FULL USE OF MATHEMATICS – FOUNDRY

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Abstract: In this work, we present the necessity of using the full mathematics in the industrial branch of machine building of the example of the foundry. Obtaining the necessary structures is accompanied by research work even in micro-foundries, which is provided by powerful and new software products, i.e. knowledge transfer with computational mathematics, physics and education.

Keywords: MACHINE BUILDING, FOUNDRY, CASTING STRUCTURES, MATHEMATICS, EDUCATION

1. Introduction

The importance of mathematics is represented by a general block diagram of “The History of the Development of Knowledge of Civilization from Antiquity to Today” of Fig. 1

Fig. 1 Block diagram - Developing the knowledge of civilization from antiquity to today [1, 3, 4].

1 follows: 1. Initial knowledge is obtained through empiricism - obtaining and classifying experimental data; 2. Collecting knowledge in philosophy; 3. Knowledge is divided into separate sciences after Christ: 3.1 Physics - 18th Century; 3.2 Mathematics - the 19th and the beginnings of the 20th century; 3.3 Mathematics - Self Development; 3.4 Mathematics - a powerful tool for research: Description of physical processes and phenomena. Any theory is obtained only by using mathematics; 3.5 The term mathematical physics includes natural and theoretical physics; 4. Mathematics is in every area of human activity; 5. Sustainable development of civilization is based on: a sustainable society and economy - a challenge for every government; 6. Civilization only evolves by overcoming crises in society and the economy; 7. The challenge is the restructuring of the world by the fourth industrial revolution [1], involving education throughout every person’s life, environmental technologies and industries.

The natural systems and the four main types of interaction forces in nature are classified in Fig. 2

Fig. 2 Scheme - Natural systems and types of interactions [2]; 1 - gravitational interaction (large-scale events in the Universe), 2 - electromagnetic interaction (holds electrons in atoms and binds atoms to molecules and crystals (chemistry, biology)), 3 - strong interaction connects the nucleons (it unites protons and neutrons in the nucleus of all elements), 4 - weak interaction determines the forces acting between the light particles (leptons: electrons, neutrinos and muons) and between leptons and heavier particles.

The purpose of this work is to present the necessity of the complete mathematics in the foundry.

2. Foundry - physical and technological processes of structure formation

The casting structures are obtained in phase transition of 1st order is shown with the characteristic scale of the scheme of Fig. 3

Fig. 3 The casting structures are obtained in phase transition of 1st order (solidification) [5]; a) Numerical experiment: technological solidification of a cylindrical cast at 902 s, graphically represented by the geometry of the solidification zone (front) – the local time of solidification. $V_i$ – chosen local volume for description of structure formation; b) Cell for determining grid – $L_{corr}$ for $V_i$, $\Delta V_i$ – changing the volume $V_i$ from melting.
(solidification), \( d \) – direction of growth 1D, 2D or 3D, \( \eta \) – pacing density coefficient, \( V_0 \) – volume of atom, \( V_{sc} \) – volume cell, Wigner-Zeitz cell and structure.

The technological system of foundry we introduced on the example by the machine – Gas counter-pressure casting method Fig. 4

The technological system (see Fig. 4) provides of macro-level to obtain the desired structure average diameter of polycrystalline grains [12]. The macro-parameters of the casting technology are the overcooling of the melt and scattering of the latent heat of melting [3, 5, 11, 12].

3. Mathematics in Foundry

It is well known, that the mathematics application in foundry is theoretical and applied thermodynamics [1, 2, 3]. The separation of each set of knowledge into science is achieved only by using mathematics, which definition is [3]: Mathematics contains mathematical knowledge, foundation of mathematics, methodology of mathematics and philosophy of mathematics in a complex interconnectivity and continuous development.

3.1 Mathematics in Thermodynamics and Foundry

The crystals are arranged in a solid state where the atoms or molecules are arranged in the form of a crystal lattice (structure). The crystals are obtained by a phase transition of first order by changing the aggregate state of the initial phase to the new solid phase. Bearer of the working properties of the castings is the crystalline structure, which is obtained in the phase transition of first order. Thermodynamics system in foundry is alloy (pure metal) crystalline structure, which is obtained in the phase transition of changing the aggregate state of the initial phase to the new solid state with minimal total surface energy for given volume.

There is contradiction theory-experiment: supersaturation and growth sides of crystal. At high supersaturation the growth is not uniformly in all directions and only of some sides.

2. Diffusion theory is on the base that there is a concentration gradient in the vicinity of the growing surface

\[ \frac{dm}{dt} = \frac{D}{\delta} \ln \left( C - C_0 \right) \]

where \( dm/dt \) is the rate the mass deposited on the crystal surface with area \( A_t \); \( D \) – diffusion coefficient; \( \delta \) – thickness layer adjacent to the crystal surface; and \( C_0 \) – actual and \( C_s \) – equilibrium concentration.

3. Surface nucleation theory is developed by Kossel [18], Stranksi [19], Volmer [21], and Kaishev [23] (model KSVK): crystal growth on the surface with inhomogeneties of the type terrace, ledge and kink; guess that the growth is discontinues process of absorption of the material layer by layer on the crystal surface. The arriving atoms (molecules) do not get directly into the grid, but they migrate over the surface in a random walk process and finally get absorbed on these sites, where its energy is a minimum. Migration distance \( x \), is

\[ x^2 = D_t \tau, \text{where } x, = a(kt/2) \]

where \( D_t \) – coefficient of migration; \( \tau \) – time of life of the absorbed particle on the crystal surface; \( k \) is the nearest interaction parameter. Migrate atoms create diffuse flow at the surface of the growing crystal, and they are called adatoms. Migrate atoms create diffuse flow at the surface of the growing crystal, and they are called adatoms. For adsorption of adatoms on the crystal surface is need description of interaction between one adatom and elements of surface relief: one adatom at kink site have three chemical bonds for six first neighbor’s atoms from of the crystal lattice surface; adatom and ledge have two chemical bonds; adatom and terrace have one chemical bond. Barton-Cabreara-Frank model (BCF) [22] gives: 1. the rate of diffusion flow of migrate adatoms \( V_{sc} \): distant migration step is much higher than between two kinks (or middle migration distance is much higher than the mean distance between two adjacent kinks); 2. When the movement step covers the whole surface completely, further growth is only possible by creating a two-dimensional nucleus circle with a radius \( r \) and a height \( h \) with the necessary energy change \( A_{G_{cr}} \). According to Volmer [21], this is possible due to heat fluctuations; 3. The growth rate of a single side is generally controlled by the degree of germ formation and the rate of step advancement \( R_{si}^{i} \)

\[ V_s \geq 2.5 \times X_s, X_{st} \exp(-W/KT), \]

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\[ J_w = C_i \exp[-\mu/\Omega kT] \]

\[ S_{cr}^{i} = \exp[\mu/\Omega kT] \]

\[ R_i^{i} = \frac{h_0^{i/2/2}}{V_{st}^{i/2}}, \]

where \( \lambda \) is a frequency factors in (1.21) and the edge free energy in (1.22)

Table 1: Phase transition in foundry: Liquid(L) ↔Solid(S)

<table>
<thead>
<tr>
<th>Liquid (L)</th>
<th>phase transition of 1st order</th>
<th>Solid (S)</th>
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THERMODYNAMICS OF THE TRANSITION L ↔ S
Continuity of bond type and electron pair bonding mechanism for maximum valence rule for polar corn pounds only; Lewis (1916) rare gas shells; Kossel (1916) Extension of ionic model. Eight as a maximum valence rule for polar corn pounds only; Lewis (1916) rare gas shells; Kossel (1916) Extension of ionic model.

Crystal growth in casting methodology – atomistic approach

1. Thermodynamics – thermodynamic driving force and work of nucleation.
2. Kinetics – nucleation rate and supersaturation number.

Examining the crystal growth methods, we find that nucleation is a critical step in the growth process. The concentration of the growth units on the surface determines the growth rate, which is proportional to the supersaturation. The BCF model depends on two parameters: C which determines the absolute value of the supersaturation, and \( \Omega \) which represents the equilibrium concentration of growth units on the surface.

\[
\Omega = \Omega_0 \left( \frac{C}{x} \right)^{1/2},
\]

where \( \Omega \) is the supersaturation, \( x \) is the rate of nucleation, and \( C \) is a constant for BCR model.

Chemical bond short history introduction on the base table 7 page 199 in [13]: Mendelev (1871) Eight as a maximum valence rule Chemical bond short history introduction on the base table 7 page 199 in [13]: Mendelev (1871) Eight as a maximum valence rule as a continuous source of steps the step provided by the screw dislocation is fixed at the point of displacement; growth is only by rotation around the point of dislocation, like the inner parts of the thread moving faster than the outer parts of the thread. This mechanism can provide a relation between the rate of growth \( R \) and the relative supersaturation \( s \) which are expressed with the equations:

\[
R = C \Omega^{1/2} \tan \left( \frac{s}{2R} \right),
\]

\[
s = \frac{1}{2} \Omega \left( \frac{C}{x} \right)^{1/2},
\]

where \( s \) is the relative supersaturation, \( R \) is the rate of growth, and \( C \) is a constant for BCR model.

As it is known, Koseel offers a kinetic theory of crystal growth [18] and Stranski offers the same model [19]. At their meeting at the suggestion of the Stranski model is a well-known Koseel-Stranski model. The 1930s saw the publishing of several important articles which Stranski co-authored with Kaishev [20, 23] and Krastanov [30], which is called Stranski-Krastanov's growth mechanism. Stranski [28] and Kaishev [23] have developed the method of average separation work, a molecular kinetic method, which has played a role in the development of the theory of crystal growth and growth. Kaishev and Stranski create the model of the crystal lattice by layering crystaline growth; have merit clarifying the relationship between the two-dimensional germ formation and spiral growth of the crystals. Kaishev summarizes Wulff's theorem of the equilibrium crystalline form, Kaishev summarizes Wulff's theorem about the equilibrium shape of the crystal formed on a foreign substrate (Wulf-Kaishev's rule); Develops thermodynamics and kinetics of electro-crystallization and electrolyte nucleation. Application the Kossel-Stranski mechanism is [17].

Nucleation. Kashchiev's book [25] presents at the same time an introduction to the theory of nucleation; the new results, their role and the interaction of the new results with the full theory of crystalline growth; the directions of the development of the complete theory. Thermodynamics and kinetics are directed to saturation (driving force), nucleus size dependence and work of nucleation. Regular spiral growth and known mechanisms of crystal growth are considered. Regular layered, spiral growth and known mechanisms of crystal growth are considered. A great potential for the application of the results in [25] to describe the first-order phase transition in the theory fundamentally is: the theorem of nucleation; and the basic kinetic equation of the formation of new phases for variable supersaturation. Epitaxy. Markov's book [26] considers in four parts the nucleation at obtaining of thin films in epitaxial growth, on the base of equilibrium between crystal and ambient phase, nucleation and crystal growth. The crystal growth mechanisms are examined, and the barrier effects on crystal growth mechanisms and on morphology analysis of the growing crystal surface are also considered. The mechanisms of Frank and van der Merwe and Stranski–Krastanov are discussed. The Mechanism of Stranski-Krastanov is the formation of several complete monolayers followed by the growth of isolated 3D islands and is well known to all epitaxial growth researchers. Barrier effects reporting require rewriting of the nucleation theory. An atom in a barrier effect like Ehrlich–Schoebelel has less close neighbors, which is important for morphology of surface growth. Morphology. The morphology of growing surface is part of the crystal growing. In [14] is presented graphical method generalized by general theorem. Has developed a new model of interaction between an internal structure and the morphology of a growing crystal surface [15]. In work [16] is study the growth and the morphology of Study of growth and morphology of precious stones.

An important moment for the foundry (but also for material science) is the natural boldness between the works of Balevski [6] and Borisov [7]. By definition [6] – By definition [6] – Metal science is the science of the relationships between structure and properties, as well as the influence that thermal, mechanical and other impacts have on the structure, and hence on the properties of metals and alloys. Metal science as a science emerges in the second half of the 19th century, originated in physics, metal physics, and so on. The introductory first part is Theory of Metals and Alloys: electronic struction of atoms; interatomic connections; crystal structure of metals; crystallization; physical – properties and methods of measurement; due to the engineering direction of [6]: deformation (elastic and plastic), mechanical properties and tests. These rigorous scientific terms clearly show the required minimum number of scientific fields in metal science, and only by the engineering need It is further clarified that the scientific ideas in [13] are not only in the theory of metal science but also in the theory of all material science. Изключително важен момент е: за описание свойствата на металите е създадена квантовата механика; използва се във фундаментални изследвания на физиката и техниката, които вече са съвпадат. An extremely important point is: quantum mechanics has been created to describe the properties of metals; used in fundamental studies of physics and technology that have already coincided. The full theory of crystalline growth covers applications such as semiconductor materials and structures for nanoelectronics [...].

In [7] the introduction of solid state physics is based on quantum chemistry, i.e. the application of quantum mechanics for explanation of the chemical connection (electromagnetic interaction see Fig. 2). The interaction of the electron (atomic core) is coulomb and the state of the electron in the atom lies as a solution to Schrödinger's amplitude wave equation. Types of solid bodies according to the type of interatomic connections [7]: ionic crystals - crystalline lattice consists of oppositely charged ions; valent crystals - the atoms are connected in a crystal lattice with a covalent (homoeopolar) bond; metals - a crystal lattice is made up of positive ions, the repulsive forces between them being equalized by the free electrons; molecular crystals - the lattice is made up of individual molecules or atoms interconnected with intermolecular (vanderals) forces. Metal alloys are the simplest chemical compounds - solutions. The crystal lattices of the alloys according to the size of the atoms are: solid substitution solutions; solid solutions of deployment. It can be said that work [7] binds work [6] with

Full mathematics is called upon to create new purely mathematical theories. The new theories are evolving because Gödel’s theorems of "incompleteness" clearly show that there is no complete mathematical theory. The history of mathematics shows the need for the development of pure mathematics, but it is challenging to suggest the assessment of the development of the necessary, for example, a "new mathematical field". A scale of 1μm is a macro-scale. Scale for nm or Å requires modern methodologies based on [8, 9, and 10]. Generalized this is the mathematics, the theoretical and the mathematical physics presented in Fig. 5.

![Scheme](image)

**Fig. 5** Scheme - Full mathematics is needed in Micro-Foundry and Industry 4.0.

**4. Conclusion**

Mathematics is a powerful tool for research. Mathematics is needed in public development, for example "virtual factories", apart from technological, legal relations between companies, based on new experimental data, evaluations are also made for research ideas for development from "artificial intelligence". Hence Industry Change 4.0: "factories without people", and people naturally need life-long education.

**5. References**

5. S. Bushev, Theoretical model of structureformation in die casting. XXII International scientific technical conference “FONDARY 2015”, 16-17.04.2015, Pleven, Bulgaria, Year XXIII, ISSUE 3(166), April 1015, p.60-63, ISSN: 1310-3946 (In Bulgarian)
20. I. N. Stranski, and R. Kaischew, 2 Phys. Chem., (B) 26 (1934) 31