Intelligent Information System for Predicting Chemicals with Interactive Possibilities

Oleksii Kudryk[a], Oleg Bisikalo[a], Yuliia Oleksii[b] and Serhii Radio[b]

[a] *Vinnitsa National Technical University, Khmel'nyts'ke sh., 95, Vinnytsya, Vinnyts'ka oblast', 21000, Ukraine*
[b] *Vasyl' Stus Donetsk National University, 600 richchya street, 21, Vinnytsya, Vinnyts'ka oblast', 21000, Ukraine*

Abstract

Urusov's crystal energy theory of isomorphous substitutions carried out in our intelligent information system (IIS) was used to calculate mixing energies (interaction parameters) and critical decomposition temperatures (stability temperatures) of solid solutions. Diagram of the thermodynamic stability of solid solutions is built that makes it possible to predict the thermodynamic stability of solid solutions. IIS provides interactive features for user convenience.

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 1

Intelligent information system, phase stability, mathematical model, interactive possibilities, image.

1. Introduction, formulation problem in general

The problem of isomorphic substitutions of atoms in crystals attracts the interest of researchers due to the fact that most new inorganic materials for phosphors, lasers [1], scintillators, photocatalysts [2], LEDs [3], etc. is created on the basis of solid solutions, which allows you to purposefully influence their properties. "Mixed" solid solutions, which contain, in addition to the activator, several other cations [4-5]. However, it is not always taken into account that solid solutions synthesized at high temperatures are prone to decomposition on cooling and can uncontrollably change the phase composition and properties. Therefore, before the synthesis and study of their properties, it is desirable to evaluate the displacement limits and thermodynamic stability of solid solutions.

It is known that some solid solutions of rare earth elements (REE) with a zircon structure can be used as luminescent materials for optoelectronics (production of displays, LEDs, etc.), biomedicine and other industries [6]. They may include several REEs that are part of both the matrix and the activator [7]. However, state diagrams, as well as the limits of component substitutions in REE solid solutions are insufficiently studied, which limits the possibility of choosing the compositions of solid solutions of appropriate systems to study their luminescent properties and further practical application. Apparently, the latter is due to the high cost of REE compounds [8]. This forces researchers studying luminescent properties to choose the composition of matrices and activators, either by analogy with related systems, or by trial and error.

You can add information about the boundaries of substitutions in two ways:

1. By experimental studies of the dependence of the boundaries of substitutions on the composition. This requires the cost of expensive reagents, equipment and significantly increases the duration of

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EMAIL: kydrikalex@gmail.com (O. Kudryk); obisikalo@gmail.com (O. Bisikalo); oleksii.i@donnu.ua (Yu. Oleksii); radio@donnu.ua (S. Radio)
ORCID: 0000-0002-0592-6633 (O. Kudryk); 0000-0002-7607-1943 (O. Bisikalo); 0000-0002-7328-6674 (Yu. Oleksii); 0000-0001-9808-0392 (S. Radio)

research. Since the number of the above systems of solid solutions exceeds one hundred, experimental studies can take many years. In addition, they can be performed only in a limited range of temperatures due to the difficulty of achieving equilibrium at both low and high temperatures [9].

2. Forecasting the boundaries of substitutions by calculation methods that do not require large expenditures of money and time [10].

To conduct research in the second direction requires the creation of a model, methods and technological means for predicting the boundaries of substitutions by the crystal chemical method in systems with isostructural components in the approximation of regular solutions. It is proposed to combine a set of appropriate models, methods and technological means in the form of an intelligent information system (IIS) for predicting the phase stability of solid solutions. The main task of IIS is the automated determination of the mixing energy of the components *Q*, the knowledge of which allows the Becker equation, setting the decay temperature (stability) *Tr* to calculate the equilibrium composition of the solid solution "*x*", or to calculate *Tr* for a given "*x*". It should also be borne in mind that material scientists, who should be the main users of IIS, when calculating the mixing energy by the method of V. Urusov may have difficulty in choosing the initial parameters. We are talking, for example, about choosing the degree of ionicity, coordination number, interatomic distances, and so on. Therefore, all initial parameters for each component must be entered in the IIS knowledge base. It is also important that the IIS provides a natural language interface with the database in order to speed up user decision-making.

The object of research is the processes of forecasting the phase stability of solid solutions and building an intelligent information system to automate such forecasting.

The subject of the research are models and knowledge bases of IIS, as well as technological tools for building IIS: Oracle Application Express (programming languages javascript, html, pl / sql) and pl / sql developer (programming language pl / sql).

2. Formulation of the purpose of the article

The aim of the work is to increase the accuracy and speed of predicting the phase stability of solid solutions based on the development of models based on knowledge and technological shell convenient for the work of IIS.

To achieve the higher goal, it is necessary to provide the following characteristics of the IIS, which provides:

- High accuracy of forecasting results;
- convenience and ease of use of IIS;
- built-in IIS interactive capabilities for user interaction;
- allow simultaneous work with an unlimited number of users;
- lack of rigid binding to specific hardware and software;
- light scalability system;
- high level of security.

3. Model of phase stability of solid solutions

The main task in calculating the limits of substitutions and thermodynamic stability of solid solutions using the crystal energy method VS Urusov [11] is the definition of the mixing energy Q (interaction parameter). In the General case, the mixing energy according to VS Urusov consists of three contributions due to the difference in the size of the substituting structural units or interatomic distances in the components (Q_R), the difference in the degree of ionicity of the chemical bond ($Q\varepsilon$) and the difference in their crystal structures ($\Delta H_{II-I}/x_1$), where ΔH_{II-I} enthalpy of the polymorphic transition from the structure of the component it replaces to the structure of the one it replaces:

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

In this paper, the substitution of REEs in isostructural groups of systems is studied. Therefore, the third term in the above equation is zero. The second term of the equation according to must be taken

into account in cases where the dimensional factor is large enough, and the difference in the electronegativity of the substitute ions is greater than 0.4; or a difference in the degree of ionicity of the chemical bond in the components of the systems greater than 0.05. Taking into account the difference in the size of the structural units to be replaced and the differences in the degrees of ionicity of the chemical bond in the components, the mixing energy will be [11]:

$$Q = Q_R + Q_\varepsilon = Cmnz_m z_x(\Delta R/R_1)^2 + 1390mz_m z_x\alpha(\Delta\varepsilon)^2/(2R_1),\ kJ/mol,$$

where:

C is an empirical parameter calculated from the expression $C = 20\ (2\Delta\chi + 1)$ [11] by the magnitude of the difference in electronegativity $\Delta\chi$ (EN) of cations and anion;

m is the number of structural units in the compounds in the pseudobinary approximation of the components;

n is the coordination number of the substituting structural unit in the pseudobinary approximation;

z_m, z_x - charge modules of structural units (Ln^{3+} and YO_4^{3-});

R is the interatomic distance of the cation - the central atom of the oxoanion;

R_1 is the smaller interatomic distance;

α is the reduced Madelung constant calculated by the Templeton formula;

$\Delta\varepsilon$ - differences in the degrees of ionicity of the chemical bond in the components, calculated by the difference in electronegativity (EN) of REE and anion cations, taken from [11]. The choice of scale [12, 13], in contrast to the scales of other authors, was due to the fact that the values of EN change in it at regular intervals, increasing in the series Ce^{3+} - Eu^{3+} from 1,348 to 1,433 and Gd^{3+} - Yb^{3+} from 1,386 to 1,479 with a sharp drop in transitions Eu^{3+} - Gd^{3+} from 1,433 to 1,386 and Yb^{3+} - Lu^{3+} from 1,479 to 1,431, which is due to the structure of their electronic shells REE;

$\Delta R/R1$ - the relative difference in the size of the structural units to be replaced (dimensional parameter).

The crystal chemical method of quantitative theory of isomorphic substitutions was first developed and tested on the example of systems formed by binary compounds - alkali metal halides. This was due to the existing theoretical developments of previous generations of scientists, as well as a large number of results of experimental studies on diagrams of states, substitution boundaries, structures, thermodynamics and other characteristics of these compounds. Formulated by VS Urus's rule of assistance allowed us to move to the characteristics of the size factor - from the relative difference in the size of structural units (tabular radii of ions), which are replaced by the difference in interatomic distances cation-anion. The latter were determined experimentally with greater accuracy and included not only the size of the structural units to be replaced, but also the total structural units. Later, the method was extended to systems formed by ternary compounds that contain complex anions isolated from each other, which can be considered as separate structural units, and the compounds themselves are called pseudobinary. Unlike alkali metal halides, pseudobinary compounds have been studied to a much lesser extent, which in many cases complicates the determination of the dimensional parameter due to the limited amount of structural data.

According to [11], in the case of using the crystal chemical method, for systems of solid solutions of compounds with a tetrahedral anion, the following options can be selected to calculate the size parameter $\Delta R/R$ as a relative difference:

1. Experimentally found interatomic distances cation-central atom of the complex anion components of the systems

$$(R\mathrm{Ln}_1 \bullet\bullet\bullet \mathrm{V} - R\mathrm{Ln}_2 \bullet\bullet\bullet \mathrm{V}) / (R\mathrm{Ln}_2 \bullet\bullet\bullet \mathrm{V}).$$

Hereinafter, the interatomic distances are denoted by the letter R, the ionic radii will be denoted by r.

2. Sums of experimentally found interatomic distances of cation-oxygen and central oxygen-atom components of systems

$$[(R\mathrm{Ln}_1\text{-O} + R\text{V-O}) - (R\mathrm{Ln}_2\text{-O} + R\text{V-O})] / (R\mathrm{Ln}_2\text{-O} + R\text{V-O}).$$

3. The sum of the interatomic distances cation-oxygen and the central oxygen atom, calculated from the values of ionic radii

$$[(R\mathrm{Ln}_1 + r\mathrm{O}) + (r\mathrm{V} + r\mathrm{O}) - (r\mathrm{Ln}_2 + r\mathrm{O}) - (r\mathrm{V} + r\mathrm{O})] / [(r\mathrm{Ln}_2 + r\mathrm{O}) + (r\mathrm{V} + r\mathrm{O})].$$

4. Cubic roots from the volumes of elementary cells (V):

$$(V_1^{1/3} - V_2^{1/3}) / V_2^{1/3}.$$

Of the presented options, the first was used as a basis for deriving the basic equation of the crystal chemical method of calculating the substitution limits in binary systems of alkali metal halides. Therefore, it should be used primarily when testing the method on pseudobinary compounds. The disadvantage of this option is the small number in the reference and periodic literature of the distances cation-central atom, even for pseudobinary compounds, the structure of which is known. While the initial data for the calculation of the other three options for most cases are in the literature.

Thus, the critical decay temperatures in solid solution systems with a tetrahedral anion, as expected, are most accurately determined when calculating the first option for selecting a dimensional parameter (the inaccuracy is approximately 1%). In the absence of data on distances Ln ••• V the accuracy of calculations should be higher when calculating the second option (inaccuracy 2%). Quite high accuracy is achieved when calculating the fourth option (inaccuracy 1.9). The use of the third option can be recommended only in the absence of the possibility of calculation of other options for an approximate estimate of the critical decomposition temperature.

The obtained results can be useful in predicting the limits of isomorphic substitutions, thermodynamic and phase stability of solid solutions, in cases where experimental studies are difficult due to the radioactive or toxic properties of the compounds.

If the values of the dimensional parameters are less than 0.1, according to the recommendation [11], the values of the critical decay temperatures of solid solutions are calculated in the approximation of regular solutions by the expression:

$$T_{kr} = Q/2kN,$$

where k is the Boltzmann constant,

N is the Avogadro number.

The decay temperature Tr was set at a given substitution limit x or the substitution limit x at the decomposition temperature using Becker's equation [14]:

$$-(1 - 2x) / \ln[x/(1 - x)] = kN \times T_p/Q.$$

According to the graphical dependences, as in [15], it is possible to estimate the decay temperature of limited series of solid solutions by setting the substitution limit, or to estimate the substitution limit of one REE to another by setting the decay temperature. In the second case, the point of intersection of the isotherm drawn from a given decay temperature with the vertical drawn from the REE number allows to determine the composition interval in which the substitution boundary is located, and the interpolation between the two nearest curves gives the substitution boundary. The limit of substitution can be clarified by constructing for a particular system the dependence of the decomposition temperatures calculated by the Becker equation on the composition, which in the approximation of regular solutions will be almost symmetric.

The novelty of the proposed mathematical model, in comparison with the basic model of Urusov in the approximation of regular solutions, is that when calculating the empirical parameter C takes into account the contribution of the electronegativity of each lanthanide. This contribution is taken into account by the product of the substitution limit and the electronegativity of the corresponding lanthanide [16].

Therefore, a more accurate expression of the calculation of the empirical parameter C:

$$C = 20\,(2[\chi(\mathrm{Ln}_1)\cdot(1-x)]-[\chi(\mathrm{Ln}_2)\cdot x] + 1),$$

since the substitution limit of the substituent lanthanide is x, and the amount of substituted lanthanide is 1, respectively [17].

Therefore, the calculation of the empirical parameter *C* is more accurate because it immediately takes into account the specific limit of substitutions and, accordingly, increases the accuracy of the calculation of the mixing energy. As a result, for each individual solid solution system with the specified substitution limit, the exact rather than the total critical decomposition temperature can be calculated. Therefore, it is proposed to put the obtained model (1) in the basis of the knowledge base of the projected IIS.

4. Ensuring the interactivity of the intelligent information system

One of the manifestations of intellectual behavior is the ability of the system to transmit information about its internal state and current needs. This ability is possessed not only by man and the artificial systems created by him, but also by representatives of the higher animal world, who lead mainly a collective way of life [18].

Known artificial systems generate only symbolic messages about the state of their own functioning, mainly in the following cases [19, 20]:

• in case of incorrect user actions (in most systems);

• to control significant system parameters (operating systems, databases and knowledge, security systems);

• in order to explain the obtained results (expert systems, automatic proof of theorems);

• to obtain intermediate data in the process of debugging algorithms and software products (programming systems);

• to signal dangerous situations (banking and security systems, support for communication services, computer games, etc.).

It is clear that only in the first and last case it is a limited internal need of the system to report outward information about the occurrence of problems in performing clearly defined functions. There are no formal statements in the literature about the generation of such messages in relation to one of the possible needs of an open system that meet the complex criteria for the functioning of this system. The approach to the formalization of the figurative meaning of natural language constructions (NLC), proposed in [21], allows to solve such a problem and, thus, to obtain a model of adequate functioning of IIS.

Consider an IIS that exchanges information with the outside world through image streams. Internal criteria for the functioning of the system, which characterize the principle of minimizing energy costs, also have a figurative nature, as they depend on the previous history of the accumulation of combinations of external images in the form of a chain of events. If we present emotions in the form of the images closest to them, then the problem is to formalize the procedures for the following messages of the system:

1. definition of the "emotional state" of IIS in the form of an ensemble of images (AO);
2. the need for external verification of the solution obtained by the system of one of the semantically dependent problems, which belongs to the model of cognitive activity;
3. obtaining the system's requirements for the external environment, for example, in the case of applying the cognitive criterion, the system should indicate that it is unclear which images still require additional definition;
4. alarm about "abnormal situations" in the operation of the system.

Let's solve the problem of generating 4 types of messages in the development of the proposed approach to determining the meaning of NLC by modeling the image processing of textual information. To this end, we will use the capabilities of the mathematical apparatus, which is designed to implement the conceptual foundations of figurative meaning, taking into account the architecture of the knowledge base of the system [21].

1. To determine the "emotional state" of the system, we will rely on the model of the mechanism of random access memory [22], according to which the IIS in each clock cycle is updated ensemble of images. At the same time, images from RAM fall into the block of emotions, the task of which is to

direct the focus of attention to one of these images based on the evaluation of the connections of the images that make up the vector of emotions. Formally, this means determining the binary code of the image in focus Focus – Bi and the weight of the image in focus Focus – Weight, which is the largest of all AO images.

To solve this problem, we will include the most emotionally colored images in the Vector-Set emotion vector. Then the vector of emotions of each image of AO is determined on the basis of the operation Evaluate – Vector, as a result of which we obtain formal signs of focus of focus Focus – Bi and Focus – Weight. Finally, the message about the "emotional state" of the system will be considered a function - the formal dependence of the change of focus Focus – Bi on the model time t

$$Focus - Bi = F_e(t).$$

The proposed approach does not preclude the continuous display of the entire composition of the ensemble of images of RAM, which will take the form of a description (protocol) of internal events that occur in the IIS right now.

2. Suppose that the IIS implies the need for external verification or "reinforcement" according to IIS Pavlov obtained by the system of solving one of the tasks of cognitive activity. We will assume that the result of such a solution is the emergence of a new paradigmatic relationship, and the formal sign is an increase in the amount of meaning in the system, for example, for a synonymous relationship according to [22]. It is clear that the tasks of cognitive activity can have a complex hierarchical structure [21], but for the elementary component of cognitive activity we take the creation of a new paradigmatic relationship. Then the purpose of generating a message to verify the solution of the problem of cognitive activity is to confirm the truth of the new paradigmatic relationship. Leaving aside the planning and initialization of cognitive tasks, we will formally present such a message for synonymy with the help of

$$\exists\ Pc_{ij} \mid Pc_{ij} \in P_c \rightarrow If - Synonim,$$

$$Se^s + Se^{Pc}_{ij} \xrightarrow{Synonim} Se^s,$$

where *If – Synonim* is a predicate that requires external confirmation; *Synonym* - the function of increasing the overall meaning of the system by adding a synonymous link.

The task is to execute the *Synonim-Plus* operator, which increases the meaning of the IIS due to the verification of the synonymous connection - if external confirmation of the synonymy is received (the predicate *If-Synonim* is true), the *Synonim* operator is executed:

$$Synonim - Plus ::= ([If - Synonim]\ \ Synonim,\ \ E),$$

where *E* is an empty operator. The graph diagram of the *Synonim – Plus* operator is shown in Figure 1:

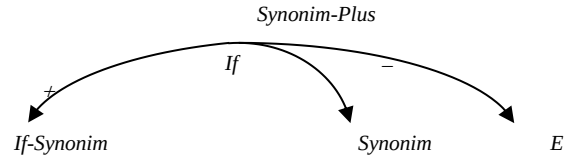

Figure 1: Graph diagram of the *Synonim – Plus* operator

The proposed approach can be applied in the process of dialogue with IIS, during which there is a natural initialization of cognitive tasks and figurative search for a species. In this case, predicates like *If-Synonym* can be considered true by default until the "teacher", as the other side of the dialogue, "corrects" the system error in solving the corresponding partial problem of cognitive activity.

3. In contrast to messages about the "emotional state", the IIS is able to generate requirements for the external environment due to the continuous analysis of the state of the internal cognitive space of

associative pairs in the form of a graph. One of the criteria for the functioning of the system can be applied, for example, the maximum increase in the total amount of IIS meaning as a model of the dominant motive of "pure" intellectual activity.

In what follows, we will consider the total amount of meaning of IIS as a cognitive criterion. Then the general task of cognitive activity is interpreted in the form

$$Se^s \to \max \mid G_z$$

To solve problem (14), the IIS can initiate a dialogue with an external "teacher", for example, to indicate which images (graph vertices) require additional definition. To this end, it is proposed to cluster the vertices of the graph by topological parameters and the value of meaning. The division of vertices into clusters can be carried out on the basis of one of the known methods [23, 24], or with the help of a specialized algorithm, which additionally initiates a dialogue with an external "teacher".

Consider the algorithm *Question – Out*, for which the average values are pre-determined and:

[Step 1] $n'_{\min} = \overline{n_i}/2$, $n''_{\min} = \overline{n_i}/2$, $Se_{\min} = \overline{Se_i}$, $Minimum - Bi = 1$.

[Step 2] Open a loop on each i-th vertex of the graph G_z.

[Step 3] If $(n'_i < n'_{\min}) \vee (n''_i < n''_{\min}) \vee (Se_i < Se_{\min})$, then $n'_{\min} = n'_i$, $n''_{\min} = n''_i$, $Se_{\min} = Se_i$, $Minimum - Bi = i$.

[Step 4] Index cycle i is closed.

[Step 5] Output (as a question object) an image with a number *Minimum-Bi.*

We will assume that the number of new connections to support the "weakest" image will be maximum. Then adding each new syntagmatic connection to the system increases the meaning parameter of the system

$$Se^s \approx Se^s + \delta + 0{,}5$$

which is the ultimate goal of the Question – Out algorithm and figurative search of the species *InsZX*

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4. Partition of vertices of the graph G_z on clusters provides the ability to generate signals to the outside of various "abnormal situations" in the work, depending on the specifics and subject area of IIS. If we do not take into account the dynamic characteristics of the system in real time, then the "abnormal situation" in the narrow sense will mean the case of defining a new cluster based on a set of information about the graph G_z ,that has changed over time.

As a result of an "abnormal situation", for example, in speech activity there is a possibility to give a name to a new cluster, which will lead to a new paradigmatic relationship such as separate-general *Pch* between all images of the cluster and increase the overall meaning of IIS. Therefore, the task is formally reduced to:

- detection of the fact of the emergence of a new cluster of images;
- notification of the external "teacher" about the composition of the new cluster;
- receiving in response the number of the vertex of the graph G_z , the corresponding image of which is determined by the name of the new cluster.

Whether or not the cluster image-name is part of a cluster, in this approach, the amount of added IIS meaning depends on the number of syntagmatic connections combined in this way.

Therefore, on the basis of the offered approach to an estimation of figurative sense of NLC formal methods of generation of 4 types of messages of IIS on types of figurative search are received *InsZX* and *InsZY* The message about the "emotional state" of the system is interpreted as a reflection of the functional dependence of the change of focus *Focus-Bi* on the model time. The message about the solution of one of the tasks of cognitive activity is reduced to the operator, which increases the overall meaning of IIS due to the external verification of the corresponding paradigmatic connection. Generation of requirements to the external environment is implemented in the form of the *Question – Out* algorithm, which is based on the search of the vertices of the graph G_z finds the "weakest" *Minimum*

– *Bi* image, which differs in the smallest values of topological parameters $n_i^{'}$ and $n_i^{''}$ and the meaning of meaning Se_i . The signal about the "abnormal situation" is reduced to the appearance with the participation of the "teacher" of a paradigmatic relationship of the type separate-common between the images of the discovered new cluster and an increase in the total number Se^S sense of IIS.

Let us consider an example of helping materials specialists, who should be the main users of IIS, when calculating the mixing energy by the method of V. Urusov may have difficulty in choosing the initial parameters. We are talking, for example, about choosing the degree of ionicity, coordination number, interatomic distances, and so on. In Figure 2 shown the ontology of the concepts of the subject area, which is proposed to form the basis of the interactive interaction between the user and the IIS knowledge base.

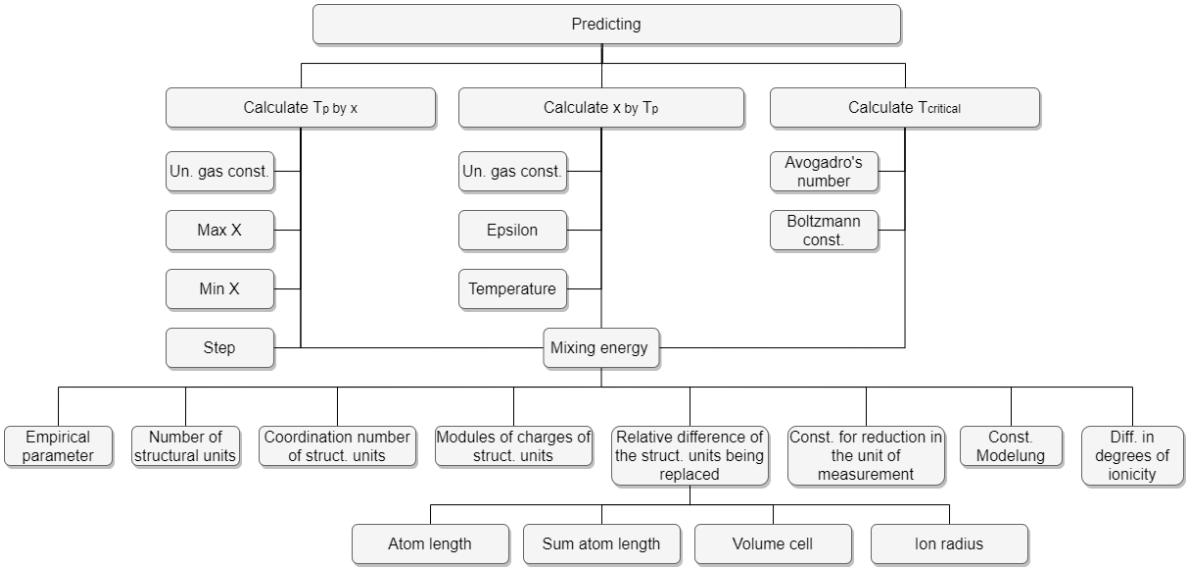

Figure 2: Ontology graph of the IIS notions

With the help of such a basic ontology, it is possible to further expand the network of concepts in the subject area, using the analysis of both texts and the results of interaction between users and IIS. After practical testing of the considered formal methods for generating 4 types of messages, the development of the proposed approach is possible in the direction of increasing the number of types of chemical reactions.

5. Software implementation and approbation of IIS

5.1. Creating an IIS architecture

We will design a system consisting of the following modules:

- software module for working with the interface;
- software module of basic logic;
- software module for working with the database.

The software module for working with the interface provides the correct display of information on the pages of the system.

The following modules are used for the interface:

- user authentication;
- work with chemical elements;
- work with groups of chemical elements;
- work with interatomic lengths;
- work with the sum of interatomic lengths;
- work with the volume of cells;
- work with the structure of solid solutions;

• work with thermodynamic systems.

The basic logic software module is required to handle client requests.

A software module that works with the database is needed to obtain data for further placement on the pages of the system. The following modules are required for the software module that works with the database:

• implementation and authentication;
• administrator check;
• obtaining data on chemical elements;
• obtaining data on groups of chemical elements;
• obtaining data on interatomic lengths;
• obtaining data on the sum of interatomic lengths;
• obtaining data on cell volumes;
• obtaining data on the structure of solid solutions;

5.2. Development of database structure

To ensure the forecast of phase stability of solid solutions, it is necessary to store data on: users, elements, groups of elements, interatomic lengths of elements, sums of interatomic lengths of elements, cell volumes, structures of solid solutions, thermodynamic systems. The ER database model (physical layer) is shown in Appendix 1.

The following structure of tables used in the developed model is offered:

1. *Element_grp* - a table in which groups of elements are stored.

This table has the following fields:

• *Elmg_id* - identifier;
• *Elmg_name* - Name;

2. *Sub_element_grp* - a table in which subgroups of elements are stored.

This table has the following fields:

• *Selmg_id* - identifier;
• *Selmg_elmg* - group identifier;
• *Selmg_name* - name.

3. *Element* - a table in which elements are stored.

This table has the following fields:

• *Elm_id* - id;
• *Elm_selmg* - subgroup identifier;
• *Elm_name* - name;
• *Elm_code* - chemical code. ;
• *Elm_count* - the number of atoms of the element.

4. *Elm2elm* - a table that is needed to create a complex element.

This table has the following fields:

• *E2e_id* - identifier;
• *E2e_che_par* - ancestor charge identifier;
• *E2e_che_ch* - daughter card identifier;
• *E2e_sort* - sort.

5. *Charge_element* - a table in which the charges of the elements are stored.

This table has the following fields:

• *Che_id* - identifier;
• *Che_elm* - element identifier;
• *Che_value* - charge value.

6. *Cordination_element* - a table in which the coordination numbers of charges are stored.

This table has the following fields:

• *Crde_id* - identifier;
• *Crde_che* - element charge identifier;
• *Crde_value* - the value of the coordination number.

7. *Atom_length* - a table in which the atomic lengths between the charges of the elements are stored.

This table has the following fields:
• *Atml_id* - identifier;
• *Atml_che_from* - charge identifier of element 1;
• *Atml_che_to* - charge ID of element 2;
• *Atml_value* - values of atomic lengths;
• *Atml_strs* - solid solution structure identifier.

8. *Sum_atom_length* - a table that stores the sum of the atomic length between the charges of the elements.

This table has the following fields:
• *Satml_id* - identifier;
• *Satml_che_from* - charge identifier of element 1;
• *Satml_che_to* - identifier of charge element 2;
• *Satml_value* - the value of the sum of atomic lengths;
• *Satml_strs* - solid solution structure identifier.

9. *Volume_Cell* - a table in which the volumes of cells between the charges of the elements are stored.

This table has the following fields:
• *Volc_id* - id;
• *Volc_che_from* - charge identifier of element 1;
• *Volc_che_to* - identifier of the charge element 2;
• *Volc_value* - volume value;
• *Volc_strs* - solid solution structure identifier.

10. *Structure_solid* - a table in which the structures of the solid solution are stored.

This table has the following fields:
• *Strs_id* - identifier;
• *Strs_name* - name;

11. *Term_System* - a table in which thermodynamic systems are stored.

This table has the following fields:
• *Tsys_id* - identifier;
• *Tsys_crde* - identification number of the coordination element;
• *Tsys_elm* - element identifier.

12. *Tsys_Crde* - a table that stores elements associated with a particular thermodynamic system.

This table has the following fields:
• *Tsysc_id* - identifier;
• *Tsysc_tsys* - thermodynamic system identifier;
• *Tsysc_crde* - identifier of the coordinate number of the element.

5.3. Confirmation of the adequacy of the mathematical model

To compare and establish the convergence of the obtained results with the literature data, a system was chosen $La_{1-x}PO_4$ with the structure of monazite, because it is for her in the literature there are a sufficient number of experimental values and calculations of the mixing energy.

To obtain forecast data in the proposed IIS, the user must:
1. Log in to the interface "Existing systems".
2. Choose the structure of the monazite.
3. Select the system $La_{1-x}PO_4$.
4. Select the lanthanide variables Gadolinium (Gd) and Europe (Eu).
5. Select the calculation step (default is 0.01).
6. Click on the "Calculate" button.

After these actions, IIS calculates based on model (1) and visualizes the graphs of the systems $La_{1-x}Eu_xPO_4$ and $La_{1-x}Gd_xPO_4$ which are shown in Figure 3.

Together with the schedule the user receives the table with calculations of systems $La_{1-x}Eu_xPO_4$ and $La_{1-x}Gd_xPO_4$ which are shown in Figure 4.

At the top of the table, you can use grouping to see which method was used to calculate the system and which variable lanthanide was used. The header of the table indicates x, x_1, x_2, t - decay temperature, T kritical - critical decomposition temperature, Q - mixing energy.

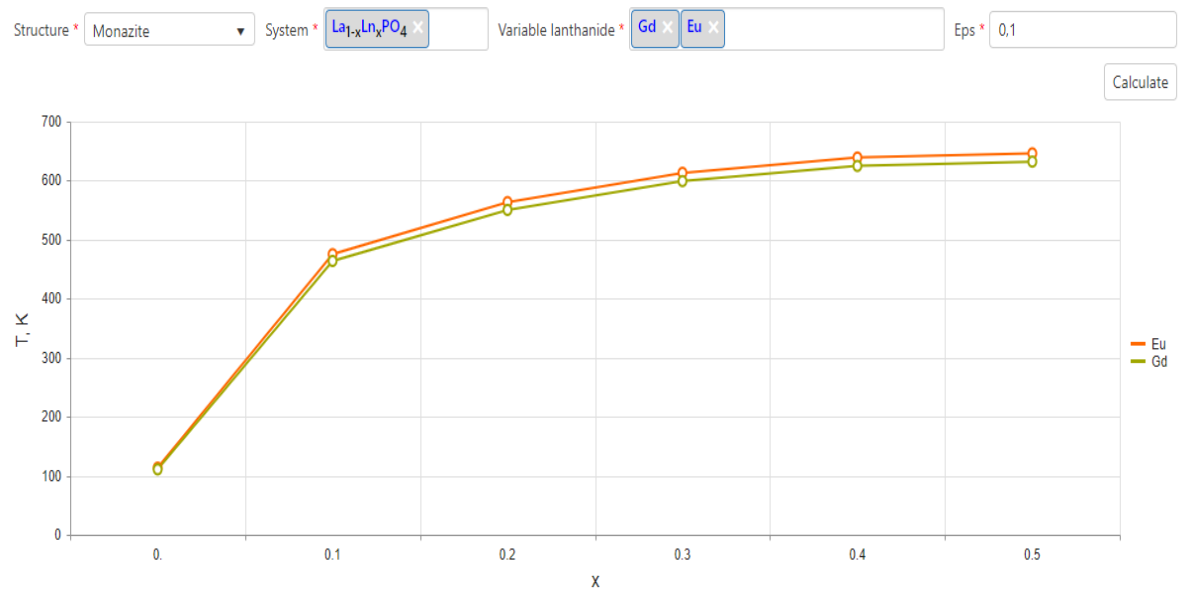

Figure 3: Graphs of systems $La_{1-x}Gd_xPO_4$ and $La_{1-x}Eu_xPO_4$

Method | Variable lanthanide

	x	x1	x2	t	T kritical	Q
Method: atom_length						
Variable lanthanide: Eu						
	0	0,99999	0,00001	113.69805	655,05177	10883,8162
	0,1	0,9	0,1	475.39922	653,38858	10856,18194
	0,2	0,8	0,2	563.67881	651,72522	10828,54491
	0,3	0,7	0,3	613.26751	650,06186	10800,90788
	0,4	0,6	0,4	639.13103	648,39851	10773,27085
	0,5	0,50001	0,49999	646.20151	646,73531	10745,63659
Variable lanthanide: Gd						
	0	0,99999	0,00001	110.88414	638,83994	10614,45336
	0,1	0,9	0,1	463.93073	637,62629	10594,28831
	0,2	0,8	0,2	550.43481	636,41252	10574,12124
	0,3	0,7	0,3	599.24566	635,19874	10553,95417
	0,4	0,6	0,4	624.9235	633,98497	10533,7871
	0,5	0,50001	0,49999	632.24904	632,77132	10513,62204

Figure 4: Table with system calculations $La_{1-x}Eu_xPO_4$ and $La_{1-x}Gd_xPO_4$

To compare the adequacy of the model taking into account the mixing energy at each step and without taking into account the mixing energy at each step, the calculation was performed, which is shown in Figure 5. On it you can see and compare the results obtained at each step.

To demonstrate how accurate the calculations of mixing energy and critical temperature are based on the scientific result (when calculating the empirical parameter C, the contribution of electronegativity of each lanthanide is taken into account by the product of the substitution limit and electronegativity of the corresponding lanthanide).).

Figure 5 shows that without taking into account the contribution of electronegativity for each substitution limit, only the total critical decomposition temperature (430.18474 K) and the total mixing

energy (7147.60549 kJ / mol) are calculated, as a result of which the accuracy of calculations decreases significantly.

Method × | Variable lanthanide ×

x	x1	x2	t	T kritical	Q
Method: atom_length					
Variable lanthanide: Eu					
0	0,99999	0,00001	74.66763	430,18474	7147,60549
0,1	0,9	0,1	312.99826	430,18474	7147,60549
0,2	0,8	0,2	372.06788	430,18474	7147,60549
0,3	0,7	0,3	405.83572	430,18474	7147,60549
0,4	0,6	0,4	424.03616	430,18474	7147,60549
0,5	0,50001	0,49999	429.82967	430,18474	7147,60549
Variable lanthanide: Gd					
0	0,99999	0,00001	61.39321	353,70641	5876,90282
0,1	0,9	0,1	257.35337	353,70641	5876,90282
0,2	0,8	0,2	305.92158	353,70641	5876,90282
0,3	0,7	0,3	333.68617	353,70641	5876,90282
0,4	0,6	0,4	348.65093	353,70641	5876,90282
0,5	0,50001	0,49999	353.41447	353,70641	5876,90282

Figure 5: Table with calculations of $La_{1-x}Eu_xPO_4$ and $La_{1-x}Gd_xPO_4$ systems without taking into account the contribution of electronegativity at each step

To calculate the limits of substitutions, decomposition temperatures and assess the stability of solid solutions, it is necessary to know the parameters of interaction (mixing energy) of solid solutions. There are several theoretical and experimental methods for determining them. During the period 2007-2017, they were repeatedly used to calculate the interaction parameters in phosphate systems $La_{1-x}PO_4$ (Ln = Eu, Gd).

This was due to the fact that solid solutions of these systems are promising matrices for radioactive waste disposal, surpassing in many respects the aluminophosphate or borosilicate glass currently in use.

Table 2 shows the values of the parameters of the interaction of the mixing energy *Q*, kJ / mol for systems $La_{1-x}Eu_xPO_4$ and $La_{1-x}Gd_xPO_4$ with the structure of monazite, obtained by various authors and methods for the period 2007-2017, as well as the results obtained using the developed IIS.

As can be seen from this table, there is a significant variation in the parameters of interaction. Obviously, the most adequate results give average values. They are 8.3 kJ / mol and 13.5 kJ / mol, respectively $La_{1-x}Eu_xPO_4$ and $La_{1-x}Gd_xPO_4$.

For the system $La_{1-x}Eu_xPO_4$ the closest value of Q = 6.2 kJ / mol to the average (Q = 8.3 kJ / mol) was obtained by the method of Ab initio / strain energy. However, this method for the system $La_{1-x}Gd_xPO_4$ gives a value of Q = 8.6 kJ / mol, which differs significantly from the average (Q = 13.5 kJ / mol).

Similarly, the Drop solution method for the system $La_{1-x}Gd_xPO_4$ received the closest to the average (Q = 13.5 kJ / mol) value of Q = 11.4 kJ / mol. At the same time for the system $La_{1-x}Eu_xPO_4$ the same method obtained Q = 2.5 kJ / mol, ie much less than the average (Q = 8.3 kJ / mol). Thus, none of the above methods can be given a definitive advantage in determining the mixing energy.

Table 1

Interaction parameters (*Q*, kJ / mol) for systems $La_{1-x}Eu_xPO_4$ and $La_{1-x}Gd_xPO_4$

Q, kJ / mol		Method
Eu	Gd	
13,4	16,5	Ab initio
5,2	6,77	Strain energy
14±8	24±9	Drop calorimetry
6,2	8,6	Ab initio / strain energy
2,5±2,6	11,4±3,1	Drop solution
10,872±0,0086	10,564±0,0050	V. S. Urusov' crystal energy method (our IIS)

A comparative analysis of the data in table 2 shows that the results obtained by the proposed IIS are between the results obtained by the method of Ab initio quantum chemical calculations, and the data obtained by calculation according to the model of regular solid solutions. Therefore, we can assume that the results obtained by crystal-energy and quantum-chemical methods are consistent, and the results of IIS are more adequate than the published results for the system $La_{1-x}PO_4$ with the structure of monazite. In particular, the obtained IIS values of mixing energies for systems $La_{1-x}Eu_xPO_4$ and $La_{1-x}Gd_xPO_4$ (10,872 kJ / mol and 10,564 kJ / mol, respectively) closest to the average values of the above methods (8.7 kJ / mol and 12.97 kJ / mol), ie adequacy for the system $La_{1-x}Eu_xPO_4$ improved within 3.77% - 46.24%, and for the system $La_{1-x}Gd_xPO_4$ - within 8.66% - 66.45%.

The speed of forecasting has increased dramatically (by several orders of magnitude), because the actual forecasting process is not carried out experimentally (months for conducting and processing an expensive experiment), but by a calculation method based on the created IIS (hours for data entry).

6. Conclusions

This research work is devoted to solving the urgent problem of predicting the phase stability of solid solutions based on the determination of the limits of substitutions by the crystal chemical method in systems of solid solutions with isostructural components in the approximation of regular solid solutions.

In order to solve this problem, the existing knowledge bases and structures of IIS are analyzed and the requirements to the system designed to solve the research problem are determined.

To build the knowledge base of IIS, a mathematical model was developed, which, in contrast to the basic model of VS Urusov (in the approximation of regular solid solutions) is that when calculating the empirical parameter *C*, the contribution of electronegativity of each lanthanide is taken into account by the product of the substitution limit and electronegativity of the corresponding lanthanide, which allows to calculate accurate rather than total critical decomposition temperature. The adequacy of the model is proved by comparing the obtained forecasting results with the published results of solving this problem by known methods.

By formalizing the natural language flows on the basis of the concepts of language image and emotional state of the system, it is proposed to lay in the IIS interactive capabilities. The new approach takes into account quantitative assessments of the figurative meaning of natural language constructions and allows to obtain formal methods of generating 4 types of IIS messages by types of figurative search.

The technological implementation of IIS is substantiated - Pl / sql and Oracle APEX programming environment (Oracle Application Express) were chosen as the programming language for the server part; HTML hypertext markup language, CSS style language and Javascript language were chosen for the client part.

The architecture of the system is offered and programmatically implemented, taking into account its functionality the physical model of ER database is presented, the IIS interface is developed taking into account the needs of end users.

Thus, based on the study and construction of easy-to-operate IIS, the accuracy (compared to the known published results in the range of 3.77% - 66.45%) of predicting the phase stability of solid

solutions is increased. At the same time, the created IIS allowed to abandon experiments, which dramatically increased the speed of forecasting by several orders of magnitude.

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