

FULL USE OF MATHEMATICS – FOUNDRY

Bushev S., Associate Professor, PhD, Eng.

Institute of metal science, equipment and technology with hydro- and aerodynamics center “Acad. A. Balevski”
Bulgarian academy of sciences, Sofia 1574, 67 “Shipchenski prohod” Str. Bulgaria Republic
stbushev@abv.bg

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

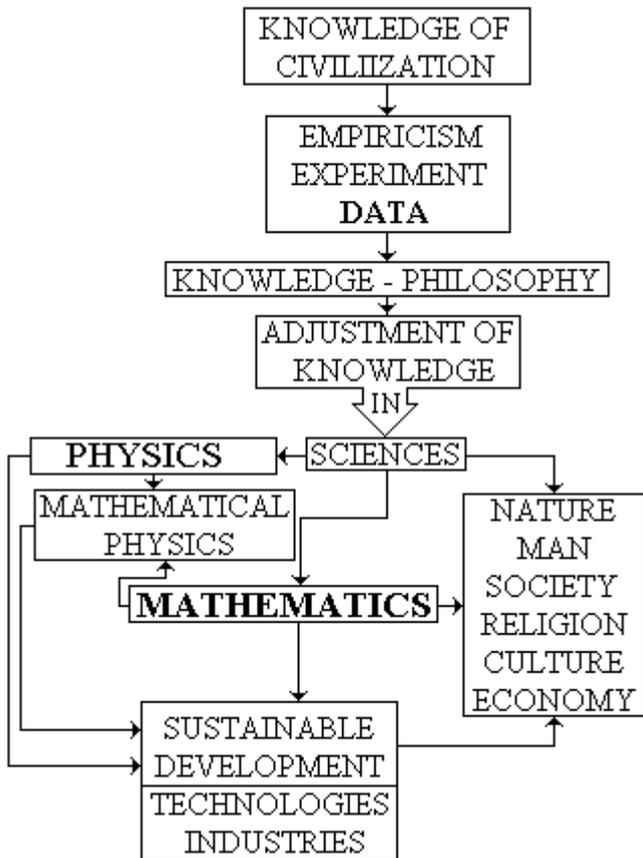


Fig. 1 Block diagram - Developing the knowledge of civilization from antiquity to today [1, 3, 4].

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

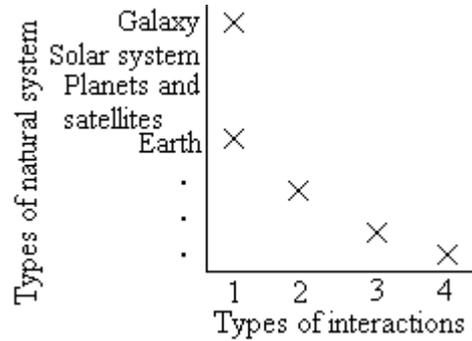


Fig. 2 Scheme - Natural systems and types of interactions [2]: 1 - gravitational interaction (large-scale events in the Universe), 2 - electromagnetic interaction (holds electrons in atoms and binds atoms to molecules and crystals (chemistry, biology)), 3 - strong interaction connects the nucleons (it 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

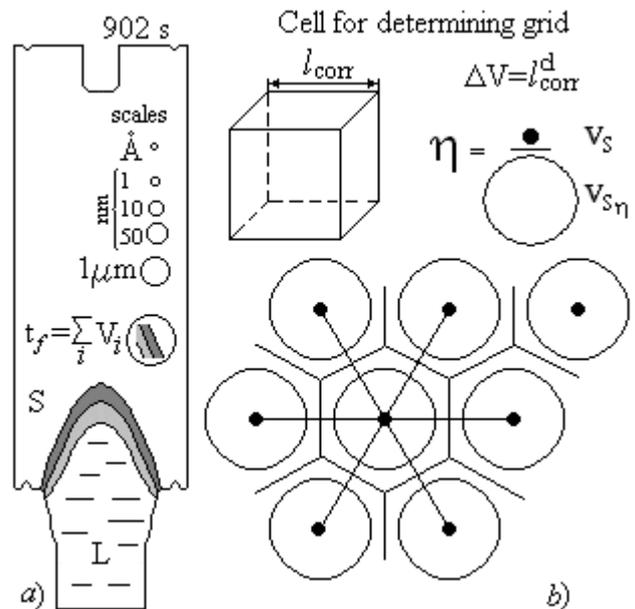


Fig. 3 The casting structures are obtained in phase transition of 1st order (solidification) [5]: a) Numerical experiment: technological solidification of a cylindrical cast at 902 s, graphically represented by the geometry of the solidification zone (front) – S between the liquid (L) and the solid (S) phases. Scales \AA , nm, $1\mu\text{m}$. t_f – local time of solidification. V_i – chosen local volume for description of structure formation; b) Cell for determining grid – l_{corr} for V_i , ΔV_i – changing the volume V_i from melting

(solidification), d – direction of growth 1D, 2D or 3D, η – packing density coefficient, v_s – volume of atom, $v_{s\eta}$ – 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

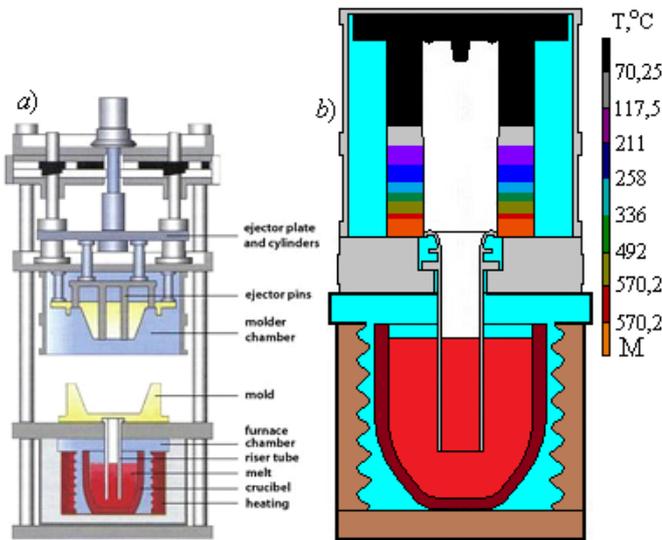


Fig. 4 Casting technology system - Gas counter-pressure casting machine: a) General appearance of the casting machine; b) Technology for producing counter-pressure cylindrical castings. The technological regime shown (see Fig. 2 a) is obtain with initial temperature of the mould without taking into account the filling process.

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) (see Fig. 3 and Fig. 4). Casting is a fundamental branch of material science. It is known that the most advantageous technology for making castings with complex geometry is casting.

The description of the first-order phase transition is presented here in its historical development, i.e. the development of the classical theory of crystallization in atomistic approach. Table 1 presents: the description of thermodynamics; the theoretical description of nucleation like: thermodynamics and kinetics; crystal growth theory: Surface energy; Dyffusion; Surface nucleation; Screw dislocation

Table 1: Phase transition in foundry: Liquid(L) \leftrightarrow (S)Solid.

Liquid (L) $\xleftarrow{\text{phase transition of 1}^{\text{st}} \text{ order}}$ Solid (S)
THERMODYNAMICS OF THE TRANSITION L \leftrightarrow S

$$G = H - TS, \text{ Gibbs free energy at } T_e \rightarrow G_L = G_S, \quad (1,1,2)$$

$$\Delta G = \Delta H - T\Delta S; \text{ and } \Delta G = G_L - G_S, \Delta H = H_L - H_S, \Delta S = S_L - S_S, \quad (1,3,4,5,6)$$

$$\Delta G = 0 \text{ is equilibrium at } T_e \Rightarrow \Delta H = T_e \Delta S, \quad (1,7)$$

$$\Delta G = \Delta H \Delta T / T_e, \text{ and } \Delta T = T_e - T, \quad (1,8,9)$$

$$\Delta G = \Delta S \Delta T \text{ for melt growth,} \quad (1,10)$$

$$\Delta G = RT \ln(S_R) \text{ growth depend to supersaturation ratio } S_R. \quad (1,11)$$

In foundry the basic thermodynamics system is material from two phases; G – Gibbs’s free energy of the system; H – enthalpy; S – entropy; T – temperature; $T_e = T_L = T_S$ – equilibrium temperature; $T_e - T$ – supercooling; Δ – change of G, H, S; R – gas constant.

NUCLEATION – IMPORTANT PHENOMENON IN CRYSTAL GROWTH

$$\Delta G = 4\pi r^2 \sigma - \frac{4}{3}\pi r^3 \Delta G_v; \quad r^* = \frac{2\sigma}{\Delta G_v}, \quad \Delta G^* = \frac{16\pi\sigma^3}{3\Delta G_v^2} \quad (1,12,13,14)$$

$$\Delta G^* = \frac{16\pi\sigma^3 \Omega^2}{3(kT \ln S_R)}, \text{ Gibbs – Tomson equation} \quad (1,15)$$

$$J = J_0 \exp\left[-\frac{\Delta G^*}{kT}\right], J = J_0 \exp\left[\frac{16\pi\sigma^3 \Omega^2}{3(kT \ln S_R)}\right], S_{R_{Cri}} = \exp\left[\frac{16\pi\sigma^3 \Omega^2}{3k^3 T^3 \ln J_0}\right], \quad (1,16,17)$$

where ΔG_v – change the Gibbs free energy of nucleus volume of new phase (L or S); r – nucleus radius; r^* ; ΔG^* - critical parameters; σ – surface energy; Ω – atomic (molecular) volume; J – nucleation rate per *unit* volume; J_0 – is the total number of particles in the new phase; $S_{R_{Cri}}$ – critical supersaturation ratio; k is Boltzmann’s constant.

CRYSTALS GROWTH THEORY

1. **Surface energy theory** is on the based to thermodynamics equilibrium 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 of 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

$$\frac{dm}{dt} = \frac{D}{\delta} A(C - C_0) \quad (1,18)$$

where dm/dt is the rate the mass deposited on the crystal surface with area A ; D – diffusion coefficient; δ - thickness layer adjacent to the crystal surface; C and C_0 – actual and equilibrium concentration.

3. **Surface nucleation theory** is developed by Kossel [18], Stranski [19], Volmer [21], and Kaishev [23] (model KSVK): crystal growth on the surface with inhomogenities 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_s is

$$x_s^2 = D_s \tau_s, \text{ where } x_s \approx a[3\phi/2kT] \quad (1,19,20)$$

where D_s – coefficient of diffusion; τ_s – life time of the absorbed particle on the crystal surface; ϕ 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-Cabrera-Frank model (BCF) [22] gives: 1. the rate of diffusion flow of migrate adatoms V_{ST} : distant migration step is much higher than distant 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 ΔG_{id} . 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 $R_{id}^{V_{ST}}$

$$V_{ST} = 2S_{x_s} x_s \gamma \exp(-W/kT), \quad (1,21)$$

$$\Delta G_{id} = 2\pi r h \gamma - \pi r^2 h \Delta G_v, \quad \Delta G_{ig}^* = 2\pi h \gamma - \pi r^2 h \Delta G_v, \quad (1,22,23)$$

$$J_{id} = C_i \exp\left[-\frac{\pi h \gamma^2 \Omega}{k^2 T^2 \ln S_{x_s}}\right] \quad (1,24)$$

$$S_{x_s, Cri}^i = \exp\left[\frac{\pi h \gamma^2 \Omega}{k^2 T^2 \ln C_i}\right] \quad (1,25)$$

$$R_J^V = h J_{id}^{1/3} V_{ST}^{2/3}, \quad (1,26)$$

where γ is a frequency factor in (1,21) and the edge free energy in (1,22)

and 23); W is the total evaporation energy; S_{x_s} is supersaturation for the mean migration distance x_s , and index cri is for critical supersaturation; C_l – concentration of liquid.

4. Burton, Cabrera and Frank [23] (BCF model) **screw dislocation theory**: on the surface of the crystal in the dislocation point a screw component with a height of the Burger vector projection acts 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 tread moving faster than the outer parts of the tread. This mechanism can provide a relation between the rate of growth R and the relative supersaturation s which are expressed with the equations

$$R = C(s^2 / s_1) \tanh(s_1 / s), \quad (1,27)$$

$$s_1 = 19\gamma\Omega / 2kTx_s; \quad C = D_s \cap_{se} \beta\Omega / x_s^2,$$

where s – relative supersaturation; s_1 – a const for BCF model; \cap_{se} – equilibrium concentration of growth units on surface; β – retardation factor; Ω – volume of the growth unit. The variation R with supersaturation thus depends on two parameters, C which determines the absolute value of growth rate and s_1 which determines actual growth rate. The BCF model predicts nucleation at edge dislocation predicts that the growth rate is proportional (\propto) to the square of the supersaturation for low supersaturation if $s \ll s_1 \Rightarrow R \propto s^2$ and changing to a linear dependence at higher supersaturations if $s \gg s_1 \Rightarrow R \propto s$.

Crystal growth in casting methodology – atomistic approach

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

MACROSCOPIC LEVEL – SOLIDIFICATION [5]

1. **Heat Conductivity analytical solution**: 1.1 1D Stefan's problems; 1.2 1D Stefan-Schwartz problems;
2. **Numerical Solidification's Problems**: 2.1 1D Stefan's problems and 1D Stefan-Schwartz problems; 2.2 3D Stefan's problems and **the most important 3D Stefan-Schwartz problem**; 2.3 Numerical Methods: 2.3.1 Finite differentials method; 2.3.2 Finite elements method; 2.3.3 Boundary elements method.

Chemical bond short history introduction on the base table 7 page 199 in [13]: Mendeleev (1871) Eight as a maximum valence rule and the sum of the hydrogen and oxygen valences for higher types; Abegg (1904) Electrochemical interpretation of Mendeleev's rule of eight in terms of electron gain and loss; Thomson: (1904, 1907) Concept of chemical periodicity in terms of recurring outer electron configurations. Rule of eight as striving for completion of stable rare gas shells; Kossel (1916) Extension of ionic model. Eight as a maximum valence rule for polar compounds only; Lewis (1916) Continuity of bond type and electron pair bonding mechanism for octet completion; Langmuir (1919-1921) Elaboration and popularization of the Lewis model. Mathematical formulation of the octet rule.

As it is known, Kossel 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 Kossel-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 crystalline growth (layered crystalline 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 crystal's form, Kaishev summarizes Wulff's theorem about the equilibrium shape of the crystal formed on a foreign substrate (Wulff-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 foundry methodologically is: the theorem of nucleation; and the basic kinetic equation of the formation of new phases for variable saturation. **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-Schwoebel 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 structure 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 (van der Waals) 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

quantum mechanics. Work [6] and [7] are expanded by [9] for electron theory in metals.

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 $1\mu\text{m}$ 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

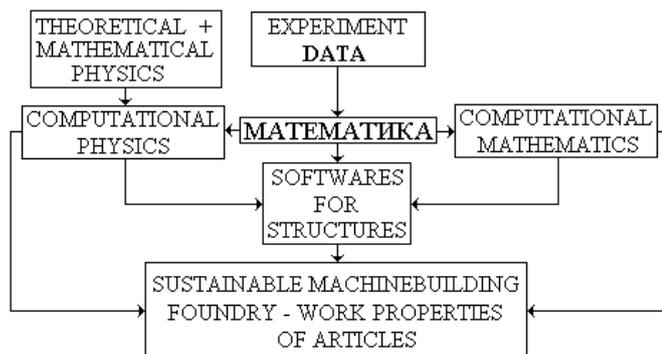


Fig. 5 Scheme - Full mathematics is needed in Micro-Foundry and Industry 4.0.

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

1. S. Bushev, Knowledge transfer Industry 4, International Scientific Journal "INDUSTRY 4.0", No 4, p.51-54, Year I, ISSUE 1/2016
2. Ch. Kittel, W. Knight, M. Ruderman, Mechanics, Berkeley Physics Course, v. I, "Nauka", Moscow, 1975. (In Russian)
3. S. Bushev, Industrial mathematics – phase transitions, scattering, structures, International Scientific Journal "INOVATIONS", p.57-62 Year V, ISSUE 2/2017, Sofia.
4. K. Schwab, The Fourth Industrial Revolution, "Hermes", 2016, ISBN 978-954-26-1630-6 (In Bulgarian)
5. S. Bushev, Theoretical model of structureformation in die casting, XXII International scientific technical conference "FOUNDRY 2015", 16-17.04.2015, Pleven, Bulgaria, Year XXIII, ISSUE 3(166), April 1015, p.60-63, ISSN: 1310-3946 (In Bulgarian)
6. A. Balevski, Metaloznanie, „Tehnika”, Sofia, 1962. (In Bulgarian)
7. M. Borisov, K. Marinova, Uvod vav fizikata na tvardoto tialo, I chast, „Nauka i izkustvo”, Sofia, 1977. (In Bulgarian)
8. E. Pavarini, E. Koch, F. Anders, and M. Jarrell (Eds.) Correlated Electrons: From Models to Materials, Autumn School organized by the Forschungszentrum Jülich and the German

Research School for Simulation Sciences, 3 – 7 September, 2012. ISBN 978-3-89336-796-2

9. U. Mizutani, Introduction to the electron theory of metals, Cambridge University Press, 2003, ISBN 0 511 01244 6
10. U. Landman, Materials by numbers: Computations as tools of discovery, PNAS, May 10, 2005, vol. 102, no. 19, 6671–6678
11. S. Bushev, Multyscales evaluation structure formation – casting, Proceed. Forth national conference with international participation "Materials science, hydro- and aerodynamics and national security'2014", p.19-23, 23-24, October, 2014, Sofia, Bulgaria
12. S. M. Bushev, Controllability problems of crystallization process in casting, Thesis of PhD, TU, Sofia, 1993.
13. W. B. Jensen, Abegg, Lewis, Langmuir, and the Octet Rule, Journal of chemical education, Volume 61, Num. 3, March, 1984.
14. P. Terpstra, W. J. van Weerden, Graphical methods for the determination of reticular densities and lattice parameters, www.minsocam.org/ammin/AM19/AM19_531.pdf
15. E. Dowty, Crystal structure and crystal growth: I. The internal structure on morphology, American Mineralogist, Volume 61, pages 448-459, 1976.
16. I. Sunagava, Growth and morphology of crystals, *Forma*, **14**, 147–166, 1999. Reprinted with permission from Mathematical Sciences, No 358, 1993, (in Japanese)
17. G. Wranglén, Bravais' and Kossel-Stranki's Theories of Homopolar Crystals and their Applications to Elements, Acta Chemica Scandinavica, **9** (1955) 661-676.
18. W. Kossel, Nachr. Ges. Wiss. Göttingen, Math. Phys. K1 11A (1927) 135.
19. I. N. Stranski, Z. Phys. Chem., 136 (1928) 259.
20. I. N. Stranski, and R. Kaischew, Z. Phys. Chem., (B) 26 (1934) 31
21. M. Volmer, Die Kinetik der Phasenbildung (Steinkopff, Dresden, 1939).
22. W. K. Burton, N. Cabrera, F. C. Frank, Phil. Trans. Roy. Soc., A243 (1951) 299.
23. R. Kaishev, Selected Works, Publishing House of the Bulgarian Academy of Sciences, Sofia, 1980. (In Bulgarian)
24. M. C. Flemings, Solidification processing, Peace, Moscow, 1977. (In Russian)
25. D. Kashchiev, Nucleation: basic theory and application, Butterworth-Heinemann, Oxford, 2000. ISBN 0 7506 4682 9
26. I. Markov, Crystal growth for beginners: fundamentals of nucleation, crystal growth and epitaxy, World Scientific, Singapore, 2004.
27. Crystal growth: Theory and techniques, www.shodganga.inflibnet.ac.in/bitstream/10603/.../08_chapter1.pdf
28. I. Stranski, www.revolvvy.co/main/index.php?s=Ivan%20Stranski
29. https://bg.wikipedia.org/wiki/Ростислав_Кашиев
30. Stranski, Ivan N.; Krastanow, Lubomir (1938). "Zur Theorie der orientierten Ausscheidung von Ionenkristallen aufeinander". Abhandlungen der Mathematisch-Naturwissenschaftlichen Klasse IIb. Akademie der Wissenschaften Wien. **146**: 797–810
31. A. Popov, Semiconductor materials and structures for nanoelectronics, University Publishing house "St. Kliment Ohridski", Sofia, 2007. ISBN 978-954-07-2539-0 (In Bulgarian)