Technological first-order phase transition base of foundry and material science

Angel Velikov, Stefan Bushev
Institute of Metal Science, Equipment and Technologies
with Hydro- and Aerodynamics Centre „Acad. Angel Balevski"
67 Shipchenski Prohod Blvd., 1574 Sofia, Bulgaria[2]
Bulgarian Academy of Science, Sofia, Bulgaria[2]
stbushev@abv.bg

Abstract: *Technological first-order phase transition is obtain base process of material science by numerical experiments at use of finite elements method (FEM). The history of movement and the geometry of the front in the first-order phase transition are investigated. A free first-order phase transition was investigated to estimate the local place of the liquid residue. Mathematical model is Stefan-Schwartz task in 3D case. The corresponding temperature fields of a free and technological first-order phase transition are presented. Engineering information is local phase transition conditions is shown of macro-level with the local transition time and volume at the front is assumed.*
Keywords*: STEFAN-SCHWARTZ TASK, 3D FEM, FREE AND TECNOLOGICAL FIRS-ORDER PHASE TRANSITION*

1. Introduction – fundamentals processes of material science

Some of the basic processes of material science are phase transitions [3, 5, 7, 12, 16, 17, 18 and 19]. Our institute has been developing technologies and equipment for foundry production for more than 40 years on the basis of the Angel Balevski and Ivan Dimov method for injection molding (certificate No.187 / 1961 y. P. 181 [12]). The gas counter-pressure casting method allows precise volume and surface formation of castings [12]. Investigation of gas-, hydro- and thermodynamic processes in conditions of gas counter pressure casting and their influence for controlling the formation of castings [7, 12].

On Fig. 1 is shown the base geometric diagram of the casting process by the method of the „GP"[19]:

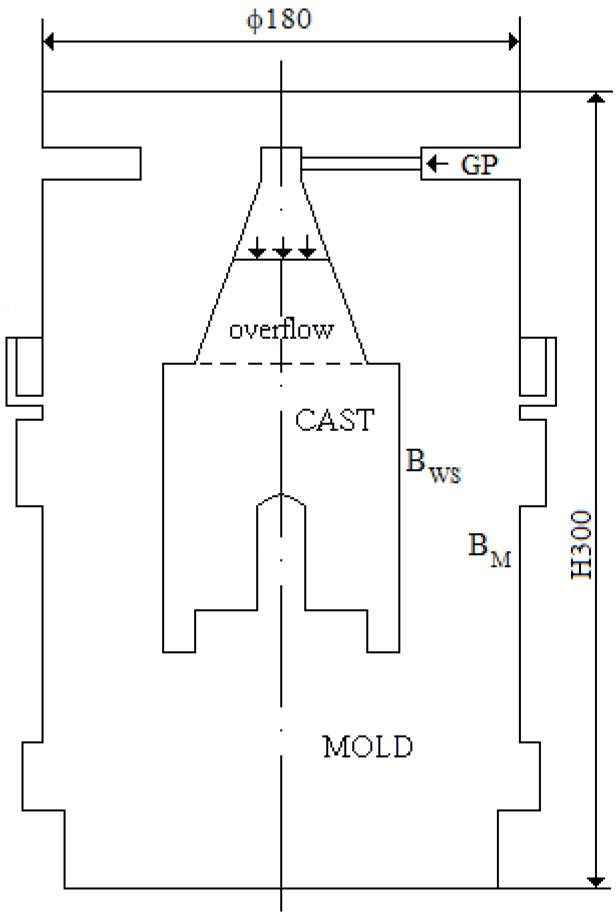


Fig. 1 *Geometrical diagram of open thermodynamics system (OTS): Mold and cavity for Cast and overflow with overall dimensions diameter ϕ = 180 mm and height H = 300 mm. The volume $\boldsymbol{V_{SYS}}$ is the sum of cast volumes of liquid $\boldsymbol{V_{CL}}$, surface front $\boldsymbol{S_{Front}}$ and solid $\boldsymbol{V_{CS}}$ phases, mod volume $\boldsymbol{V_M}$ with it boundary surfaces $\boldsymbol{B_{WS}}$ and $\boldsymbol{B_M}$.*

The casting method „GP", the first-phase phase method runs under high gas pressure [19].

The mathematical base of the casting is mathematical tasks of Stefan [1] and Schwartz [2]. The open thermodynamic system (OTS) of Fig. 1 is:

$$\boldsymbol{V_{SYS} = (V_{CL} \cup S_{Front} \cup V_{CS}) \cup B_{WS} \cup (V_M \cup B_M)}$$

The task of Stefan-Schwartz in 3D for numerical investigation by Finite Different Method, Finite Elements Method and so on is:

- Equation of the heat conductivity:

$$\boldsymbol{(c + SFQ_m)\frac{\partial T}{\partial t} = \lambda \Delta T} \quad \text{in } \boldsymbol{V_{SYS}}, \qquad (1, 1)$$

- Stefan's boundary condition (S_F):

$$\boldsymbol{-\lambda_L \nabla T_{L|S_F} = \rho_S R Q_m - \lambda_S \nabla T_{S|S_F}}, \qquad (1, 2)$$

And growth velocity of solid phase:

$$\boldsymbol{R = \left[\lambda_L \nabla T_{L|S_F} - \lambda_S \nabla T_{S|S_F}\right] / \rho_S Q_m}, \qquad (1, 2, 1)$$

- Boundary condition at the mold's work surface (B_{WS}):

$$\boldsymbol{-\lambda_C \nabla T_{C|B_{WS}} = \alpha_{B_{WS}}\left(T_{C|B_{WS}} - T_{M|B_{WS}}\right) = -\lambda_M \nabla T_{M|B_M}}, \qquad (1, 3)$$

- Boundary condition mold-environment (B_M):

$$\boldsymbol{-\lambda_M \nabla T_{M|B_M} = \alpha_{B_M}\left(T_{M|B_M} - T_{En}\right)}, \qquad (1, 4)$$

- Initial conditions at t = 0:

$$\boldsymbol{T_L(x, y, z, t) = const_L, T_M(x, y, z, t) = const_M}, \qquad (1, 5)$$

where T is the temperature with indexes for the cast (C) liquid (L) and solid (S) phases and mold (M); $\mathbf{V_{SYS}}$ is the sum of cast volumes of liquid $\mathbf{V_{CL}}$, surface front $\mathbf{S_{Front}}$ and solid $\mathbf{V_{CS}}$ phases, mod volume $\mathbf{V_M}$ with it boundary surfaces $\mathbf{B_{WS}}$ and $\mathbf{B_M}$. the thermophysical coefficients of the (OTSF) are: thermal conductivity (λ), thermal capacity (c), density (ρ); S_F is function of the heat source, Q_m is latent heat of the melting at the melting temperature T_m.

The mold (Fig. 1) is for "GP" casting method [19], in which the cast is formed under high gas pressure. The study of temperature changes in operation [19] was made using the MAGMAsoft software package. The solution of Stefan-Schwartz task is for maximum heat transfer: coefficient of heat transfer α = 56000 w/m^{2}sK at the mold boundary $\mathbf{B_{WS}}$ and $\mathbf{B_M}$; mold initial temperature T_M(x, y, z, 0) = 72^o C is introduce on Fig.2, where the initial temperature of the mold and the temperature field of the first-order free phase transition at a time are shown The technological model of eq.(1) is solved by using a software package of (FEM) created at our institute of M. Dimitrov and S. Bushev.

The purpose of this work is to consider the phase transition of the first order of basic process in foundry.

2. Free process of first-order phase transition in foundry

*A free first-order phase transition process in the casting process is carried out by **uniform and constant heat exchange** throughout the working and external surfaces of the mold.*

In Fig. 2 is shown cross section of car wheel formation at FREE first-order phase transition

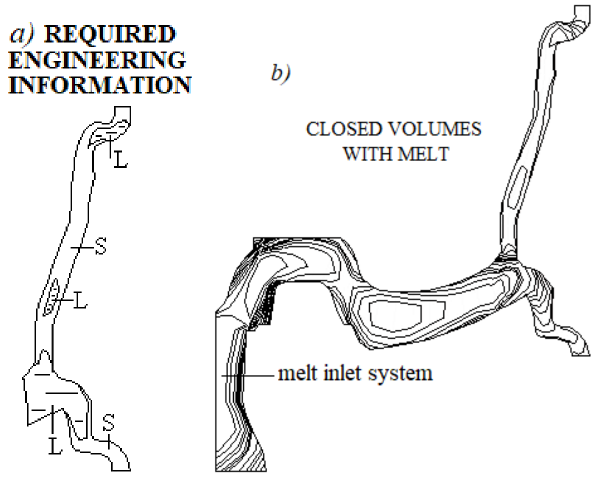


Fig. 2 *Methodology of the example of the car wheel formation at free first-order phase transition and heat unit (closed volumes with melt): a) ice cast [20]; b) history of phase transition of Al [21].*

A major engineering interest (Fig. 2) is the temperature field of a first-order phase transition is the location and geometry of the interfacial surface [1, 2, 3, 5, 7 and 12] separating the volumes of the liquid and solid phases in the formed cast. In Fig. 3, the initial temperature of (OTC) and the temperature field of a free first-order phase transition with the front (zone) of phase transformation at time t = 0, 6475 sec are presented:

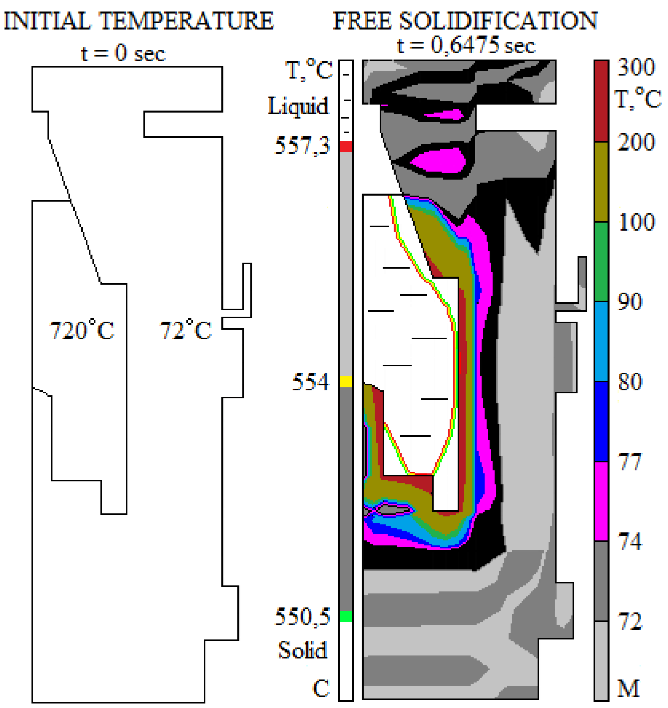
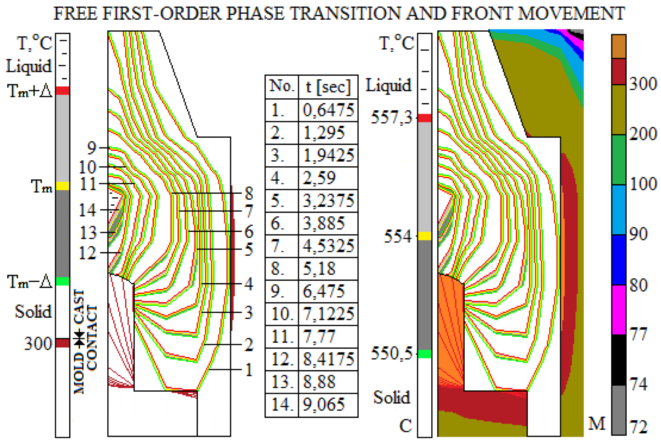
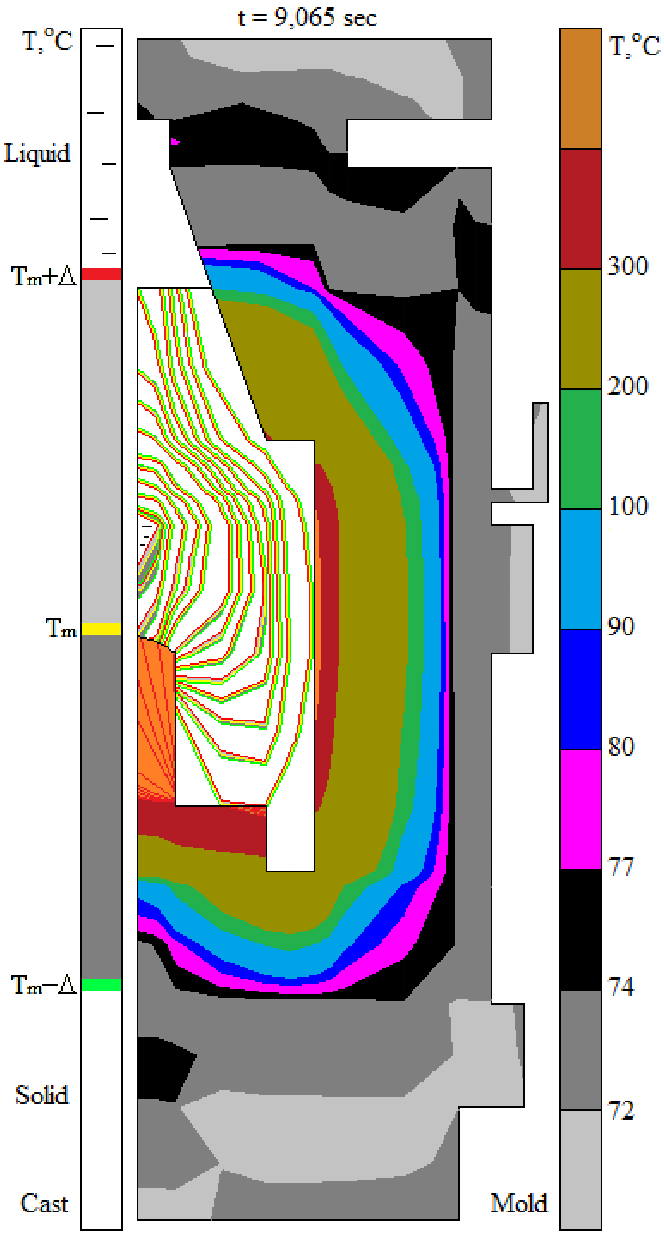


Fig. 2 *Initial (OTC) casting temperature and shape with a temperature field of free first kind of phase transition at time t=0.6475 sec together with the volumes of liquid and solid phases separated by the phase transition front (zone).*

The correct engineering answer is the history of the phase transition front (zone) movement from free first-order phase transition in the time is present:



a)



b)

Fig. 3 *Initial condition and a temperature field of free first-order phase transition in the end time t = 9,065 sec of numerical experiment: a) history of the movement boundary phase transition front (zone) with 14-in transition; table with 14-in times; the temperature field in a little layer at the mold work surface contact; b) full temperature field of the system at the end time = 9,065 sec of the numerical experiment.*

The overflow does not fulfill its purpose.

3. Technological first-order phase transition in foundry

In Fig. 4 is the methodology for a technological first-order phase transition based on [20]:

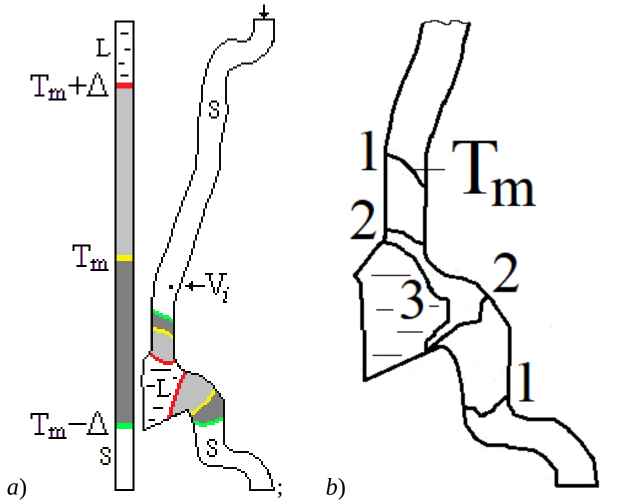


Fig. 4 *Technological first-order phase transition in foundry [20]: a) ↓ is cooling place; the volumes of liquid (L) and solid (S) phases separated by the phase transition front (zone) (T_m-Δ, T_m, T_m+Δ) with removable of thermal unit; V_i is micro-volume; b) sketch for work [20] history of movable isothermal surface (front) T_m in tree time 1, 2, 3 at technological removal of thermal unit.*

The basic purpose of the foundry methodology is to move the front of a first-order phase transition: from a cold region to a warm region without closed liquid volumes. Here (see Fig. 1) we have an overflow whose volume must to finish the first-order phase transition in the warm overflow. On Fig.5 we used initial temperature of the mold:

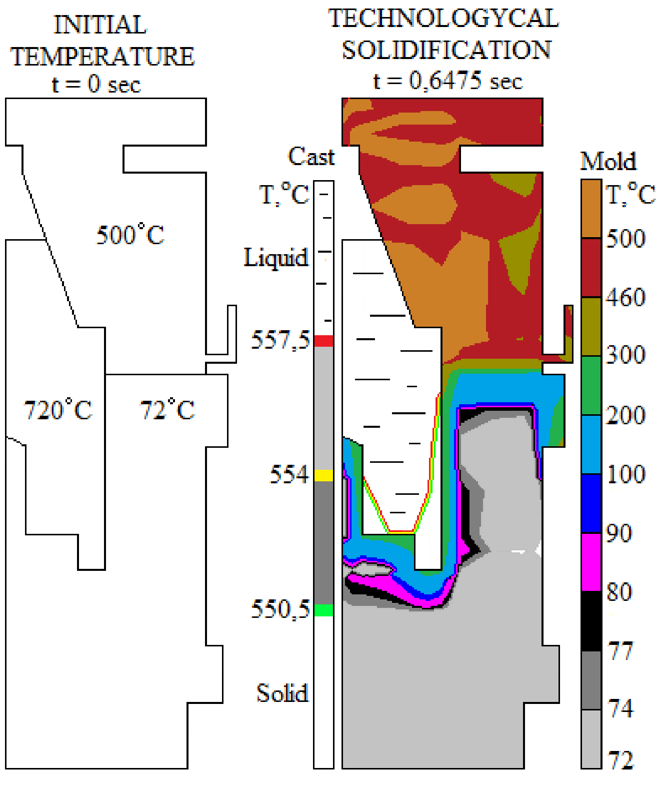
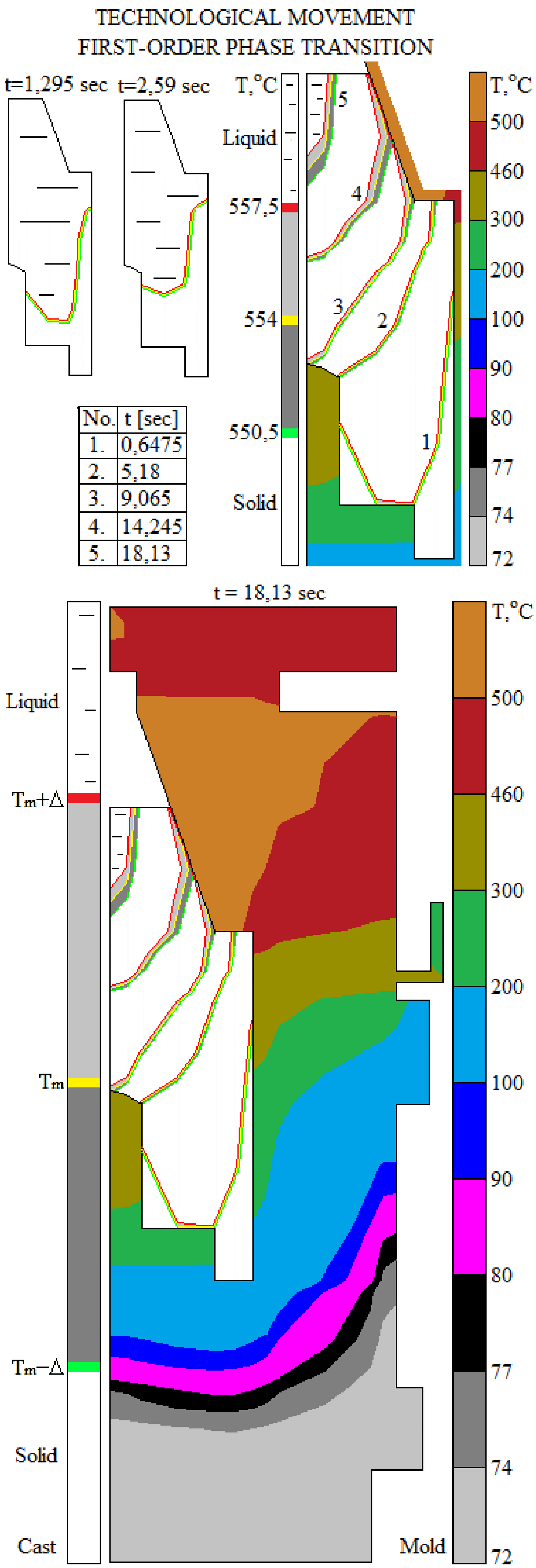


Fig. 5 *Initial temperature of the mold is of two area cold with 72° C and hot – 500° C. In hot part of the mold is located the overflow. The temperature field of the OTS in the time t = 0,6475 sec.*

The numerical experiment is the same - the history of the motion of the first-order phase transition front and is presented in Figs. 6:



No.	t [sec]
1.	0,6475
2.	5,18
3.	9,065
4.	14,245
5.	18,13

Fig. 6 *History of the front moving the first-order phase transition:*

a) detailed history of front moving and ***is ending in the overflow volume****; the last temperature field at the contact surface cast/mold; b) the last temperature field of the OTS in the time t = 18,13 sec.*

From Fig. 6 follows that the overflow in the hot area of the mold we have technological first-order phase transition and is ending in the overflow volume.

4. Technological first-order phase transition – cast structure

Engineering information [6, 3, 5, 7, 9, 12] from calculated *front* of first-order phase transition is: geometry, thickness, correlation volume V_i, characteristic time τ_{ch} (or local t_f) of phase transition on Fig. 7:

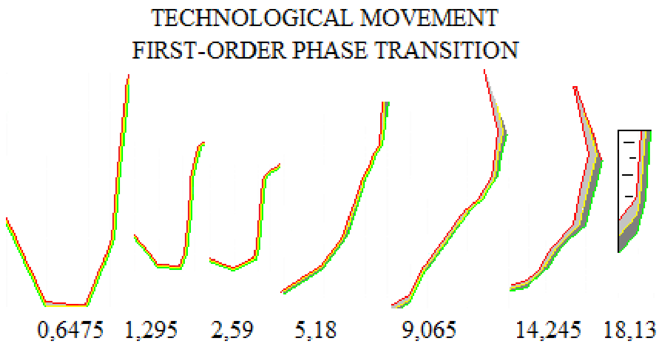


Fig. 7 *The history of the technological first-order phase transition and local difference between the two temperatures T_m-Δ and T_m+Δ in the fronts at: 0,6475sec; 1,295sec; 2,59sec; 5,18sec; 9,065sec; 14,245sec; 18,13sec;*

$$t_f = \Delta\mu / R\nabla T_{S|Front}, \qquad (2, 1)$$

$$\tau_{ch} = V_i^{2/d} / D = \Delta\mu / R\nabla T_{S|Front} = t_f, \qquad (2, 2)$$

where Δμ is thermodynamic driving force; d = 1, 2, 3; D is Diffusion coefficient. The volume V_i we suggest it to be considered as a cell needed to work with the CASTEP [22] software product, which is available for crystallization processes. CASTEP is software to perform calculations on the first principle of quantum mechanics for the study of the properties of the crystal surfaces in the solid state [22]. This software can calculate five tasks: energy; geometry optimization; molecular dynamics; elastic constants; study of transition-state [22]. The task of CASTEP – study of transition-state is connect with [3, 5, 6, 7, 9, 11, 12, 20 and 21]. Elastic constants task of CASTEP is connect with [8]. Technological first-order phase transition is two levels: 1. Macro-level Stefan-Schwartz [1, 2] and eq. (1) and eq. (2); 2. Meso-level [4, 6, 10, 13, 14, 15].

Stefan-Schwartz problems and CASTEP software covered theoretical and applied material science [16, 17 and 18].]. From all of this it follows that even the smallest family foundry requires scientific support based on the Stefan-Schwartz problem and [1 and 2], which can be provided by a relevant industrial branch, such as MACHINE BUILDING.

. Conclusion

The technological process of a first-order phase transition is obtained at the macro-level based on the history of geometry and the movement of its front. A local volume is defined at the front to describe this transition and at meso-levels using CASTEP software.

6. References

1. J. Stefan. ¨ Uber die verdampfung und die aufl¨osung als vorgüange der diffusion. Annalen der Physik und Chemie, 277(12):725–747, 1890.
2. C. Schwarz, *Arch. Für Eisenhüttwesen*, H. 3, p. 139- 148, Sept. 1931.
3. A. Balevski, Metal science, Technics, Sofia, (1962) (In Bulgarian)
4. M. Borisov, K. Marinova, Introduction to Solid State Physics 1, Science and art, Sofia, 1977. (In Bulgarian)
5. M. Flemings, Solidification processing, Peace, Moscow, 1977. (In Russian)
6. Enrico Fermi, Thermodynamics, Prentice-Hall, New York, 1937, second stereotype edition, Publishing House of Kharkov University, 1973. (In Russian)
7. S. M. Bushev, Thesis of PhD Controllability problems of crystallization process in casting, Technical University – Sofia, 1993.
8. S. Vodenicharov, Dynamic destruction of metal structures, Bulged Ltd. ISBN 978-954-92552-3-2
9. A. S. Maneva, Thesis of PhD Investigation of the structure and properties of castings of under eutectic aluminum alloys as a function of the ratio of primary and secondary alloys, Technical University – Sofia, 1993. (In Bulgarian)
10. Ts. Uzunov, Physics of metals, Technical University, Sofia, 2004.
11. I. M. Parshorov, Thesis of Dr.Sc. Processes and conditions associated with dynamic relaxation in alloy martensite, Technical University, Sofia, 2001.
12. Y. Arsov, E. Momchilov, K. Daskalov, G. Bachvarov, Theoretical and technological fundamentals of gas counter-pressure casting, "Prof. M. Drina" Acad. Pub. House, Sofia, 2007.
13. G. Schulze, Metallphysik, Peace, Moscow, 1971. (In Russian)
14. J. Blakemore, Solid state physics, Metallurgy, 1972. (In Russian)
15. Ch. Wert, R. Thomson, Physics of solids, Peace, Moscow, 1960. (In Russian)
16. W. D. Callister, Jr. D. G. Rethwisch, Fundamentals of materials science and engineering an integrated approach 3 Ed., John Wiley & Sons, Inc. 2008.
17. W. D. Callister, Jr. D. G. Rethwisch, Material science and engineering 9 Ed., John Wiley & Sons, Inc. 2014.
18. J. Campbell, Complete Casting Handbook, Butterworth-Heinemann, 2011.
19. Georgiev G., Velikov A., Stanev S. Maneva A., Thermal processes for the formation of aluminum casting by the method "GP", XXII International Scientific Technical Conference „FOUNDRY 2015“, 16.-17.04.2015, Pleven, Bulgaria. ISSN: 1310-3946 (In Bulgarian)
20. S. Bushev, N. Miloshev, G. Batchvarov, L. Stanev, M. Dimitrov, N. Stoichev. Analysis of a Real casting Solidification Under Different Cooling Conditions. Proceedings of the 12th International Metallurgy & Material Congress and Fair, 28.09.-01.10.2005, Istanbul, Turkey, 2007-2014.
21. A. Maneva, S. Stanev, S. Bushev, M. Georgiev, Low pressure casting micro-foundry – investigation of the care wheels, International Journal „NDT Days“, vol. I, Issue 1, Year 2018. ISSN: 2603-4018
22. www.castep.org