

Information System to Forecasting the Steadiness of REE OOS Solid Solutions for Environmental Monitoring

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Abstract

V.S. Urusov's crystal-energy theory of isomorphic replacements accomplished in our information system was used to calculate mixing energies and critical temperatures of disintegration (steadiness) of solid solutions in the systems $(Sc_{1-x}Ln_x)[(SiO_4)_{0.5}O_{0.5}]$, where Ln is rare-earth elements (REE) of Terbium – Lutetium row, and Yttrium. Steadiness temperatures of some solid solutions at $x = 0.01, 0.03, 0.05, 0.10, \text{ and } 0.20$ were established. Based on the given calculation results, a diagram was created to estimate the areas of sustainability of solid solutions and forecast the replacement limits based on the steadiness temperature depending on the obtained replacement limits. The results of the research can be helpful for choosing the ratio of the components in the host materials and the amount of dopant in newly “hybrid” REE OOSs (OOS) $(Sc_{1-x}Ln_x)[(SiO_4)_{0.5}O_{0.5}]$, where Ln represent REEs of Terbium – Lutetium row, and Yttrium.

Keywords

Information system, phase steadiness, solid solutions, mathematical modeling, model, OOSs.

1. Introduction

Solid solutions based on Scandium-OOS Sc_2SiO_5 are innovational materials for creating efficacious lasers for medicine, laser ranging [1], military purposes, metalworking [2], and what is important for environmental monitoring [3-5] since they have become an attractive research topic due to their huge benefits. For example, such lasers are not dangerous for eye and it has fine transparency in the atmosphere, can serve as efficient sources in optical measurements, for example, weather conditions (wind measurement), as well as the determining of the concentration of atmospheric atoms. They serve as host materials, while the triple charged Ln^{3+} ions, which are contained in small amounts (up to 5 at%), act as dopants. In addition to OOSs containing only Scandium cations in their matrices [6-7], we also studied materials based on “hybrid” OOS with two different cations – Sc and REEs, which are solid solutions of

$Sc_2SiO_5 - Ln_2SiO_5$ systems [8-11]. The use of “hybrid” Sc and REE OOS is due to the purpose of synthesizing materials with better properties compared to Ln_2SiO_5 , and which are cheaper compared to Sc_2SiO_5 , since the cost of Sc is higher than one of REE.

No analysis of physical and chemical foundations for the receiving of solid solutions – state diagrams and, in particular, areas of solubility based on the components of the Sc_2SiO_5 and Ln_2SiO_5 systems – has been carried out, while this result is necessary for choosing the compound of materials. As far as we know, only data about the $Lu_{2-x}Sc_xSiO_5$ [12] and $Er_xSc_{2-x}SiO_5$ [13] systems are available. In [12], it was reported that three compositions of polycrystalline solid solutions with $x = 0.5, 0.8, 1.0$ at a temperature of 1670 K were obtained, while in [13] the synthesis of $Er_xSc_{2-x}SiO_5$ in the form of films within the temperature range 1173 – 1373 K was studied. In [13], it was also reported that $Er_xSc_{2-x}SiO_5$ films could be used to

ISIT 2021: II International Scientific and Practical Conference «Intellectual Systems and Information Technologies», September 13–19, 2021, Odesa, Ukraine

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CEUR Workshop Proceedings (CEUR-WS.org)

create a light source with high optical gain since they have a higher Erbium concentration compared to Silicon-based materials doped with Erbium. Nevertheless, no information on the replacement limits in the $\text{Lu}_{2-x}\text{Sc}_x\text{SiO}_5$ and $\text{Er}_x\text{Sc}_{2-x}\text{SiO}_5$ systems are available.

It is very important to determine experimentally areas of solubility in the solid phase, which requires expensive equipment, additional reagents, large energy and time consumption. This forces researchers who study the properties of “hybrid” REE OOS to choose the composition of host matrix materials and activators either by analogy with similar systems or by selection method that is trial and error.

It is often not taken into account that “hybrid” REE OOS tend to decay and modification their phase composition and properties upon cooling. This can lead to the damage of materials based on them if used in applications. Accordingly, before carrying synthesis and studying it, it is recommended to evaluate the steadiness of solid solutions in the corresponding systems during their obtaining and intended use.

In view of this, the aim of this research is to forecast the phase steadiness and replacement limits in materials based on solid solutions of OOS of Scandium and REEs of Terbium – Lutetium row, and Yttrium.

Yttrium subgroup REEs and Yttrium were chosen as second cations due to the same structure with Sc_2SiO_5 , as well as the proximity of crystalline ionic radii of Sc^{3+} (0.885 Å) and triply charged cations of Yttrium subgroup REEs and Yttrium (1.063 – 1.001 Å [14]), which suggests the wide presence of isomorphic replacement of Scandium by these REEs. The radii of the Cerium subgroup REE cations (1.172 – 1.078 Å) vastly differ from the ionic radius of Scandium, and their OOS are not isostructural with Sc_2SiO_5 [15], which, according to the theory of isomorphic miscibility [16-18], should vastly limit the solubility of components in systems with Scandium and REEs of the Lanthanum – Gadolinium series.

2. Calculation method and results

The main aim in establishing the replacement limits of solid solutions using the crystal energy method by Urusov [16-18] is to determine the mixing energy E_{mix} . As to components with the same structure of the system and the possibility of

their pseudo-binary representation, there are two contributions to the mixing energy, which are caused by the difference in the size of the substituting structural units E_δ and the difference in the degree of ionicity of the chemical bond E_ε :

$$E_{\text{mix}} = E_\delta + E_\varepsilon = Cmnz_mz_x\delta^2 + 1390mz_mz_x\alpha(\Delta\varepsilon)^2/(2D), \quad (\text{kJ/mol}), \quad (1)$$

where: C is a constant calculated from the equation $C = 20(2\Delta\chi + 1)$ [18] based on the difference in electronegativity χ of Ln^{3+} cations and anions [19]. The value $\chi(\text{SO}_4^{4-})$, as recommended [20], was accepted equal to $\chi(\text{O}^{2-})$ [19]; m is the number of formula units in the pseudo-binary approximation of components. Since the anionic sublattice of the crystal structure of OOS contains Orthosilicate and Oxide anions that are not bonded to the Silicon atom [15], and the replacement limits are calculated per one mole of the replaceable ion, the OOS formulas will be presented below as a pseudo-binary compound $\text{Ln}[(\text{SiO}_4)_{0.5}\text{O}_{0.5}]$; n is the coordination number of the replaceable structural unit in the pseudo-binary approximation of the structure; z_m, z_x is the formal charges of the replaced and general structural units in the components; δ is a dimensional parameter, which for each system is characterized by the relative difference of cube roots of unit cell volumes taken from [15, 21-22], calculated by the formula:

$$\delta = (V^{1/3}_{\text{Ln}} - V^{1/3}_{\text{Sc}})/V^{1/3}_{\text{Sc}} \quad (2)$$

α is the reduced Madelung constant calculated by the Hoppe formula [23]: $(\alpha/n)^2 + \alpha$; $\Delta\varepsilon$ is the difference in the degree of ionicity of the chemical bond in the components of the systems.

For example, using an information system for forecasting the phase steadiness of solid solutions, which based on the crystal-energy theory of isomorphic miscibility, were calculated the energies of mixing E_{mix} and critical temperatures of disintegration T_{cr} of $(\text{Sc}_{1-x}\text{Ln}_x)[(\text{SiO}_4)_{0.5}\text{O}_{0.5}]$ solid solutions (where Ln is a REE, $\text{Ln} = \text{Tb} - \text{Lu}$ and Y). Some initial data and calculation results are summarized in Tables 1, 2 and Fig. 1. The Table 1 shows that as the number of REE in the Terbium – Lutetium row increases, the contributions of E_δ values to the total mixing energy become smaller (from 34.5 to 10.8 kJ/mol), which is explained by smaller differences in the size of substitutable structural units – Scandium and REE.

Table 1

Sourced data for the calculation of mixing energies and critical temperatures of disintegration of solid solutions $(Sc_{1-x}Ln_x)[(SiO_4)_{0.5}O_{0.5}]$, $Ln = Tb - Lu$ and Y

Ln	V, Å ³	δ^*	$E\delta$, kJ/mol	χ_{Ln}	ϵ	$\Delta\epsilon$	T _{cr} , K
Tb	876.80 [21]	0.0535	34.5	1.410	0.708	0.001	2060
Dy	856.57 [15]	0.0453	24.8	1.426	0.706	0.003	1480
Ho	843.04[15]	0.0398	19.1	1.433	0.704	0.005	1150
Er	836.70[15]	0.0372	16.7	1.438	0.703	0.006	1010
Tm	828.59 [15]	0.0338	13.8	1.455	0.699	0.010	860
Yb	824.07 [15]	0.0319	12.3	1.479	0.694	0.015	810
Lu	819.31[15]	0.0299	10.8	1.431	0.705	0.004	650
Sc	749.97 [22]	–	–	1.415	0.709	–	–
Y	852.25 [21]	0.0435	22.8	1.340	0.722	0.013	1400

*Note: according to the recommendations in [17-18] and considering the dependence of the interaction parameter on the difference in volumes of the unit cells of components [29], the calculation of the dimensional parameter was carried out according to the volumes of the unit cells

Contributions due to different degrees of ionicity of chemical bonds in the components of the E_ϵ systems are substantially smaller (in most cases, two-three times smaller) than in E_δ , and they can be neglected in this case. This agrees with the recommendation not to consider them, provided that $\Delta\epsilon \leq 0.05$ [16-18] (in this case, $\Delta\epsilon \leq 0.015$). Consequently, it is accepted that $E_{mix} = E_\delta$.

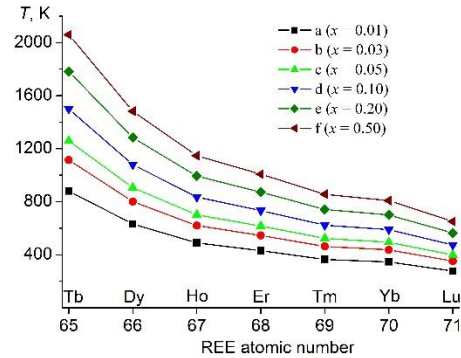


Figure 1: The diagram of thermodynamic steadiness of solid solutions in the systems $(Sc_{1-x}Ln_x)[(SiO_4)_{0.5}O_{0.5}]$, where $x = 0.01$ (a), 0.03 (b), 0.05 (c), 0.10 (d), 0.20 (e) and 0.50 (f)

Table 2

Temperatures of disintegration of $(Sc_{1-x}Ln_x)[(SiO_4)_{0.5}O_{0.5}]$ solid solutions for $x = 0.01, 0.03, 0.05, 0.10,$ and 0.20

x	Tb	Dy	Ho	Er	Tm	Yb	Lu
0.01	880	630	490	430	370	350	280
0.03	1110	800	620	550	469	440	350
0.05	1260	910	700	620	520	490	400
0.10	1500	1080	840	730	620	590	470
0.20	1780	1280	990	870	740	700	560

In all systems, the size parameter (δ) does not exceed 0.1 with its maximum value of 0.0535 (Table 1). This, according to [16-18], makes it possible to use the approximation of regular solutions when calculating the temperatures of disintegration of solid solutions. In this case, the curve showing the dependence of the

temperatures of disintegration on the system composition will be nearly symmetric. Therefore, to calculate T_{cr} , the following equation was used:

$$T_{cr} = E_{mix}/2kN, \quad (3)$$

where k is Boltzmann constant, N is the Avogadro number. In order to calculate the replacement limits for a given disintegration

temperature of a solid solution (T_d), or the disintegration temperature for a given replacement limit [24], the Becker's equation was used [24]:

$$-(1 - 2x) / \ln[x/(1 - x)] = RT_d/E_{\text{mix}}, \quad (4)$$

where R is universal gas constant; E_{mix} is a mixing energy (or interaction parameter), x is a replacement limit.

As can be seen from the Table 1 and Fig. 1 (curve f), the values of maximum temperatures of disintegration, as expected, become smaller as REE number increases. The Becker's equation was also used to calculate the temperatures of disintegration of solid solutions for the replacement limits $x = 0.01, 0.03, 0.05, 0.10,$ and 0.20 (Table 2), and to build their dependences (Fig. 1) on the REE number (curves a, b, c, d and e, respectively). The latter can be used to determine the replacement limit of Scandium for REE based on a given temperature or calculate the disintegration temperature based on the replacement limit. In the first case, it is necessary to draw an isotherm from a given temperature to the intersection with the vertical line for this REE. The intersection point makes it possible to estimate the range of x values within which the replacement limit lies. The replacement limit should be defined by interpolating the vertical segment between the closest to the intersection point dependencies of the replacement limit on the REE number. In the second case, based on the given composition the point is determined on the vertical line of the REE, and then the horizontal line is drawn until its intersection with the temperature axis. More precise results can be obtained if using the Becker's equation.

It is generally known that as the temperature depression, the movability of the structural units in solid solution becomes smaller due to a decrease in the diffusion rate, while the areas of solubility become narrower [17]. This happens until the diffusion rate becomes so low that the decrease in the areas of solubility practically ceases, i.e. spontaneous quenching occurs, and solid solutions become metastable. If we assume that the hardening temperature is close to the minimum temperature at which the interaction of the components in the solid phase begins that leads to the formation of a solid solution, we can estimate the temperature of spontaneous hardening and the area of metastability in the system.

It was previously established (Table 3) that the temperature during the synthesis of solid solutions of $\text{Sc}_{2-x}\text{Er}_x\text{SiO}_5$ OOS as a part of the preparation

of multilayer films is in the range of $1173 - 1373$ K, while the temperature during the synthesis of Gadolinium, Lutetium and Yttrium OOS using the solution combustion synthesis method is 1273 K, and the temperature during solid-phase synthesis of REE OOS of the Terbium – Lutetium row, and Yttrium, using the sol-gel method is in the range of $1173 - 1323$ K.

Table 3

Methods and temperatures for the synthesis of REE OOS

Method of synthesis	Composition	T, K
Calcination of multilayer films [13]	$\text{Sc}_{2-x}\text{Er}_x\text{SiO}_5$	1173 – 1373
Solution combustion synthesis (SCS) [25]	$\text{Lu}_2\text{SiO}_5:\text{Ce}$ $\text{Gd}_2\text{SiO}_5:\text{Ce}$ $\text{Y}_2\text{SiO}_5:\text{Ce}$	1273 1273 1273
Sol-gel method followed by calcination [26]	Y_2SiO_5 Tb_2SiO_5 Dy_2SiO_5 Ho_2SiO_5 Er_2SiO_5 Tm_2SiO_5 Yb_2SiO_5 Lu_2SiO_5	1323 1323 1323 1273 1273 1273 1223 1173

In this way, at a temperature of less than 1173 K, the diffusion rate of structural units is apparently insufficient for the synthesis of REE OOS and solid solutions based on them. Consequently, it can be assumed that the disintegration of solid solutions at temperatures below ~ 1173 K is unlikely to occur, hence, the solid solution will be metastable.

The diagram also makes it possible to evaluate the areas of thermodynamic steadiness of solid solutions of Scandium OOS and REEs of the Terbium – Lutetium series. In the $(\text{Sc}_{1-x}\text{Ln}_x)[(\text{SiO}_4)_{0.5}\text{O}_{0.5}]$ systems with $\text{Ln} = \text{Tb}, \text{Dy},$ and Y , unlimited solid solutions are thermodynamically stable in the entire range of concentrations $0 < x < 1$ at temperatures above the critical one ($2060 - 1400$ K; Table 1, Fig. 1); when the temperature depression to the range between T_{cr} and ~ 1173 K, they become thermodynamically unstable and can decay. At $T < 1173$ K, solid solutions will not decay, i.e.

spontaneous hardening will occur, and they will become metastable.

In the systems containing REE from Erbium to Lutetium, the maximum temperatures of disintegration (1010 – 650 K) are lower than the spontaneous quenching temperature (~1173 K), unlimited solid solutions do not decay upon cooling, and remain stable at temperatures higher than critical one and metastable at temperatures lower than critical one.

The difference between the critical temperature for a system containing Holmium (1150 K) and the temperature of spontaneous quenching (~1173 K) is less than the calculation error (± 100 K [17]); therefore, it is difficult to forecast disintegration of an unlimited solid solution in this system.

Likewise, limited solid solutions with $x = 0.01, 0.03, 0.05, 0.10,$ and 0.20 in the areas above the curves a, b, c, d, and e, respectively, are thermodynamically stable (Fig. 1), in the areas below the curves they are unstable and can decay, while at $T < 1173$ K they are metastable.

Notwithstanding there are numerous publications, which study the laser properties of Scandium OOS, doped with, for example, 0.5 at% of Holmium [3], 1 at% of Neodymium [9, 27], 4 at% of Thulium [7], 5 at% of Ytterbium [28] and others, and some papers on the properties of “hybrid” OOS $Y(Lu,Sc)_2SiO_5$ [2], $(Sc_{0.5}Y_{0.5})_2SiO_5$ [8, 10], $(Sc_{0.2}Y_{0.8})_2SiO_5$ [11], there is practically no data on the limits of isomorphous replacements in the corresponding systems. This, of course, makes it difficult to assess the reliability of our calculations. But, they do not contradict the experimental data obtained previously for $Lu_{2-x}Sc_xSiO_5$ and $Er_xSc_{2-x}SiO_5$ solid solutions. For example, in the $Lu_{2-x}Sc_xSiO_5$ system, a mixture of Lu_2O_3, Sc_2O_3 and SiO_2 was calcined to synthesize solid solutions for compositions with $x = 0.5, 0.8, 1.0$ at a temperature of 1670 K [12], i.e. in the area of continuous series of solid solutions, which are thermodynamically stable according to the results of our calculation (Fig. 2).

In [13], the $Er_xSc_{2-x}SiO_5$ solid solutions were received by calcination of atomized multilayer films in the temperature range 1173 – 1373 K; i.e. also in the area of continuous series of solid solutions above the disintegration curve calculated by us (Fig. 3).

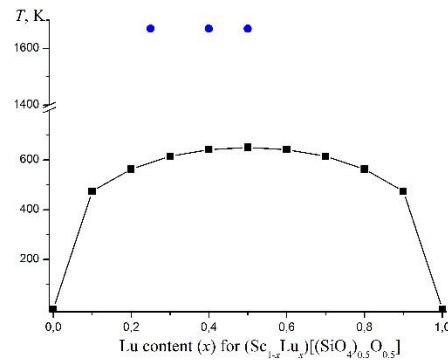


Figure 2: Dependence of the calculated temperatures of disintegration of solid solutions for the system $(Sc_{1-x}Lu_x)[(SiO_4)_{0.5}O_{0.5}]$ (■) on the molar fraction of Lutetium, and experimental data on the synthesis temperatures (●) for the compositions with $x = 0.25, 0.4,$ and 0.50 [12]

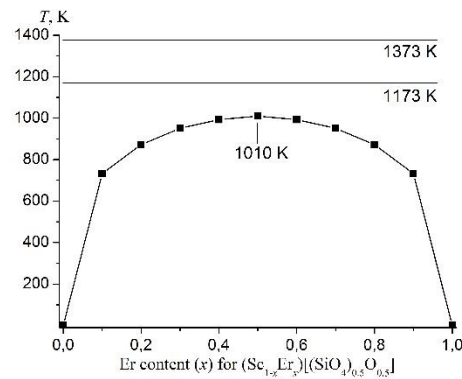


Figure 3: Dependence of the calculated temperatures of disintegration of solid solutions for the system $(Sc_{1-x}Er_x)[(SiO_4)_{0.5}O_{0.5}]$ (■) on the molar fraction of Lutetium, and experimental data on the synthesis temperatures (●) for the compositions with $x = 0.25, 0.4,$ and 0.50 [12]

3. Conclusions

The crystal-chemical approach in the approximation of regular solutions was used to calculate the interaction parameters E_{mix} of solid solutions based on Scandium OOS $(Sc_{1-x}Ln_x)[(SiO_4)_{0.5}O_{0.5}]$, modified with REEs with $x = 0.01, 0.03, 0.05, 0.10, 0.20,$ and 0.5 . With an increase in the number of the rare earth element, the calculated mixing energies and critical temperatures of disintegration of solid solutions become smaller, which is due by the decrease in the ionic radii of REE in the series from Lanthanum to Ytterbium.

The diagram of thermodynamic steadiness makes it possible to evaluate not only the steadiness of $(Sc_{1-x}Ln_x)[(SiO_4)_{0.5}O_{0.5}]$ solid solutions in a wide range of compositions and temperatures, but also to forecast for some solid solutions the replacement limits at a given disintegration temperature, or the disintegration temperature at a given replacement limit.

In the systems $(Sc_{1-x}Ln_x)[(SiO_4)_{0.5}O_{0.5}]$ with $Ln = Tb, Dy, \text{ and } Y$, unlimited solid solutions are thermodynamically stable at temperatures above critical one (2060 – 1400 K), and if the temperature depression to the range between critical temperature and ~1173 K, the solutions become thermodynamically unstable and can decay. At a temperature of $T < 1173$ K, solid solutions will not decay, since they become metastable. In the systems containing REE from Erbium to Lutetium, where the critical temperatures of disintegration are vastly lower (1010 – 650 K) than the temperature of spontaneous quenching (~1173 K), unlimited solid solutions do not decay upon cooling, and they remain stable at temperatures higher than critical one and metastable at temperatures lower than T_{cr} .

The calculation results obtained do not contradict the experimental data obtained previously for $(Sc_{1-x}Lu_x)[(SiO_4)_{0.5}O_{0.5}]$ and $(Sc_{1-x}Er_x)[(SiO_4)_{0.5}O_{0.5}]$ solid solutions, since the temperatures of their synthesis are in the limits attributed by us to thermodynamically stable ones.

Materials based on such solid solutions have budding prospects in optical remote environmental sensing, differential absorption light detection.

4. Acknowledgements

The authors note that the research results presented in the article were obtained while working on the research topic “Prediction of phase stability and isomorphic substitutions in solid solutions of different structural types” of the Department of Inorganic, Organic and Analytical Chemistry, Vasyl’ Stus Donetsk National University (Ukraine, Vinnytsia). The authors are grateful to the staff of this department and personally to the lecturer of the Department of Inorganic, Organic and Analytical Chemistry PhD, Associate Professor, Serhii V. Radio for facilitating the research.

The authors also note that the research results presented in the article were obtained while

working on the research topics “Identification of hidden dependencies in online social networks based on methods of fuzzy logic and computational linguistics” and “Information and communication technologies for solving semantic-dependent problems” of the Department of Automation and Intelligent Information Technologies of Vinnytsia National Technical University (Ukraine, Vinnytsia).

The authors are especially appreciative to the staff of the Department of Automation and Intelligent Information Technologies, personally to the head of the Department, Doctor of Technical Sciences, prof. Roman N. Kvyetnyy also personally to the professor of the Department of Computer Science and Information Technology, Vasyl’ Stus Donetsk National University, Doctor of Technical Sciences, prof. Sergiy D. Shtovba for consultations on theoretical and applied aspects of the research.

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