near the gate, where the stream of the poured melt comes into contact with the walls of the metallic mold, enhanced heat transfer occurs, leading to the erosion of the mold wall or the previously formed shell. This results in localized heating and, consequently, slows down the solidification process [5], [6]. After the melt completely fills the mold cavity, solidification begins approximately uniformly from all surfaces except for those where the initial stage of solidification has been inhibited. In the vicinity of the gate, there is a likelihood of the formation of some volume of unsolidified melt, which may lead to the development of shrinkage cavities. The extent of this defect depends on the level of melt superheat and the duration of flow through the gate [7], [8].

In cases where the nucleus forms not in the space but on a solid surface or substrate, it may take the shape of a spherical segment with a radius of curvature that provides stability with significantly fewer atoms or volume (Figure 2a). Therefore, the formation of such a heterogeneous nucleus will require less undercooling than for a homogeneous nucleus of the same volume [9], [10].



**Figure 2:** Formation of a nucleus on flat (a) and curved (b) surfaces of the mold; V - volume of the sphere, VC - volume of the segment, h - height of the segment,  $\theta$  - edge angle

Most often, such surfaces will be the forming surfaces of the mold, and sometimes small solid particles of impurities in the melt. The conditions of interaction between the materials of the mold, the poured melt, and the forming solid phase have the greatest influence on the formation of the embryo [11], [12].

It is worth noting that the shape of the solid surface affects the stability of the embryo if the surface curvatures are comparable to the dimensions of the embryo. Various depressions and indentations contribute to the formation of stable embryos at smaller sizes even under slight undercooling (Figure 2 b), and vice versa.

In addition, the blurred particles of the metal mold or shell, when further introduced into the flow of the melt, will act as nucleation centers, starting their growth slightly earlier than the main volume of the poured melt. The grain size depends on the rate of crystallization and the rate of nucleation. If we assume that in a certain plane, the filling with solid phase occurs such that the rates of crystallization and nucleation are constant, and that after a certain time, two nucleation centers will form at random locations, then as the crystals grow in the shape of squares around each of them, there will be a growth of the crystal in the form of layers of constant thickness (see Figure 3).



Figure 3: Crystallization Model on a Plane

The solution to the problem of covering a solid phase of such a plane made it possible to formulate the relationship that grain size increases with an increase in the rate of crystallization and a decrease in the rate of nucleation, and vice versa [13], [14]. An important point from a practical perspective is that the nucleation rate in pure metals is lower than that in their alloys.

The specified planar model is simplified and does not take into account certain negative aspects associated with defects during shrinkage [15]. When crystallizing castings with equiaxed structures, defects are most easily formed in a high-concentration suspension when the casting transitions from a liquid state to a solid. This occurs when the average amount of solid phase exceeds 50% and depends on the size and shape of the grains. At this stage, the risk of microcrack formation, porosity, and other defects that impair key performance characteristics increases. Such defects arise as a result of grain movement under the influence of pressure, vibration, or stresses due to hindered shrinkage.

This circumstance becomes particularly important during the crystallization of castings with a two-phase and multi-layer structure, as well as for alloys prone to dendritic liquation. In such alloys, which exhibit selective solidification, the remaining liquid will have a composition corresponding to the eutectic or a second phase with a lower crystallization temperature. During this period, the crystallization process may slow down or even halt entirely, despite continuous heat removal, until the alloy reaches the solidification temperature of the eutectic or second phase. This stage poses a certain danger, as intergranular cracks may form that are not always easily welded. This largely depends on the volume of residual liquid and its distribution among solid grains. When there is a sufficient amount of eutectic or a second phase, effective filling of the formed micropores is possible, making such an alloy less hazardous, as the resulting microcracks and tears can be successfully filled and welded when large volumes of liquid move. However, the most significant danger arises from a small amount of eutectic or a second phase (less than 15%), which may lead to a slowdown in crystallization at such residual liquid content. The tendency to form the described defects also depends on the distribution of the residual liquid phase. A structure in which grains are completely surrounded by thin shells of the liquid phase will not withstand significant stresses, leading to typical intercrystalline destruction. Microcracks and tears that occur during shrinkage compensation or vibrations are not always repairable and remain within the solid material, which may cause leaks during pressure testing and reduce mechanical properties. The fracture characteristics of samples from such alloy resemble a break under tension within the solidification range of the alloy, further confirming the link between defect formation and the specified temperature range.

The situation changes when a small amount of residual liquid alloy of eutectic composition or

a second phase does not surround the solid grains but exists between them as separate isolated areas. In this case, grains touch each other at their edges, forming a rigid structure that significantly better withstands stresses from shrinkage, vibrations, metallostatic, and other pressures. Shrinkage during the crystallization of the last portions of the liquid alloy, in this case, manifests as discrete, isolated pores. Such pores (usually oval in shape) have a negligible effect on the occurrence of leaks and the mechanical properties of the alloy.

Primarily, the shape and position of the liquid phase are influenced by the interfacial tension at the boundary between the crystal and the residual liquid. At low interfacial tension, the liquid, even in a small volume, envelops the grain from all sides. Conversely, at high interfacial tension, the residual liquid forms a significant angle with the face of the forming crystal, promoting the formation of separate areas of liquid phase.

Figure 4 shows a schematic representation of the layer-by-layer growth process of three crystal nuclei, resulting in the formation of a residual liquid phase in a three-grain junction. Subsequently, crystallization — the filling of this liquid phase region — can occur primarily through one of the following mechanisms:

1. Crystallization mainly occurs along the faces of the growing crystals, while this process slows down at the edges forming the angles of the crystals. The slowdown of crystallization in the two-grain junction is due to the accumulation of liquid with an increased concentration of the alloying component. This enrichment in the two-grain junction arises from selective solidification at the faces of the two crystals, where the two growing faces push the impurity into the narrow space between them. When the wetting angle is small, interfacial tension also facilitates this distribution. The liquid enriched with the alloying component has a lower freezing temperature (according to the normal phase diagram), which further slows down crystallization in the two-grain junction.

2. Crystallization occurs mainly in the two-grain junction, meaning that it happens at a greater rate along the edges than on the faces of the growing crystals. In this case, due to selective solidification, the liquid becomes enriched with a component that increases interfacial tension. Here, the alloying element or the alloy enriched by capillary forces (surface tension) is continually expelled from the two-grain angles. An alloy with a lower impurity content from the central part of the liquid enters the void of the two-grain junction, facilitating further filling of the two-grain junction during continuous circulation of the liquid phase. The driving force behind this process is the potential difference arising from the surface tension.



Figure 4: Planar Model of Crystallization Considering the Residual Liquid Phase

If dendritic liquation is often observed in alloys, micro-voids can also form in them. Alloying and modifying additions can significantly alter the surface tension of liquid metals and, consequently, the interfacial tension at the boundary between the solid crystal and the residual liquid. This opens up the possibility for controlling the feeding mechanism of the solidifying alloy. This change can be illustrated using the example of the tin bronze OC10-2. The bronze, by its structure, is two-phase: the eutectoid, which represents a more fusible fraction, is located along the grain boundaries of the  $\alpha$ -solid solution of tin in copper. Depending on the amount of added

elements (such as Ni, Ti, Ce, and others), the shape and position of the eutectoid in the alloy's structure, as well as its density and mechanical properties, change [1].

Considering the studied relationship between interfacial tension and the location of the fusible component, the dihedral angle formed by the faces of two  $\alpha$ -solid solution grains in the region of the eutectoid inclusion can serve as a measure of the magnitude of interfacial tension. If the additions increase the angle of the eutectoid component formed by the faces of two solid solution crystals, thus increasing interfacial tension, it leads to a compact and isolated arrangement of the eutectoid. Conversely, if the additives decrease the dihedral angle and reduce interfacial tension, favorable conditions are created for an elongated position of the eutectoid along the grain boundaries [2].

When studying the microstructure of samples on microsections, it is important to consider that the plane of the section is usually not perpendicular to the faces of the oriented crystals, leading to distortion of the visible angles in the section. Nevertheless, it can be statistically demonstrated that the most frequently observed angles in the planar section represent the true magnitude of the spatial angle. This implies the necessity of conducting several measurements for each structure and subsequent statistical processing of the obtained data.

Based on structural analysis, it has been found that various additions can increase, decrease, or have no effect on the wetting angle of solid grains by the residual liquid at the final stages of crystallization. This, in turn, affects the shape and position of the eutectoid within the structure. At the very final stages of solidification, solid crystals are surrounded by the liquid and are not rigidly connected to each other, creating conditions for the movement of the entire two-phase mass. If the structure forms with a large dihedral angle at the final stages of solidification, the crystals become rigidly interconnected, and the liquid occupies isolated compact regions, which enhances the alloy's resistance to shear stresses and complicates two-phase feeding. Changes in the shape and position of the eutectoid in bronze, with a constant relative amount of the eutectoid phase, predetermine changes in the dominant feeding mechanism and, consequently, influence the ratio of isolated to transitive porosity of the alloy, which, in turn, determines its tightness, mechanical properties, and other characteristics.

The cooling rate of castings affects defect formation in the following ways. At very high cooling rates, dendritic liquation is reduced due to the suppression of segregative diffusion. On the other hand, at very low cooling rates, castings also show reduced dendritic liquation as a result of the homogenizing diffusion process. At moderate cooling rates, there is an increased tendency for dendritic liquation and the formation of micro-voids. High cooling rates, as well as sharp temperature gradients, contribute to minimizing the suspended and solid-liquid states. Additionally, the nearest zone of fully solidified metal is subjected to all stresses. At very slow cooling rates, when a polycrystalline structure with randomly oriented grains is formed, the reduction of defects is associated with the increased time available for their healing due to the prolonged solidification process.

### **III.** Summary

Thus, the improvement of the operational properties of castings obtained in metal molds depends on the formation of the casting as it transitions from a liquid state to a solid one. The degree of superheating is one of the most important factors influencing the cooling and solidification process of the melt. In this case, the most optimal variant involves significant superheating, which helps eliminate the negative effect of premature crystal formation on the surface of the metal mold. However, the greatest impact is exerted by the volume of the liquid phase and its distribution among the solid phases. With a sufficient amount of eutectic or a secondary phase, it is possible to effectively fill the formed microvoids, making such an alloy less hazardous because the resulting microcracks and tears can be successfully filled and welded when large volumes of liquid are moved.

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