MATERIALS – ADDITIVE KNOWLEDGE PROPERTIES AND TECHNOLOGIES

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Abstract: Two tasks are enumerated: a task of hardening spheres with a radius of 50 nm and a task of crystallization - the underlying kinetic equation of formation of new phases. These tasks are rational bridges for multi-scale approach.

Keywords: ADDITIVE MANUFACTURING GAS COUNTER-PRESSURE, „CORRELATION VOLUME“, 3D PRINTING

1. Introduction

Definition of the thermodynamics: Thermodynamics (from Greece) [1] is called the general science of energy dealing with the relationship between heat and mechanical energy and heat transformations at work and vice versa. The purpose of the article in [1] is to show the application of the two general principles (1) the Joule’s Law on Heat and Work Equivalence, and (2) the Carnot principle that the efficiency of a reversible engine depends only on the temperatures between which it does work;

The main content of thermodynamics - this is a description of the conversion of heat into work and, conversely, the conversion of mechanical work into heat [2]; Thermodynamics: the science that deals with heat and temperature and their relationship to energy, work, radiation, and the properties of the bodies of matter [3]. The main meaning in all definitions is preserved, which is an example of accurate knowledge.

The classical thermodynamics presented in the essay of Table 1:

Table 1: Thermodynamics [1, 2, 4, 6]

| 1. LIQUID IS HOMOGENEOUS OR HETEROGENEOUS OPEN THERMODYNAMICS SYSTEM; 2. PARAMETERS: VOLUME V, PRESSURE PARAMETERS P, TEMPERATURE T AND AGGREGATE STATE, 3. FOR A SUBSTANCE VARIABLES V, P, T AND ARE NOT INDEPENDENT BUT ARE CONNECTED IN THE STATE EQUATION \( f(p, V, T) = 0 \) AND THE SOLUTION FOR EACH VARIABLE IS A FUNCTION OF THE OTHERS TWO; 4. EXTENSIVE QUANTITIES ARE: VOLUME \( v \), MASS \( m \), ENERGY \( U \), ENTROPY \( S \), ENTROPY \( S \), ENTROPY \( S \), BECAUSE THEY ARE PROPORTIONAL TO THE QUANTITY OF MATTER. INTENSIVE QUANTITIES ARE: DENSITY \( \rho = \frac{n}{V} \) AND TEMPERATURE T, WHICH DO NOT SATISFY WITH THE CONDITION OF EXTENSIVE; 5. ANALYSIS APPROACH THE HETEROGENOUS SYSTEM IS DISTRIBUTED AT THE END OR EXTREME NUMBER OF HOMOGENEOUS VOLUMES (PARTS). 6. THE STATE OF THERMODYNAMICS EQUILIBRIUM OF A SYSTEM IS SIMULTANEOUSLY THE THREE THERMAL, MECHANICAL, AND CHEMICAL EQUILIBRIUM, THE DYNAMICALY-THERMODYNAMIC STATE IS A COMBINATION OF DYNAMIC STATES THROUGH WHICH THE SYSTEM RAPIDLY MIGRATES AS A RESULT OF MOLECULAR MOVEMENT, 7. THE SYSTEM HAS A STEADY EQUILIBRIUM WITH A MINIMUM OF FREE ENERGY; 8. THE CONVERSION OF THE SYSTEM STATUS IS EXCHANGED UNDER AN INCREASING RANGE OF INTERMEDIATE CONDITION. THE REVERSIBLE TRANSFORMATION IS WHEN THE ARRAY OF INTERMEDIATE STATES ARE INFINITELY CLOSE TO THE EQUILIBRIUM; 9. INTERNAL ENERGY \( U \) IS THE SUM OF: THE TOTAL KINETIC ENERGY \( \sum_{i} E_{kine} \) OF THE MOVEMENT OF MOLECULES AND THE FULL POTENTIAL ENERGY \( \sum_{i} E_{pote} \) OF ELECTROMAGNETIC INTERACTION KEEPS THE ELECTRONS IN THE ATOMS AND CONNECTS THE ATOMS IN MOLECULES AND CRYSTALS U = \( \sum_{i} E_{kine} + \sum_{i} E_{pote} \).|

10. LAWS OF THERMODYNAMICS: ZERO LAW: IF THERMODYNAMICS SYSTEM A IS IN THERMODYNAMIC EQUILIBRIUM WITH SYSTEM B AND IN TURN SYSTEM B IS IN THERMODYNAMIC EQUILIBRIUM WITH SYSTEM C, THEN A AND C ARE ALSO IN THERMODYNAMIC EQUILIBRIUM. PHYSICAL PRINCIPLE EXPRESSING THE TRANSITIVITY OF THERMODYNAMIC EQUILIBRIUM AND DEFINING TEMPERATURE, FIRST LAW: THE CHANGE IN THE INTERNAL ENERGY \( U \) OF A THERMODYNAMIC SYSTEM IN AN ARBITRARY THERMODYNAMIC PROCESS WITH INITIAL AND FINAL STATE IS EQUAL TO THE QUANTITY OF HEAT Q INPUT OR OUTPUT FROM THE SYSTEM AND THE OPERATION W PERFORMED ON THE SYSTEM \( \Delta U = Q + W \) OR \( \Delta U = \mu + pV \). CHANGE BETWEEN TWO EQUILIBRIUM STATES: CLOSED SYSTEM \( \Delta E = \Delta H_{eq} + \Delta P_{eq} + \mu \Delta N + \mu_{N_{A}} \), WHERE MASS \( m \), MASS \( m \), MASS \( m \), WHERE MASS \( m \), MASS \( m \), MASS \( m \), MASS \( m \), MASS \( m \), MASS \( m \), MASS \( m \), MASS \( m \). |
22]. is the extended form of I. Prigogine's second law of thermodynamics [18] in the view:

\[
\text{Entropy of OTS} = \left[ \frac{\text{Internally entropy production of irreversible processes}}{\text{Time}} \right] + \left[ \frac{\text{Externally entropy flow by Interaction OTS with environment}}{\text{Time}} \right] = \frac{dS}{dt} = \frac{dS_{\text{mix}}}{dt} + \frac{dS_{\text{ex}}}{dt}.
\] (1)

The thermodynamic driving force \( \Delta \mu > 0 \) of the phase transition of first order and at crystallization of melts [15, 16, and 17]

\[
\Delta \mu = \Delta S_m(T_m - T).
\] (2)

Where \( T_m \) – the temperature of phase transition. Temperature of undercooling is defined from Stefan’s problem. The work \( W_n \) for the formation of n-atoms complex in the system \( \Delta V \) under the influence of the case eq. (2) we have

\[
W_n(\Delta \mu) = -n\Delta \mu + F_n(\Delta).
\] (3)

For description the nucleation and growth we use fundamental kinetic equation phase transition of Kashchiev [30]. It expresses a balance between the distribution function \( Z_n(t) \) of new phase complex of n-atoms and its total change \( dZ_n(t)/dt \)

\[
\frac{dZ_n(t)}{dt} = \sum_{m=1}^{n} \left( f_{nm}(t)Z_m(t) - f_{mn}(t)Z_n(t) \right) + \kappa_n(t) - L_n(t) \text{ at } t \in [0, t_f].
\] (4)

With a suitable definition of the transition frequencies \( f_{nm}(t) \) the equation (4) is valid not only for the initial stage of nucleation, but also for coagulation from unified point of view. The general number \( N(T) \) of the over-nuclei complex in the subsystem \( \Delta V \) is obtained. So as the rate of nucleation \( J(t) \)

\[
N(t) = f[Z_n(t)], J(t) = \frac{d[N(t)]}{dt} \text{ at } t \in [0, t_f].
\] (5)

The equations (2–5) introduce the phase transition of first order of the three levels [31]. The local function

\[
\sigma_5 = F[N(t), J(t)] \text{ at } t \in [0, t_f].
\] (6)

We separate the volume of the open thermodynamic system in macroscopic cells \( \Delta V_i, i = 1, \ldots, N \) and the phase transition of first order is

\[
\sigma_5 = \sum_i \frac{d_3}{2t_i}, \text{ for time: } t = \sum_i t_i.
\] (7)

Thus with eq.(7) a generalized model of phase transition of first order in the complex casting process is present.

In order to have a technology we can reproduced in every local volume \( \Delta V_i \) degradation of energy and condition.

\[
\sigma_5 \leq J_i(t) \text{ at } t \in [0, t_f].
\]

The functional relation between kinetic motion and velocity of crystallization \( V_{\text{sys}} \) is driving force of crystallization \( \Delta T_k \) at three growth mechanisms: 1. 2D nucleus formation \( V_{\text{sys}} \sim \Delta T_k \); 2. through screw dislocation \( V_{\text{sys}} \sim \Delta T_k \); 3. Continuous growth \( V_{\text{sys}} \sim \Delta T_k \). Character macro- and micro-scales on the base of \[11\] in \[8 and 9\] is obtained:

\[
\Delta v_{\text{corr}} = d_{\text{corr}} \Delta T_k = \theta \Delta T_k / d = 1, 2, 3
\] (8)

where \( \Delta v_{\text{corr}}, d_{\text{corr}} \) are correlations scales and local characteristics volume and time \( \tau_{\text{ch}} \) d is growth directions; and from \[2\] we accept

\[
\tau_{\text{ch}} = t_f \sim \Delta T_k / D = 2 \mu / \Delta T_k V_f,
\] (9)

where \( D, \Delta T_k, V_f \) are coefficient of diffusion, locals temperature gradient and velocity of solidification. On Fig.1 present gas counter-pressure technology.
2. Materials science in foundry – sciences and technologies

Bridge to unite science and technology in materials science is the basic process - the phase transition of the first order is the fundamental task at foundry Stefan-Schwarz problem (St-Sch) Fig. 2 and 3 are shown the choice of $\Delta \theta_{corr}$ and $\tau_{ch}$ two bridge tasks: solidification of spheres with radius 50 nm and solution of eq.(4)

![Graph showing solidification and solution processes](image)

**Fig. 2.** Determination of correlation volume $\Delta \theta_{corr}$ and characteristic phase transition time $\tau_{ch}$ of first order. We use a multi-scales approach.

**Fig. 3.** Additive manufacturing gas counter-pressure casting machines: Castings with simple geometry and final operation with 3D printer.
From Fig. 1, 2 and 3, the correlated volume and the characteristic phase transition time \(\Delta t_{\text{corr}}\) and \(\tau_{\text{nd}}\) we take for a drop size of a 3D printer. This way we can preserve the capabilities of the machines, technologies and materials of our institute. Tasks for solidification of spheres with a radius of 50 nm are key, and the solution of eq.(4) represents the number of nuclei-forming particles. This information is very close to the actual structure of the material. Using quantum mechanics allows you to get complete information about the real structure i.e. the properties of the material.

The multi-scales approach by the bridge tasks of solidification and crystallization are shown interacts with thermodynamics [1, 2, 3, 4, 5, 6]; material science [12, 13, 14]; synergy and methodology of science [18, 19, 20, 21, 22]; metal science [8, 9, 11]; metallography [23]; solid state physics and quantum physics [7, 10, 24, 29]. By choosing a correlation volume, phase transition conditions [25, 26, 27, and 28] allow to transfer through a 3D printer.

### 3. Conclusions

Bridged tasks such as solidification a sphere with a radius of 50 nm and a crystallization task are selected.

Nano-scale and number of nuclei-forming particles are robust scientific and technological tools in multi-scale approach and additive production.

An additive manufacturing methodology is created by choosing a drop size for a 3D printer.

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