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# INTELLIGENT INFORMATION SYSTEM FOR PREDICTING THE PHASE STABILITY OF SOLID SOLUTIONS WITH ZIRCON STRUCTURE

**Анотація.** Запропоновано створення проєкту інтелектуальної інформаційної системи прогнозування фазової стабільності твердих розчинів. У проєкті передбачено розроблення інтерфейсної частини та побудова математичної моделі, на основі якої буде можливим прогнозування фазової стабільності твердих розчинів зі структурою циркону.

**Ключові слова:** інтелектуальна інформаційна система, фазова стабільність, тверді розчини, математичне моделювання, модель, структура циркону.

**Problem.** Information that some solid solutions of rare earth elements (REEs) with zircon structure can be used as luminescent materials from optoelectronics (production of displays, LEDs, etc.) to biomedicine. They can include several REEs, which will be part of both the matrix and the activator. However, state diagrams, as well as substitutions of substituted components, in solid REE decompositions have been insufficiently studied, which limits the possibility of choosing the composition of complex solid soluble appropriate systems for studying their luminescent authorities and further practical application. Apparently, the last shoes are high-cost REE compound. This forces researchers who study the luminescent properties to choose the composition of matrices and activators, either by analogy with related systems, or by trial and error.

**Solution.** For this purpose, we have created a program for predicting the limits of substitutions by the crystal chemical method in systems with isostructural components in the approximation of regular solutions. The main task of the method is to determine the mixing energy of the components Q, the knowledge of which allows Becker's equation, setting the decay temperature (stability) $T_r$ to calculate the equilibrium composition of the solid solution "x", or for a given "x" to calculate $T_r$. However, when calculating the mixing energy by the method of V. Urusov [1], material scientists, for whom the model was created, may have difficulty in choosing the initial parameters (eg, degree of ionicity, coordination number, interatomic distances, etc.), so all the initial parameters for each components are listed in the program database.

The following programming environments were chosen as the software design environment: Oracle Application Express (programming languages javasript, html, pl / sql) and pl / sql developer (programming language pl / sql) [2].

**Brief description of the proposed Information System.** The proposed information system will consist of three main parts. The first part will carry out a detailed analysis of the latest technologies, with the help of which, it will be possible to achieve the desired result. The next main part in the calculation between the substitution and thermodynamic stability of solid solutions using the crystal-energy method by V.S. Urusov determines the mixing energy Q (interaction parameters) [1]. In the general case, the energy content according to V. S. Urusov using three contributions, educational changes in the size of the substituting structural units or interatomic distances in the components ($Q_R$), the distribution of the degree of ionicity of the chemical bond ($Q\varepsilon$) and the difference between their crystalline structural structures ($\Delta H_{II-I} / x_1$), where $\Delta H_{II-I}$ am the enthalpy of a polymorphic transition from structural components that replaces the structure of the one it replaces:

$$Q = Q_R + Q_\varepsilon + \Delta H_{II-I} / x_1.$$

The final part will be the development of a software solution for the Intelligent information system for predicting the phase stability of solid solutions using Oracle Application Express [3].

**Results.** The proposed information system should have a reliability of results, convenience and ease of use, lack of rigid binding to specific hardware and software. The developed mathematical model should describe the work of the information system in full.

**References**

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