MESURMENT OF FOUNDRY STRUCTURES – MATHEMATICS

Maneva A., Chief Assistent, PhD, Eng., 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
anna13@abv.bg , stbushev@abv.bg

Abstract: Mathematics is a technological necessity for manufacturing but casting in micro-foundry. The need to describe the first-order phase transition process is based on physical experiments with this transition based on theoretical and mathematical physics. The natural basis of any science is the use of mathematics, which is a basic motivation for its self-development.

Keywords: MATHEMATICS, FOUNDRY, MICROSTRUCTURE, INFRASTRUCTUR OF KNOWLEDGE TRANSFER

1. Introduction

The capabilities of foundries and computational mathematics are presented very clearly in Fig. 1

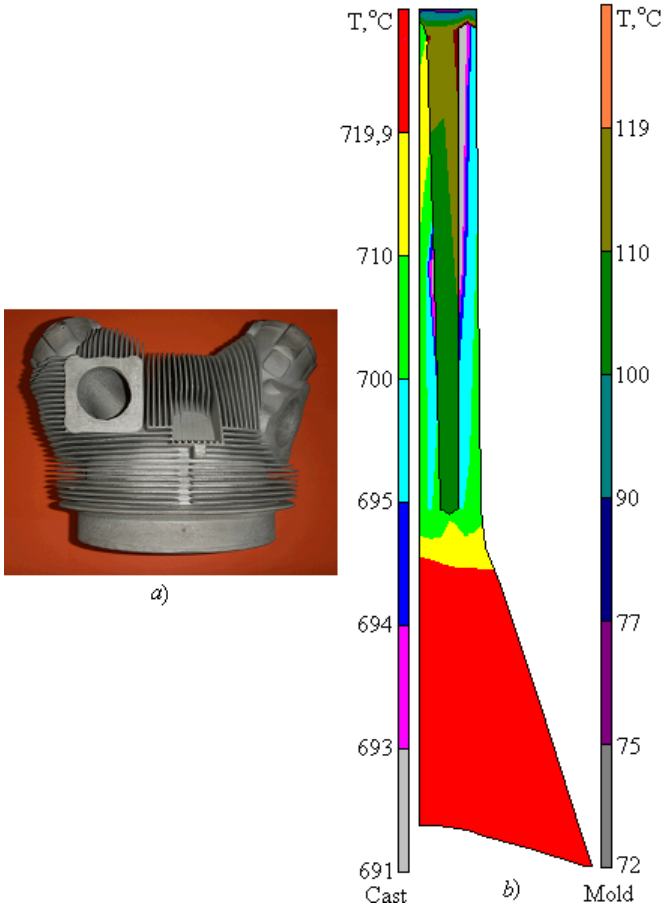

Fig. 1 *The possibilities of die-casting and computational mathematics:a) Cast cylinder head for an aircraft engine produced by the gas counter-pressure process according to [1]; b) Non-stationary temperature field cooling of a local melt volume (rib) and an adjacent local volume of format at the start of a melt cooling process. Computational mathematics allows detailed numerical study of contact heat transfer in volume with complex geometry according to [2]*

This communication presents the need to use computational physics through the necessary software for foundry structures of the meso- level (Quantum Mechanics) and in micro-foundry.

2. Computational physics – foundry structure formation

The structure of metals and alloys at the micro-level we present through the location of the atoms in 2D an ideal crystal lattice composed of Wigner-Seitz cells. By definition, it is well known that the volume of this cell may be located only a single atom. The degree of density of the atomic locations in the crystal lattice is represented by the density of the packing density coefficient in Fig. 2

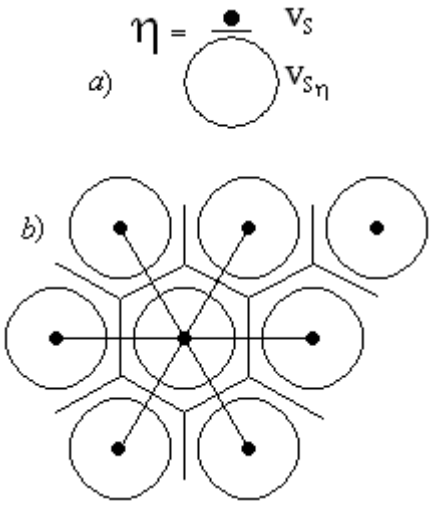

Fig. 2 *Scheme – casting structure of meso- level [3]: a) η – packing density coefficient, v_S – volume of atom, $v_{S\eta}$ – volume of cell, where have only one atom; b) 2D an ideal crystal lattice composed of Wigner-Seitz cells.*

The calculations of the casting structure at the meso-level are carried out at scales of Å and nm. It is well known that a scale of 1 μm is a macro size. The theoretical model [3] includes the tasks: Stephan and Stephan - Schwarz; the atomic level is the model of Kosel-Stranski-Folmer-Kaishev and the basic equation of Kashchiev with variable thermodynamic driving force and thermodynamics of supesaturation (supercooling). This is the classical theory of crystallization, but an important nuance applicable to a certain minimum scale. The classical theory of atomic crystallization is applied to the nuclei of ten atoms through the Kashchiev equation.

In the [4] mathematical theory of heat conduction it is proposed to use these nuclei sizes when it is possible to apply the postulates of quantum mechanics.

M. Borisov makes the main step for metal science by associating it with the physics of the solid body [5]. In particular, it shows „the metal bond" and the need for quantum mechanics in the engineering of metals and alloys. It should not be forgotten that quantum mechanics arises to describe the properties of metals - Drude's theory.

In the textbook of U. Mizutani is presented the electronic theory of metals [6]. Electrons are responsible for the physical, chemical and transport properties of metals. This textbook gives a complete account of electron theory in both periodic and non-periodic metallic systems.

At the Correlated Electrons: From Models to Materials Conference [7], mathematical modeling and simulation of correlated electrons in the electronic structure of quantum systems in materials is presented.

Def. Electronic correlation is the interaction between electrons in the electronic structure of a quantum system.

Work [8] presents the capabilities of computational physics as a research tool especially and for nano-sized materials. This work has a methodological significance.

Opportunities for observation and measurement of structures of electron microscopy materials are known. At work [9], single atom observation and a specific defect are presented in a 3D aberration-corrected electron microscope, with information being limited to 0.5-Å.

Let us summarize: Fundamental knowledge is needed directly in the details of the market in the particular consideration these are micro-foundries. Knowledge requires specification of the specific requirements for each manufacturer.

3.1 Computational physics in Materialscience

The theory of metals [10] spreads us to the physics of the solid body [5]. The phase transition from the first order creates the structure that carries the working properties of each cast. The description of the first-order phase transition processes requires scientific areas: the classical theory of crystal growth in the present state; quantum mechanics, which is used to describe the chemical bond and structures.

The types of solids according to the chemical bond in the crystal lattice are 5: ionic crystals; valent crystals; metals; molecular crystals. The metallic connection [5]: the crystal lattice is made up of positive ions, the repulsive forces between them being equalized by the free electrons. The description of the chemical bond is obtained after the decision of the amplitude wave equation of Schrödinger we show no relativistic time-dependent (Schrödinger, 1, 2) and time-independent (Schrödinger, 3, 4) view

$$i\hbar\frac{\partial\psi(r,t)}{\partial t}=\left[\frac{-\hbar^2}{2\mu}\nabla^2+V(r,t)\right]\psi(r,t), \quad \text{(Schrödinger, 1 and 2)}$$

$$i\hbar\frac{\partial\psi(r,t)}{\partial t}=\hat{H}\psi(r,t)$$

$$\left[\frac{-\hbar^2}{2\mu}\nabla^2+V(r)\right]\psi(r)=E\psi, \quad \text{(Schrödinger, 3 and 4)}$$

$$\hat{H}\psi(r)=E\psi$$

where ħ - Planck's constant; μ – particle reduced mass; ∇^2 is the Laplacian; ψ is wave function; $\hat{H}$ – Hamiltonian operator; V - potential energy; E – energy of the state ψ.

For real crystals it is necessary to describe the defects [5]: Schottky (1), Frenkel (2) and dislocations (3)

$$p=\frac{Z!}{(Z-x)!x!}, \quad (Schottky) \qquad \text{(Points Defects)}$$

$$x=\sqrt{ZZ'}\exp\left(-\frac{E_2}{2kT}\right), \quad (Frankel)$$

where Z – total number of atoms occupying places in the crystal lattice; Z' – number of gaps in the crystal lattice; p – Schottky's defects; x – Frenkel's defects; E_2 – the energy of the atom to pass from its normal to the intermediate state of the crystal lattice, k and T – Boltzmann's constant and temperature; Degression of ionic crystals from the ideal crystal lattice and the stoichiometric ratio by two parameters [5]: Degree of deviation of ionic crystals from the ideal crystal lattice and stoichiometric ratio by two parameters: μ – degree of deviation of the actual grid from the ideal, ν – degree of deviation from the stoichiometric ratio and criteria for observing the stoichiometric number

$\mu = (Y_M/Z_M+X_R/Z_R) + (X_M/Z_M+Y_R/Z_R)$ (Grid deviation)

$\nu = (Y_M/Z_M+X_R/Z_R)–(X_M/Z_M+Y_R/Z_R)$ (Stoich. ratio deviation)

$\nu = N_M/Z_M – N_R/Z_R$, (Stoichiometric ratio criteria)

where X_M and X_R are the number of cations and anions vacantions; Y_M and Y_R – the number of ions and metal and the metalloid in the gaps; Z_M and Z_R – the total number of metal and metalloid ion sites in the ideal crystal lattice; N_M and N_R – the total number of metal and metalloid ions in the ideal crystal lattice. Example [5]: Let the crystal lattice consist of (m) the number of metals (M) and (r) the number of metalloid (R) ions and the grid composition and that of the molecules of the substance being determined by the formula M_mR_r. (Grid and molecules formula)

In pure ionic relation m/r = p/q, where p and q are the charges of the positive and negative ion in elementary electric charges.

There are various combinations of point defects in crystal crystals of ionic crystals [5]. For example, [5]: anion vacation with a connected electron called the F-center; pair adjacent in the direction [$e_1e_2e_3$] the F-center (M-center); triple adjacent to the plane ($e_1e_2e_3$) the F-center (P-center), etc.

Other defects in the lattices of real crystals are dislocations [5, 10]. This term means a heterogeneous elastic strain centered on a line to explain the plasticity properties of the crystals. The two simplest dislocations are threshold and screw. *Threshold dislocation* [5, 10] is characterized by the presence of an "excess" atomic plane in a part of the crystal lattice. *Screw dislocations* [5, 10]. Crystal in the form of a cylinder with a height H and a radius r is cut in a plane defined by the height ... and the radius ... and is perpendicular to the two bases. Then the two crystal parts are slid against each other along the plane of cut, with the outer parallel to the height side being offset at a distance equal to the Burger's $\vec{b}$ vector. Finally [5], the two parts of the crystal are glued and the outer forces are removed again. As a result, a non-uniform deformation, centered on the center height of the cage, occurs. As a result, a non-uniform deformation, centered on the center height of the cage, occurs. As a result of the screw dislocation the family of parallel crystallographic planes, perpendicular to the axis of the screw dislocation. When only one screw dislocation occurs, growth is due only to it, because it is much more energy efficient. Random dislocations in crystal lattices [5]: In general, the line of dislocation is a random curve, and the "sliding plane" is an arbitrary spatial surface. Dislocation defects: *energy* of dislocations such as a hollow cylinder (Dis. Def. 1), occurrence of *threshold* dislocation (or *movement*) (Dis. Def. 2), *interaction* of two dislocations (Dis. Def. 3)

$$E_S\approx\int_0^{2\pi r_\infty}\int_{r_0}\frac{1}{r^2}rdrd\vartheta=2\pi\ln\frac{r_\infty}{r_0}, \qquad \text{(Dis. Def., 1, 2, 3)}$$

$$F=\tau\vec{b},$$

$$dW\approx(\tau_1+\tau_2)^2=(\tau_1^2+2\tau_1\tau_2+\tau_2^2),$$

where E_S – energy of dislocations; r_∞ and r_0 – outer and inner radius of dislocation; F – force for occurrence of threshold dislocation; τ – the limit voltage required for plastic deformation of the crystal sliding; $\vec{b}$ – vector of Bürges; τ_1^2 and τ_2^2 – the energies of the individual deformations; $2\tau_1\tau_2$ – the energy of their interaction.

Crystal lattice of the alloys [5 and 10]: Metal alloys can be regarded as the simplest chemical compounds. They are solid solutions which can be obtained by replacing the atoms of the crystal lattice of one metal with other metal alloys or by introducing atoms of the second metal between the atoms of the crystal lattice of the parent metal.

The shortest can be said that work [5] is the development of work [10] in the direction of fundamental knowledge of foundry. This is confirmed by the current state of economic development - **the fourth industrial revolution**.

Summary: Fundamental knowledge is needed directly by the market-makers who are the micro-foundries. Knowledge requires specific specification for each manufacturer, which has to be

implemented by a specific infrastructure – such as R. Georgiev's office [14] for transfer of knowledge presented in Fig. 3

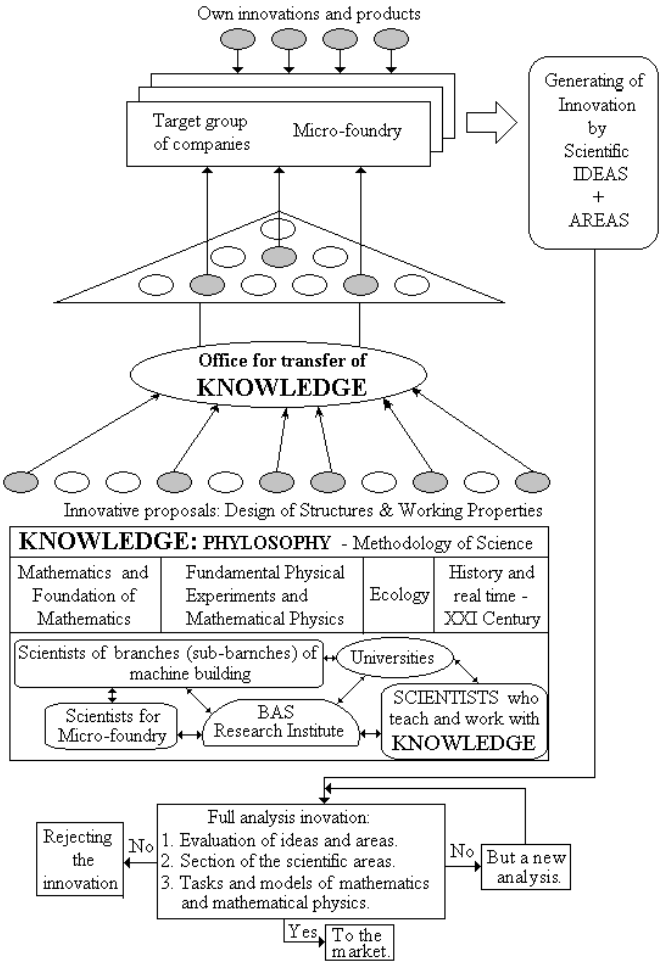

Fig. 3 *Principle scheme of Georgiev's office of knowledge transfer to innovation the subject of cast technology – Design of structures & Working properties. Knowledge: philosophy – methodology of science of: Mathematics and Foundation of mathematics; Fundamental experiments and Mathematical Physics; Ecology; History and real time of XXI century; Scientists, who teach and work with knowledge; Institutions - Universities and thoroughly Researches Institutes of the Bulgarian academy of sciences; Business branches; Office for transfer of knowledge; full knowledge are whites and innovations ideas + areas of our transfer are the grays; Target group of companies; Full analysis of generated innovation – micro-foundry [14].*

Date for phase transition of first order in foundry process:

Experiment and measurements: Alloy composition; Obtaining the alloy – fresh or using secondary alloys; Phase transition process of first order: melting; casting – thinness, degassing; pour temperatures, temperature range transferred to the melt; temperature interval of filling the mold cavity; true phase transition – precise thermocouple measurement of the hardening temperature field; Differential thermal analysis – solidification of the alloy in small volume; obtained polycrystalline structure – micro-, macro-grinding and medium grain diameter; measuring the temperature field of solidification in a large volume – an experimental task of Stefan-Schwarz.

Phase Transition Process of First Generation: Classical Theory of Crystal Growth – Mechanism; Contemporary Description Quantum Mechanics - Postulates; The polycrystalline structure of the cast material: mean grain diameter; Crystal lattice - parameters; A full description of the properties of the solid in the alloy, i.e. the working properties of the castings.

Scientific areas related to the description of the processes of formation of the structures of new phases Meso-level is **Quantum mechanics**. Nano-level are: **Quantum nanoscience** [11] is the research area and the branch of nanotechnology and physics that uses methods of quantum mechanics to the design of new types of nanodevices and nanoscale materials, where functionality and structure of quantum nanodevices are described through quantum phenomena and principles such as discretisation, superposition and entanglement; **Nanomechanics** [12] is a branch of *nanoscience* studying fundamental *mechanical* (elastic, thermal and kinetic) properties of physical systems at the nanometer scale. Nanomechanics has emerged on the crossroads of classical mechanics, solid-state physics, statistical mechanics, materials science, and quantum chemistry. As an area of nanoscience, nanomechanics provides a scientific foundation of nanotechnology.

On the basis of work [14], the data on the micro - foundry are presented on Fig. 4

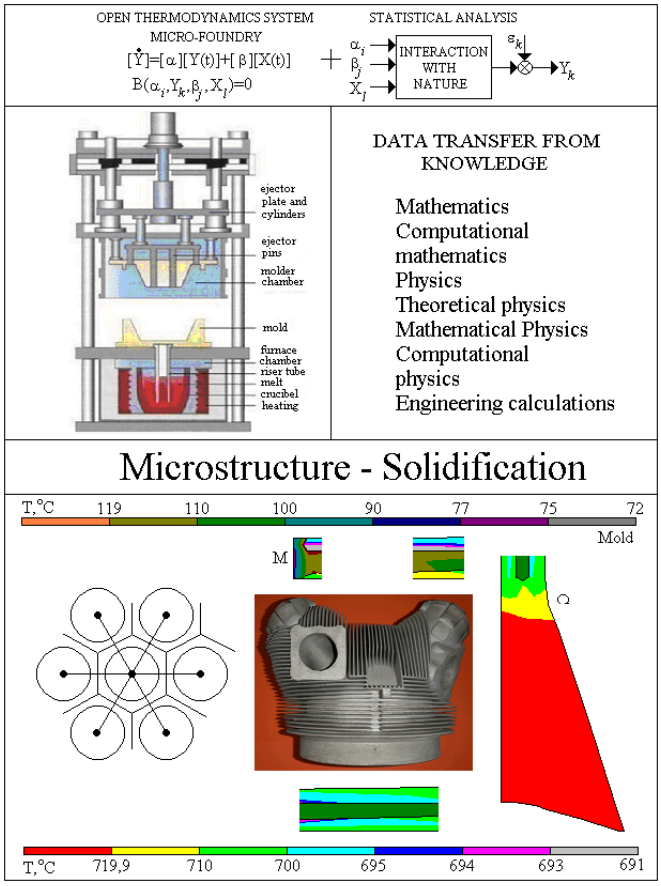

Fig.4 *Date from Knowledge transfer to Ecology–economics complex of "Smart Micro-foundry" for Phase transition of first order in Gas counter pressure casting method – Industry 4*

Micro-foundry is Open Thermodynamics System (OTS) is describe by stochastic differential equation in the subject of Ito – Stratonovich, which introduce transformation input materials and energies flows, where matrixes α_i, β_j – physical and constructive parameters, and i, j =1,…, m; matrixes column X(t), Y(t) – input, output parameters, and k, l = 1,…n; equation B is operator of controllability of OTS, which is support in zero by change of some parameters of control ; Statistical analysis ε_k – ecological complexity interaction micro-foundry with nature , Date transfer from office to micro-foundry.

It is clear that the information interesting for the particular technology should use the infrastructure (see Figure 3) and economic restructuring through serious investments such as the change – INDUSTRY 4.0. Filtering the necessary information is only possible through mathematics.

The methodology is work-based [8]: software for computing physics is continually being created by a new one based on the development of mathematics. Using mathematics to describe the meso-level is working [6, 7 and 8].

An example of the role of mathematics in quantum mechanics is work [13]. From the works [6, 7, 8 and 13] follows that every

question posed by a physical experiment passes a long and complicated mathematical interaction with theoretical and mathematical physics.

Measurements of example structures are works [9 and 15]. It has long been known to see the bottom, according to Feynman [15], the development of measuring instruments follows the development of the necessary technological possibilities, non-standard creation of equipment. A direct example of Bulgarian participation is a work [9], electron microscope with optimized aberration and monochromatic source with high brightness is a significant resolution of the instrument and contrast. Achieved is an information limit of 0.5-Å (angstrom).

Finally, in this paragraph, we need to say that a macro-level (solidification) relation and meso-level (quantum mechanics) is mathematics.

3. Conclusion

Mathematics is a complex technological necessity in the field of education and knowledge transfer infrastructure.

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