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THE DYNAMIC STRUCTURE PLOTTING DURING EXPERIMENTAL RESEARCH INTO THE BEHAVIOR OF SYSTEMS WITH COMPLEX ORGANIZATION

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The paper presents holistic approaches for experimental data processing during research into the behavior of a complex system of self-propagating high-temperature synthesis such as the Metal1 – Metal2 – Nitrogen system. The holistic approach takes into account that the combustion characteristics during self-propagating high-temperature synthesis are the characteristics for a high temperature chemical environment with heterocatalytical processes. Dissipative structures are plotted on the basis the following factors: analogies with well-known types of phase portraits, using known invariants, and observance of symmetry.

Keywords: self-propagating high-temperature synthesis, chemical environment, dissipative structures, phase portraits.

Introduction

By the present time, the main principles of a new approach for investigation of complex systems have been thoroughly developed [1,2,3]. The main point is to understand that the properties of a particle, small part, and subsystem do not correspond to the properties of all system consisting of the parts under study. Studying a subsystem, it is not considered an interaction and self-matching of all parts, which cause absolutely unexpected new properties on macrolevels. Although this fact is obvious, nevertheless, it is widely used the research methods that divide the system into the smallest parts to investigate processes taking place on the surfaces of nanosized formations, considering that it will help to understand the mechanism of processes in the whole macrosystem comprising the set of these formations. Series of standard experiments are still conducted when only two parameters are varied and the others are constant. Firstly, it is complicated to realize such constancy, and secondly, all other "constant" parameters vary during the interaction and changing initial parameters.

By using the holistic approach, the system is studied as a whole, not in parts. For graphical plotting the experimental points are plotted on a two-dimensional surface with co-ordinates XY obtained for different variations of external (and internal) parameters, i.e., more then 5-6 parameters in different variations correspond to each point (XY). These 5 - 6 parameters are not the constants for each point, and have the values determined by self-matching of other parameters. The points on the plot are placed chaotically, especially on small scales. Therefore, there is a need to plot experimental phase portraits (for dynamic, dissipative structures) on large scales, not less then 1/2 of A4. All the points in this imaginary chaos form a series of trajectories; in addition the constant value of a parameter corresponds to each point of one trajectory. The whole sum of trajectories forms a strictly ordered structure.

According to the classics of a new scientific paradigm, the freedom degree and values of critical fluctuations are low in the system with complex organization. Therefore, a very small departure from the equilibrium position along a trajectory can be admitted. If the values of fluctuations are higher than the critical values, «a condition point» (experimental point) "jumps" on the other trajectory, that reflects the random nature of the process but with the rigidly programmed quantity of trajectories and their location in the chosen system of coordinates. It is a harsh law of evolution. Therefore, the developed methods of averaging are not used in the holistic approach. We consider that standardization of experiments and averaging of received data are often absurd, unnecessary, and take too much time and material resources. It is possible to conduct thousand experiments for nonlinear systems, and receive less than 40 – 50 significant experimental points. Similar results were received by Stoems [4].

Results and discussion

Systems with complex organization have been studied for a long time and in different fields of science. Diagrams are often plotted in XY coordinates and represent a series of parabolas or other functional curves. Each curve is plotted for the one chosen parameter. It often reminds a dissipative structure in the form of a "knot".

SHS systems are the very convenient systems to obtain the regularities for plotting of dissipative structures. In particular, it is the «Ti - Mo - N» SHS system. The chemical reaction proceeds layer-by-layer along the porous sample. Each point on the plots corresponds to a separate experiment, i.e. new filling, mixture pressing, firing by a spiral and burning in a reactor under nitrogen up to the product formation in the whole sample. The relative density and initial structure were varied, and the combustion rate was measured.

Fig. 1 represents the plot constructed according to the "classical" principles described above. Figure shows the combustion rate versus an initial density for several compositions. Next we fit curves to the standard experimental curves. We removed all the points located far from an equilibrium curve and obtained as a result of an inaccurate experiment. It is observed the intertangling of curves. We deeply analyzed the plot presented in Fig. 2 that was constructed for all the points without any exceptions and averaging.

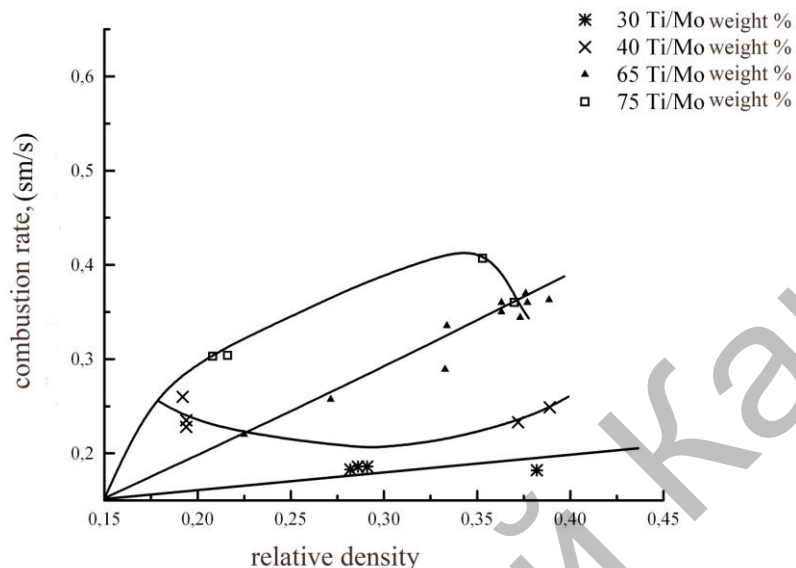


Fig.1. Graphic chart of combustion rate as function of relative density for same compositions of start mixture

We found out that the compositions chosen as invariants of a constant variable did not combine in the one curve representing the combustion rate versus a relative density. However, the points from different compositions formed the single curve for which it was necessary to search its invariant. The search of a new invariant was an important point to understand the physics of processes in a combustion wave. Each trajectory was found to correspond to the same formula of intermediate nitrides of molybdenum. It should be noted that we reduced all curves in Fig. 2 to the origin of coordinates $y=0.10$; $x=0.15$. This origin of coordinates corresponds to the actual limits of combustion in our experiments. According to the rules of synergetics, trajectories in a dissipative structure are directed toward a balance point (attractor) mostly with zero coordinates.

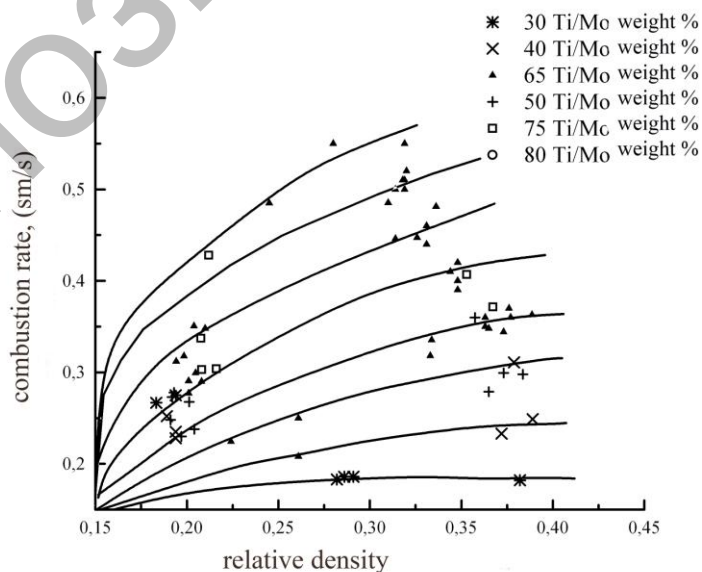


Fig.2. Reflection of condition of chemically active environment of combustion wave for Mo-Ti-N, system with different start compositions for coordinate space “combustion rate - – relative density” with point attractor $(x,y)=0$

For plotting of a dissipative structure with found invariants we chose the coordinate space with a scale of the abscissas, starting with zero. As is seen from Fig. 3 the points were located on the straight lines converging in the origin of coordinates. Each straight line had its invariant K_i that was equaled to the atomic ratio of absorbed nitrogen to atoms of molybdenum.

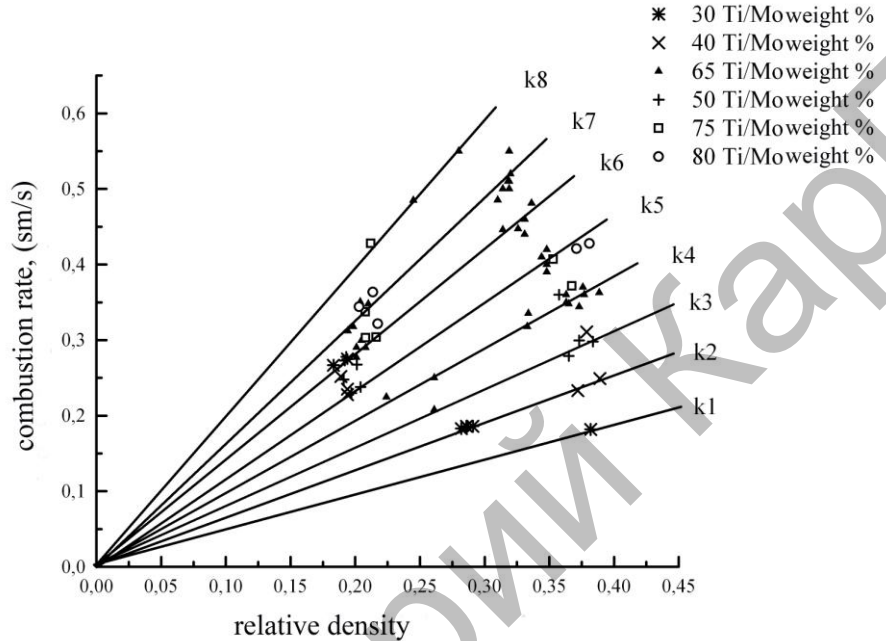


Fig.3. Dissipative structure of chemically active environment of combustion wave with point attractor $(x,y)=0$. Each straight line had its invariant $K_1 - K_8$

In the same system of coordinates, the values of experimental combustion rate were combined and another invariant was found, in particular, the values of conversion degree (Fig. 4).

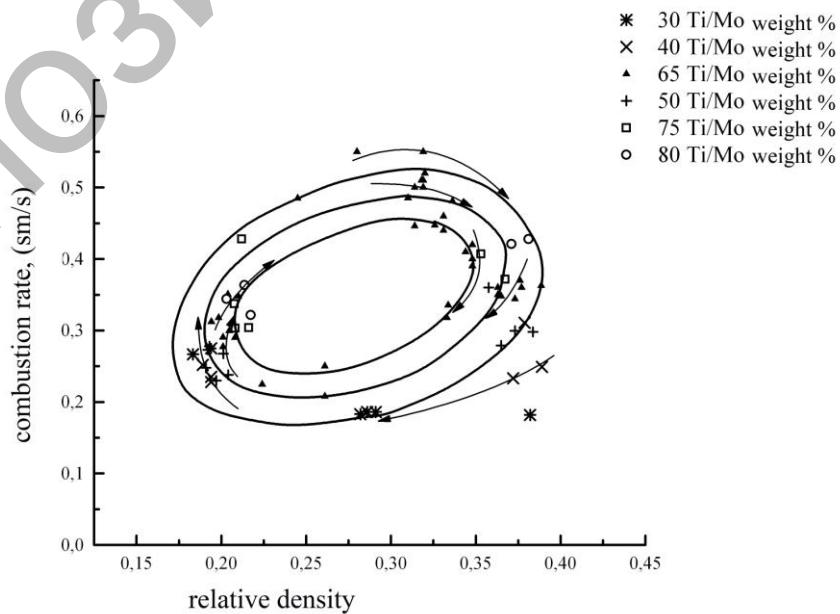


Fig.4. Dissipative structure of chemically active environment of combustion wave. Each trajectory, that formed a closed cycle, had its value of conversion degree

Figure shows three closed cycles which are attractors, and the other trajectories try to combine with these attractors. In this case, each trajectory, that formed a closed cycle, had its value of conversion degree.

Finally, we found the coordinate space «the absorbed quantity of nitrogen is the atomic ratio of absorbed nitrogen to initial quantity of molybdenum» where combustion rates were combined into linear trajectories with chosen compositions.

Conclusions

The plotting and analysis of dissipative structures representing a set of trajectories can provide an actual description corresponding to a reality.

Each set of trajectories represents a phase portrait that is defined by chosen and found invariants.

We have found the invariants that are the formulas of intermediate nitrides for one phase portrait and the conversion degree for another one in the same coordinate space for the Titanium - Molybdenum - Nitrogen system.

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