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INTELLIGENT INFORMATION SYSTEM FOR PREDICTING THE STABILITY OF ORTHOARSENATES $Sc_{1-x}Ln_xAsO_4$ AND $Tb_xLn_{1-x}AsO_4$ SOLID SOLUTIONS

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Анотація

В рамках кристалоенергетичної теорії ізоморфних заміщень Урусова, в нашій інтелектуальній інформаційній системі проведено розрахунок енергії змішування(параметри взаємодії) та критичних температур розкладання (температур стабільності) твердих розчинів у системах $Sc_{1-x}Ln_xAsO_4$*, Ln = Sm – Lu, Y та Tb1 – x*Ln_xAsO_4*, Ln = Y, Tm із структурою циркону.*

Наведені результати можуть бути корисними при виборі співвідношення компонентів у «змішаних» матрицях, кількості активатора в люмінесцентних, лазерних та інших практично важливих матеріалах, а також у матрицях для іммобілізації токсичних та радіоактивних відходів.

Ключові слова: інтелектуальна інформаційна система, фазова стабільність, тверді розчини, математична модель, структура циркону.

Abstract

Urusov's crystal energy theory of isomorphous substitutions carried out in our intelligent information system was used to calculate mixing energies (interaction parameters) and critical decomposition temperatures (stability temperatures) of solid solutions in the systems $Sc_{1-x}Ln_xAsO_4$*, Ln = Sm–Lu, Y, and* $Tb_{1-x}Ln_xAsO_4$*, Ln = Y, Tm with zircon structure.*

The present results can be useful in choosing the ratio of components in "mixed" matrices, the amount of activator in luminescent, laser, and other practically important materials, as well as in matrices for immobilization of toxic and radioactive waste.

Keywords: intelligent information system, phase stability, solid solutions, mathematical model, zircon structure.

Introduction

Even though the rare-earth element (REE) orthoarsenates in composition and crystalline structure are analogs of the REE orthophosphates and orthovanadates, which are currently being intensively studied as phosphors, lasers, light emitters, catalysts, ionic conductors, matrices for radioactive waste, much less attention is paid to orthoarsenates, apparently, due to the toxicity of arsenic compounds. However, it is known that REE orthoarsenates possess ferroelectric and electroluminescent properties and can also be used as matrices for immobilization of toxic wastes of arsenic and selenium.

Calculational approach

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, 3].

Results

The crystal-chemical approach in the approximation of regular solid solutions was used to calculate the mixing energies and critical decomposition (stability) temperatures of systems of $Sc_{1–x}Ln_xAsO_4$, Ln = Sm–Lu, Y, and $Tb_{1–x}Ln_xAsO_4$, Ln = Y, Tm solid solutions with zircon structure. With increasing in REEs charge nuclei, the calculated mixing energy and critical decomposition temperature of solid solutions naturally decrease, which is caused by the decrease in ionic radii in the lanthanide series from Sm to Lu. The differences in the degrees of ionicity of the chemical bond in the components of the systems are small and practically do not affect the calculation results.

The obtained diagram of thermodynamic stability allows one to evaluate the stability of $Sc_{1–x}Ln_xAsO_4$ solid solutions in a wide range of compositions and temperatures, as well as to predict the substitution limits for limited series of solid solutions at a given decomposition temperature, or their decomposition temperature at a given substitution limit.

In $Sc_{1–x}Ln_xAsO_4$ systems with REEs from Sm to Ho, unlimited solid solutions are thermodynamically stable at temperatures above critical (2363–1224 K). By lowering the temperature in the range between the T_{cr} and about 1073 K these systems have become thermodynamically unstable and decompose, forming a limited range of solid solutions. At lower temperatures, these solid solutions become metastable. In systems with REEs from Er to Lu, unlimited solid solutions are thermodynamically stable at temperatures above critical (790–528 K); at lower temperatures than critical, they become metastable and will not decompose.

The obtained results of the critical decomposition temperatures (56 and 139 K) in $Tb_{1–x}Ln_xAsO_4$, Ln = Y, Tm systems are consistent with the experimental results described previously within the accuracy of the calculation method.

REFERENCES

1. Grechanovsky A. E., Eremin N. N., Urusov V. S. Radiation resistance of LaPO4 (monazite structure) and YbPO4 (zircon structure) from computer simulation data. Physics of the Solid State. 2013. Vol. 55, N 9. P. 1929–1935. DOI: 10.1134 / S1063783413090138.

2. Feuerstein S.Oracle PL/SQL Programming / S. Feuerstein, B. Pribyl – Sebastopol: O'Reilly Media, 2014. – 1340 p. – ISBN 5-8459-0384-4.

3. Loney K. Oracle Database 11g DBA Handbook / Loney K. – NY.: McGraw-Hill Education, 2007. – 670 p. – ISBN 5-93286-032-4.

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