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«Почин генома материалов», «Проект генома материалов» и генотип материалов

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Аннотация
Проанализировано происхождение терминологии по наследственности материалов. Термины “проект генома материалов” и “инициатива генома материалов” возникли в 2008 и 2011 г.г., а “гетерогенный дизайн” и “генотип гетерогенного материала” - в 1998 и 2001 г.г.
Ключевые слова*:* геном материалов, генотип, наследственность, гетерогенный дизайн (ГД), концентрационный поля, фазовая диаграмма (ФД), траектории фаз, схема кристаллизации, микроструктура, конкуренция кристаллов различной размерности

"Materials genome Initiative", "Materials Genome Project" and Materials Genotype

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Abstract
Origin of terminology on materials heredity has been analyzed. Keywords “materials genome project” and “materials genome initiative” appeared in 2008 and 2011, and “heterogeneous design” and “genotype of heterogeneous material” − in 1998 and 2001.
Keywords: materials genome, genotype, heredity, heterogeneous design (HD), concentration fields, phase diagram (PD), trajectory of phases, crystallization scheme, microstructure, crystals of different sizes competition

History of the materials heredity was presented for the participants of the 5th International Conference on nanomaterials and technologies [1].

As many opinions exist in this field, main results of the two RFBR projects have been summarized: # 98-03-32844 “The design of the microstructures of multi-component materials according to the equations of the boundaries of single-phase regions” (1998-2000) and # 01-03-32906 “The genotype of heterogeneous material (boundary of concentration domains with the unique schemes of phase transformations and thermodynamically unstable fragments of phase fields in the multidimensional diagrams of the known and forecasted topological types)” (2001-2003).

Both these projects were fulfilled by the employee of the Materials computer-aided engineering sector at the Institute of Physical Materials Science (Siberian Branch of the Russian Academy of Sci.) in Ulan-Ude: http://ipms.bscnet.ru/ http://ipms.bscnet.ru/labs/skkm.html

Along with the well-known and wide-spread "molecular design" and "structural design", this new approach in solid state chemistry and physics – heterogeneous design (HD), materials genotype decoding - opens up new opportunities for multiphase materials engineering.

Computer model of a constitutional phase diagram (PD) is becoming an important tool to investigate multicomponent system, to correct the graphics of its sections, to design the miscrostructures of heterogeneous material, to decipher the genotype of ceramics and alloys. As a computer model of PD saves information about system in compact form and permits to receive any projection, isotherm and isopleth with the decoding of intersected surfaces and phase regions, it helps to discover the errors and incorrectly interpreted experimental data, especially in the cases of surfaces degeneration because of negligibly small sizes of homogeneous regions.

Thermodynamic calculation doesn’t guarantee an accuracy of PD in whole. E. g., in the system Au-Sb-Bi two surfaces of solidus and solvus were lost, and later they were found by means of our PD computer model. 3D model of PD may confirm original data, otherwise it will open (explain) the reasons for the errors.

If 3D model is formed as a set of surfaces, it may be used only to check the geometrical features of PD. If 3D model consists of phase regions, it permits to analyze the mass balances and to design the microstructures, confirming the results by mass balances: vertical ones for the given centre of masses and horizontal ones - for the isothermal states on the isopleth.

A competition of tiny eutectical crystals with more large primary crystals of the same phase in the

invariant reaction with melt was investigated, and different variants of microstructures with more large and and with tiny crystals, and with the mixture of these crystals have been located in different concentration domains.

When the phase regions are projecting on the concentration simplex, the latter is dividing into the concentration fields with the individual set of phase reactions and appropriate microstructures. Then the fields, which belong to the 3-phase regions, are dividing additionally by the surfaces of 2-phase reaction into the fragments with the different dynamics of phase masses increment. Every 3-phase region has 1-3 these surfaces of 2-phase reaction, and the sections of them are to be fixed on the isopleths and on the isothermal cuts. Analogously in the fields, connected with the invariant phase reactions, the domains with different results of the large and small crystals competition are allocated too. Like this thrice-repeated segmentation of concentrations space forms a genotype of multicomponent material.

Main results of HD are published in [2-24] and presented at the international scientific forums [25-30].

For the last six years a special session "Phase Diagram as a Tool of Materials Science" [31] are organizing by our research team for the 2^{d} , 3rd and 4th International Conferences on Competitive Materials and Technology Processes: http://www.ic-cmtp2.eu http://www.ic-cmtp3.eu http://www.ic-cmtp4.eu

The aim of this session is to discuss the key areas in material science and engineering based on phase equilibrium investigation: Thermodynamic calculations and experimental determinations produces sometimes PD with problems. The general Calphad produces PD by combining ab initio results, thermodynamic measurements data and phases simulation and lead to obtain a general view of the stabilities in the systems. Idea to assemble PD from phase regions develops additional effective instrument for specialists in materials science and technology. In these diagrams all 3-phase regions are divided into the fragments with eutectic (eutectoid) and peritectic (peritectoid) reactions. Concentrations fields of invariant reactions permit to design microstructure of heterogeneous material. Competition of crystals with different dispersity produces alloys and ceramics which differ by microstructure. Any experimental or simulated section of phase diagram (isotherm and isopleth) may be corrected and verified. New technologies are offered to optimize experimental investigation.

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References

1. Lutsyk V.I. Materials Genome and Nanotechnologies // Nanomaterials and Technologies: Proceed. 5th International Conference (Ulan-Ude, August, 27-29, 2014). Ulan-Ude: BSU Publ. Department. 2014. P. 176-183.

2. Lutsyk V.I., Vorob'eva V.P. Heterogeneous Design: Concentration Fields Determination with the Unique Crystallization Schemes and Microstructures // MRS Proceed. 2003. V. 755. P. 227-233.

3. Lutsyk V.I., Zyryanov A.M. Microstructures design in the ternary systems with the only solubility gap // Ibid. 2004. V. 804. P. 279-283.

4. Lutsyk V.I., Vorob'eva V.P. Heterogeneous Design: Structural Diagrams of Ternary Systems // Ibid. 2004. V. 804. P. 321-326.

5. Lutsyk V.I., Vorob'eva V.P. Phase and Structural Diagrams for Inorganic Materials Microstructures Design // Electrochemical Society Proceed. 2004. V. 2004-11. P. 204-213.

6. Lutsyk V.I., Vorob'eva V.P. Domains with the Reaction Type Change in the 3-Phase Regions of the Ternary Salt Systems // Ibid. 2004. V. 2004-24. P. 141-150.

7. Lutsyk V.I., Vorob'eva V.P., Zyryanov A.M. Contradictions between 3-phase region eutectical and peritectical fragments borders determination methods in monographs by A.Prince and D.Petrov // J. of Guangdong Non-Ferrous Metals. 2005. V. 15. No 2, 3. P. 174-178.

5. Lutsyk V.I., Zelenaya A.E., Savinov V.V. Melt solidification in the ceramic system $CaO-Al_2O_3-SiO_2$ // IOP Conf. Ser.: Mater. Sci. Eng. 2011. V. 18. No 11. http://iopscience.iop.org/1757-899X/18/11/112005/pdf/1757-899X_18_11_112005.pdf.

6. Lutsyk V.I., Zelenaya A.E., Savinov V.V. Phase Trajectories in $CaO-Al_2O_3-SiO_2$ melts // Crystallography Reports. 2012. Vol. 76. No 7. P. 71-74.

7. Lutsyk V.I., Nasrulin E.R. Competition of Primary and Eutectic Crystals in Invariant and Univariant Reactions // Crystallography Reports. 2012. V. 57. No 7. P. 106-110.

8. Lutsyk V., Zelenaya A., YaZhou Dai. Li,Na,K,La||F System for Molten Salt Reactor: 3D and 4D Computer Models // Advanced Materials Research. 2013. Vol. 704. P. 349-352.

9. Lutsyk V.I., Vorob'eva V.P. 3D computer models of Mo-Zr-V, Ti-C-V, Ti-Ir-Ru T-x-y diagrams with three-phase reaction type changing // Scientific Journal "Proceedings of the International Conference NANO Materials: Applications & Properties". 2013. V. 2. № 4. P. 04NAESP07-1 – 04NAESP07-4.

10. Lutsyk V.I., Zelenaya A.E. Ternary Systems for the Liquid Immiscibility Gap Technology // Ibid. P. 04NAESP09-1 – 04NAESP09-4.

11. Lutsyk V., Zelenaya A. Crystallization Paths in $SiO_2-Al_2O_3-CaO$ System as a Genotype of Silicate Materials // IOP Conf. Ser.: Mater. Sci. Eng. 2013. V. 47. 012047. http://iopscience.iop.org/1757-899X/47/1/012047/pdf/1757-899X_47_1_012047.pdf. 1-4.

12. Lutsyk V., Vorob'eva V. New Phase Regions of Ir-Ru-Ti System with Eutectic-Peritectic Transformation // Ibid. 012049.

http://iopscience.iop.org/1757-899X/47/1/012049/pdf/1757-899X_47_1_012049.pdf. P. 1-4.
13. Lutsyk V.I., Vorobeva V.P., Sumkina O.G., Tsyngeev B.V. Three-Phase Reaction Type Changing in Mo-Zr-V and Ti-Ir-Ru Systems // IFAC Proceedings Volumes (IFAC-PapersOnline). 2013. 15 (Part 1). P. 365-370.
14. Lutsyk V., Zelenaya A. Crystallization Paths and Microstructures in Ternary Oxide Systems with Stoichiometric Compounds // Solid State Phenomena. 2013. V. 200. P. 73-78.
15. Lutsyk V., Zelenaya A., Parfenova M. Solidification Paths in the Ceramic Systems // Advanced Materials Research. 2013. V. 704. P. 173-178.
16. Lutsyk V., Zelenaya A., YaZhou Dai. Li,Na,K,La||F System for Molten Salt Reactor: 3D and 4D Computer Models // Advanced Materials Research. 2013. V. 704. P. 349-352.
17. Lutsyk V.I., Vorob'eva V.P., Shodorova S.Y. Definition of Conditions for Changing the Type of 3-Phase Reactions in Systems V-Zr-Cr // Russ. J. Phys. Chem. A. 2015. V. 89. No 13. P. 2331-2338.
18. Lutsyk V.I., Vorob'eva V.P., Zelenaya A.E. 3D Reference Book on the Oxide Systems Space Diagrams as a Tool for Data Mining // Solid State Phenomena. 2015. V. 230. P. 51-54.
19. Lutsyk V., Zelenaya A. Crystallization paths in SiO_2-Al_2O_3-CaO system as a genotype of silicate materials // Építőanyag - Journal of Silicate Based and Composite Materials. 2013. V. 65. P. 34-38.
20. Lutsyk V., Zelenaya A., Zyryanov A., Nasrulin E. Computer Models of Phase Diagrams for Ceramic Systems. TiO_2-SiO_2-Al_2O_3 and ZrO_2-SiO_2-Al_2O_3 // Ibid. 2016. V. 68. P. 52-55.
21. Lutsyk V.I., Vorob'eva V.P. 3D Model of the T-x-y Diagram of the Bi-In-Sn System for Designing Microstructure of Alloys // Russ. J. Inorg. Chem. 2016. V. 61. P. 188-207.
22. Lutsyk V. Solidification paths confirmation by the mass balances // Abstracts XIV Intern. Conf. on Physics of Thin Films and Nanostructures. Ivano-Frankivsk, Ukraine. 2013. P. 50. http://www.pu.if.ua/inst/phys_che/start/conference_14/abstracts/pdf/14_pr_31.pdf
23. Lutsyk V. Heterogeneous materials genome decoding within the ternary systems // Abstracts 13th Intern. Symp. on Physics of Materials (ISPMA 13). Prague, Czech Republic. 2014. Section C. P. 168.
24. Lutsyk V. Heterogeneous design: multicomponent systems engineering by means of equations for the homogeneous regions borders // Proceed. 12th Intern. Conf. on Fundamental and Applied Aspects of Physical Chemistry. Belgrade, Serbia. 2014. V. 1. P. 49-56.
25. Lutsyk V.I. Mathematical Support for the Materials Genome Initiative // Mathematics, its application and mathematical education: Proceed. V Intern. conf. Ulan-Ude: Publ. House of ESSTU. 2014. P. 367-371.
26. Lutsyk V. Materials genome decoding by means of phase diagrams // Proceed. All-Rusian Scientific Conf. with International Participation «II Baikal Materials Science Forum». Ulan-Ude: BSC Publ. House. 2015. V. 1. P. 81-82. http://www.binm.ru/books/2015/02_BMF2015_Vol1.pdf
27. Lutsyk V., Vorob'eva V. Computer models of phase diagrams to design the materials of additive technologies // Proceed. Intern. Conf. "Additive Technologies: Present-day and the Future". Moscow, VIAM. 2015. http://conf.viam.ru/conf/163/proceedings (In Russian)
28. http://www.iccmtp4.eu/iccmtp4.php?title=Plenary%20and%20Keynote%20Speakers&contr=&kod=&idu=26
29. http://www.iccmtp4.eu/subjects.php?contr=&kod=&ide=13&title=Phase%20Diagram%20as%20a%20Tool%20of%20Materials%20Science

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Трехмерные компьютерные модели t-x-y диаграмм и их роль в создании новых материалов

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Аннотация
В статье представлены примеры эффективного использования трехмерных (3D) компьютерных моделей фазовых диаграмм металлических систем (сульфидно-металлических подсистем) при разработке бессвинцовых припоев, оптимизации технологии получения меди и никеля, анализе участия фаз Лавеса в смене типов фазовых превращений и ее влияния на микроструктуру сплавов.

Ключевые слова: фазовые диаграммы, трехмерные компьютерные модели, бессвинцовые припои, смена типа трехфазной реакции, сульфидно-металлические системы, компьютерное конструирование материалов.