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DIFFERENTIAL - THERMAL ANALYSIS APPLICATION IN COMPLEX METHODOLOGY OF STUDING POLYCOMPONENT SYSTEMS

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ABSTRACT

The efficiency of the differential-thermal analysis (DTA) application is shown on the example of a great number of subjects, this analysis being the main exoerimental method in the suggested general algorithm for investigating polycomponent salt systems. The large volume of information obtained by the DTA makes possible its application in differentiating the systems into the phase unit blocks, in the process of building crystallization trees, defining the affiliation of non-variant balance points to particular phase unit blocks (PUB), defining also the parameters of phase balance, and describing the chemical interaction of the components of the system.

The peculiarity of polycomponent systems lies in their poly-aggregation, diversity of their morphological types and poly-phase character. The existing methods of investigation do not ensure optimal studies, thereby restraining the application of polycomponent systems in solving scientific and technological problems. A complex methodology of polycomponent system investigation was suggested by the authors. It is based on the distribution of all obtained and applied data through a number of informational levels, different in their volumes and contents, though logically connected[1].

One of the main operations in the general algorithm of studying diagrams of state is the process of revealing unit components of polycomponent systems and their adequate geometrical image. Since the therminology used in the field of breaking up the polyhedrons of compounds is misleading, the authors suggest general concept - a phase unit block (PUB) as a single component of a system. PUB is a concentrated field of the diagram of

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compounds characterized by its own complexity of jointly crystallized phases, which correspond to individual substances forming the block, or to solid solutions on their base.

Revealing the PUBs of a system and their combination in the diagram of compounds is called a system differentiation process.

A series of algorithms for differentiating and forming phase trees in polycomponent systems was worked out. These algorithms are based on algebraic signs of recognizing geometrical situations, on the fields of the greatest volume of information, on the graph theory, on using the matrices of phase indices, thermodynamic data and topological peculiarities of physical-chemical systems. At this stage the DTA is used to define the correspondence of non-variant balances points to the revealed PUBs and to build afterwards a phase crystallization tree[2].

The investigation includes:

1. Combining the DTA and measurements of electric conduction to define the temperatures of phase transitions, including those corresponding to complete disappearance of the liquid.

2. Using the DTA to study one compound on each secant element.

3. To reveal the character of non-variant balance points, to define whether they correspond to particular PUBs; all that by comparing the temperatures of complete crystallization of melts on secant elements and in the adjoining PUB reveals the point of peritectic balance, their non-coincidence - the point of eutectic balance.

The complexity of the revealed non-variant balance points in PUBs makes it possible to build a phase crystallization tree. It determines stable products of the chemical interaction among the components of the system.

A most complicated task of the polycomponent system investigation is that of defining the compositions and the temperatures of non-variant balance points and the parameters of one-, two-, e.t.c. variant balances. The investigation becomes less complicated when one applies the suggested projection-thermographical method. It is based on using the laws of phase crystallization and advantages of the DTA[3].

The DTA allows to fix the temperatures of all the phase transitions taking place during melt crystallization. Thus, having heating and cooling thermograms for a number of compounds of a

chosen section one can build its polythermal diagram of state. The geometrical images of phase balances shown on the diagram of state are out of the section plane. Thus, the diagram of state of the polythermal section is a projection of the geometrical image of phase balances of the system on its cross-section. It was shown [4] that the direction of the projecting rays is connected with the laws of phase crystallization. In the geometrical models the direction of phase crystallization is defined by the direction of vectors going from the corresponding poles. The direction of the vectors by phase crystallization of a non-stoichiometric compound can be easily defined by experiment. Knowing the direction of phase crystallization one can observe the movements of any figurative point of a polythermal section in a polyhedron of compounds up to the concentration point corresponding the end of crystallization. If the polythermal section, therefore, is chosen according to the laws of phase crystallization, its diagram, built with the help of the DTA data, gives necessary information for defining the parameters not only of non-, but also of one-, two-, e.t.c. balance states. They are defined by projecting particular points of diagrams of state of polythermal sections onto a polyhedron of compounds. To define a point in a three-dimensional space there must be two projections of the point on one or two sections, in a four-dimensional space - three projections, e.t.c. The application of the projection-thermographical method showed its high expressiveness with minimal excessive information.

CONCLUSIONS

The DTA application in the general algorithm of the polycomponent system investigation made it possible to reduce temporal expenses in dozens and hundreds times. The more components has a system, the higher is the economy.

Widely and effectively applying the DTA and complex methodology the authors studied about 50 threefold, 30 fourfold and 10 fivefold systems for rather a short period.

REFERENCES

1 A.S.Trunin, Kompleksnaya metodologiya issledovaniya khimicheskogo vzaimodeystviya i geterogennykh ravnovesiy v mnogokomponentnykh

systemakh. J."Applied Chemistry", 1982, 10, p. 3297
2.A.S.Trunin, A.S.Kosmynin, G.E.Shter, Vyjavlenie kharaktera i mestopolozheniya tochek nonvariantnogo ravnovesiya. J."Applied Chemistry", 1983, 4, p. 964
3 V.I.Posypaiko, A.S.Trunin, A.S.Kosmynin, G.E.Shter, Proiektsionno-termograficheskiy metod issledovaniya trojnykh i chetvernykh vzaimnykh sistem. Report of AS USSR, series Chemistry, 1976, 4, p. 911-913
4 V.I.Posypaiko, Prognozirovanie khimicheskogo vzaimodeystviya v sistemakh iz mnogikh komponentov. M., "Nauka", 1984, p. 216