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Author's Information

Nadezhda N.Kiselyova – A.A.Baikov Institute of Metallurgy and Materials Science of Russian Academy of Sciences, senior researcher, P.O.Box: 119991 GSP-1, 49, Leninskii Prospect, Moscow, Russia, e-mail: kis@ultra.imet.ac.ru

THE DISTRIBUTED SYSTEM OF DATABASES ON PROPERTIES OF INORGANIC SUBSTANCES AND MATERIALS

Nadezhda Kiselyova, Victor Dudarev, Ilya Prokoshev, Valentin Khorbenko, Andrey Stolyarenko, Dmitriy Murat, Victor Zemskov

Abstract: The principles of organization of the distributed system of databases on properties of inorganic substances and materials based on the use of a special reference database are considered. The last includes not only information on a site of the data about the certain substance in other databases but also brief information on the most widespread properties of inorganic substances. The proposed principles were successfully realized at the creation of the distributed system of databases on properties of inorganic compounds developed by A.A.Baikov Institute of Metallurgy and Materials Science of the Russian Academy of Sciences.

Keywords: database, distributed information system, inorganic substances and materials, reference database.

ACM Classification Keywords: H.2.4 Distributed databases, H.2.8 Scientific databases.

Introduction

Now hundreds thousand of inorganic compounds are known. Every year thousands of new substances are added to them. In connection with diversity of applications of inorganic materials, the information on them is scattered over the most various publications. Therefore a search for the information about properties of inorganic compounds, especially if they have been synthesized recently, frequently makes a considerable difficulty and not always it achieves success. A consequence of it is the duplication of investigations on synthesis and research of inorganic substances. In addition, the experts not always can find already synthesized substance that is the most suitable for certain applications. The necessity of acceleration of researches on development and application of new materials were the reasons of creation of numerous databases (DB) on properties of inorganic substances. Thousand of such databases considerably have improved information service for the experts in the field of inorganic chemistry and materials science however there was another problem - problem of a search for DB, in which the needed information on the certain inorganic substances is stored.

Structure of the Distributed System of Databases on Properties of Inorganic Substances and Materials

One of ways of the solution of this problem is the development of some reference database (RDB), which would store the information on where to search for the necessary information on the substance. The distributed system of databases of A.A.Baikov Institute of Metallurgy and Materials Science of the Russian Academy of Sciences (IMET RAS) (fig.1), submitted in the present paper, is a prototype of such information system.

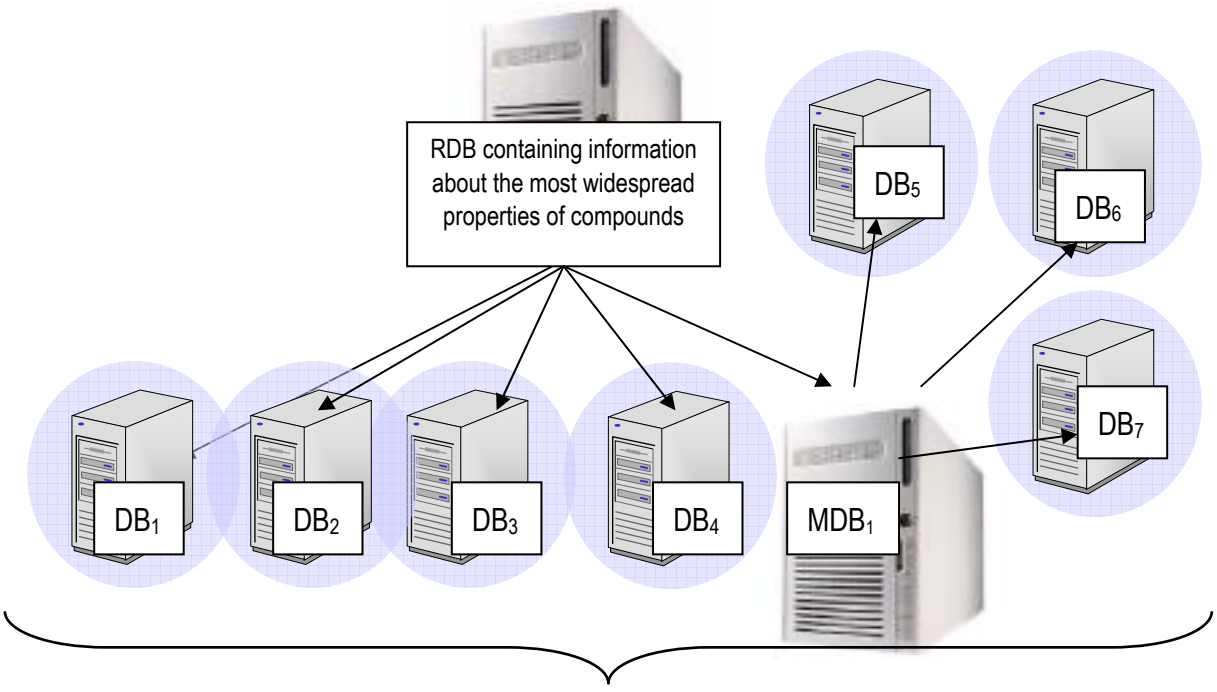

Fig.1. Principles of design of the distributed system of databases on properties of inorganic substances and materials

In this case the DB on properties of inorganic substances «Phases» [Kiseleva et al., 1996], which contains not only data on a site of the various information in other DB but also brief information on the most widespread properties of tens thousand of compounds, for example, melting and boiling points, symmetry of a crystal lattice, etc. (fig.2), carries out the role of a reference database. RDB provides a search for the relevant information

on chemical substances and their properties. The detailed information on substances, which have practical importance, is stored in ordinary DBs, for example, in DBs on properties of materials for electronics [Kiselyova et al., 2004; Khristoforov et al., 2001] developed by us. Thus, the distributed information system, integrated at a level of Web-interfaces, is created.

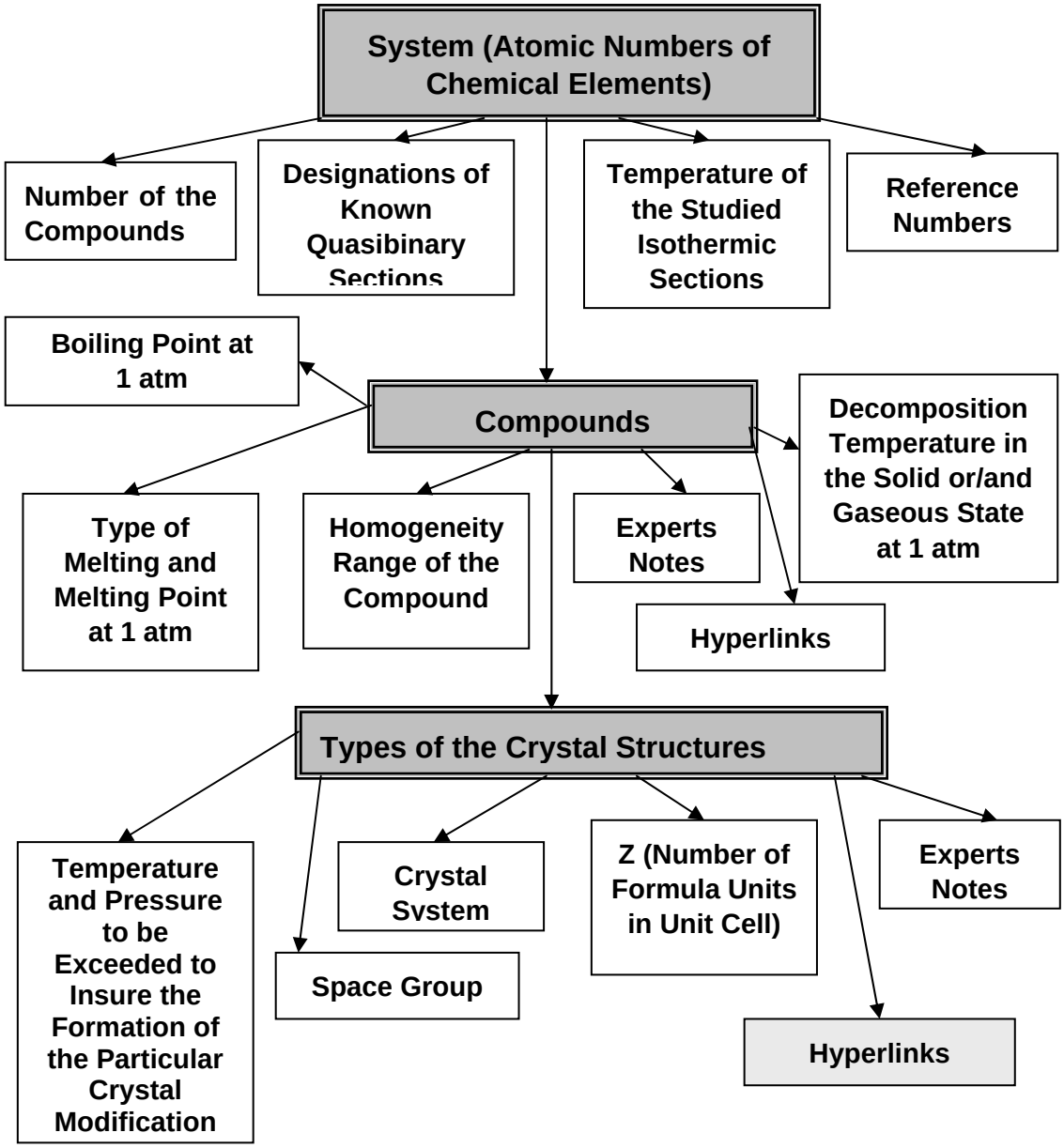

Fig.2. Structure of RDB «Phases»

The concept of design of a special reference database - metabase (MDB) - in the distributed system of the Russian databases on materials for electronics is considered in the terms of the set theory in the paper [Kornyushko et al., 2005]. As shown in this work the search for the relevant information on certain system s can be reduced to definition of the relation R being a subset of Cartesian product, $S \times S$ (in other words, $R \subset S^2$). Here set S is information on substances and systems stored in MDB. The relation R is symmetric at design of the distributed system of DBs on materials for electronics [Kornyushko et al., 2005], since the information of integrated DB mutually supplements each other. Let's note that not always relation R should be strictly symmetric.

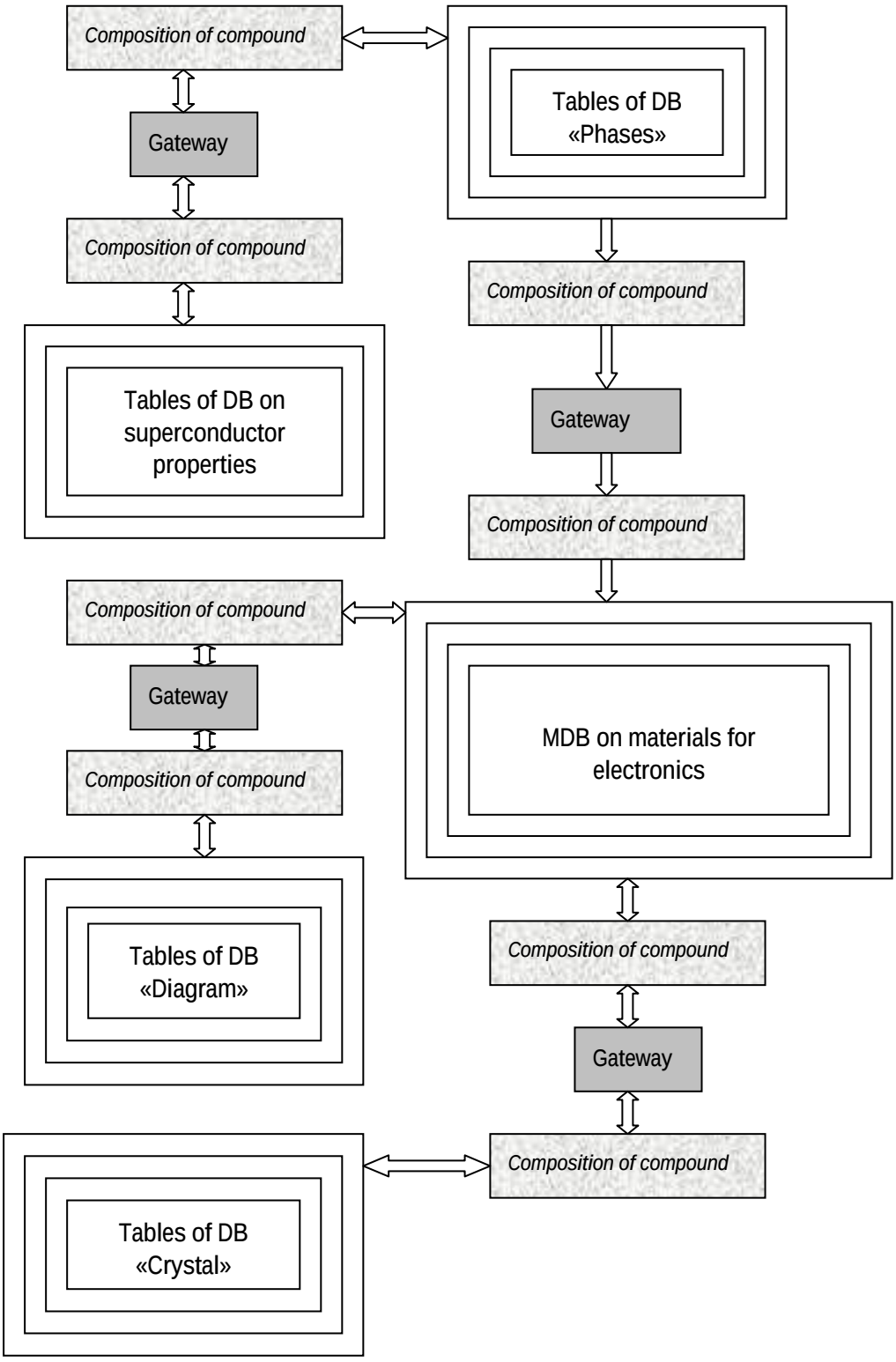

Fig.3. Structure of the distributed system of DBs of IMET RAS

For example, RDB on properties of inorganic substances “Phase” [Kiseleva et al., 1996] contains only brief information on tens thousand of chemical compounds, but specialized DB on properties of acoustic-optical, electro-optical and non-linear optical substances “Crystal” [Kiselyova et al., 2004] or DB on the phase diagrams of semiconductor systems “Diagram” [Khristoforov et al., 2001] contain the detailed information on hundreds substances promising for practical applications. Certainly, the users of the specialized systems own more detailed data in comparison with the information stored in RDB “Phase”. Hence, the users of RDB “Phase”, who search for the relevant information, must have an access to the data in specialized DB, and users, for example, of DB “Diagram” do not have the access to the relevant information on properties of compound from RDB “Phase”.

Hence, in this case relation of relevance, given in [Kornyushko et al., 2005], requires the certain updating. Assume that we have relation N, which describes inadmissible transitions from determined DB into others DB (transitions of a kind $d_1 \to d_2$). Here set D is information on databases. That is if $d_1, d_2 \in D$ and pair $(d_1, d_2) \in N$, the transition from integrated information system d_1 into system d_2 is inadmissible.

For example, if user looks through the information on certain property of compound in one of DB (i.e. actually there is an access to the information determined by a pair (d_1, s_1)), he can have the relevant information on some property of chemical system from another DB, determined by pair (d_2, s_2). As a result, user receives the required new relation of relevance RN as $RN \subset (d_1, s_1) \times (d_2, s_2)$, where $d_1, d_2 \in D; s_1, s_2 \in S$. Thus, the new relation of relevance RN can be constructed on the basis of the old relation R and set N according to the following rule: for any chemical systems $s_1 \in S, s_2 \in S$, if $(s_1, s_2) \in R$ and $d_1, d_2 \notin D$, then $(d_1, s_1), (d_2, s_2) \in R$.

Such decision of a problem of the search for relevant data about properties of substances has many advantages main of which are: simplicity of expansion of the distributed information system, independence on software and hardware platforms, opportunity of actualization and administration of DBs by different organizations which are located in different cities and even in different countries, reduction of traffic, an use of not so powerful, inexpensive servers.

The data on chemical composition (the list of chemical elements and their ratios) are external keys of RDB and various DBs in the distributed system of databases of IMET RAS on properties of inorganic substances and materials (fig.3). It is the most general characteristic of substances, which is inherent in all inorganic objects. Now the distributed system includes besides DB «Phase», in which now the information on properties of ternary compounds is stored, the DB on properties of ternary compounds-superconductors, the DB on properties of acoustic-optical, electro-optical and non-linear optical substances “Crystal” [Kiselyova et al., 2004], DB on phase diagrams of semiconductor systems “Diagram” [Khristoforov et al., 2001] and DB on bandgaps of semiconductors “BandGap”. The latest three DBs, functioning with the use of various software and hardware platforms, were integrated on the basis of the use of special metabase on properties of materials for electronics [Kiselyova et al., 2004; Kornyushko et al., 2005]. Further the distributed system of databases will include other Russian DBs on properties of materials for electronics: DB on intermolecular potentials for components of the CVD processes in microelectronics (Joint Institute of High Temperature of the Russian Academy of Sciences), information system for modeling processes of preparation of epitaxy of hetero-structures of semiconductor materials by the method of liquid epitaxy (M.V.Lomonosov Moscow State Academy of Fine Chemical Technology), etc.

Conclusion

The system of databases of IMET RAS is accessible for the registered users of the Internet: http://www.imet-db.ru.

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Authors' Information

Nadezhda N.Kiselyova – A.A.Baikov Institute of Metallurgy and Materials Science of Russian Academy of Sciences, leading researcher, P.O.Box: 119991 GSP-1, 49, Leninskii Prospect, Moscow, Russia, e-mail: kis@ultra.imet.ac.ru

Victor A.Dudarev – A.A.Baikov Institute of Metallurgy and Materials Science of Russian Academy of Sciences, programmer, P.O.Box: 119991 GSP-1, 49, Leninskii Prospect, Moscow, Russia, e-mail: vic@osg.ru

Ilya V.Prokoshev – A.A.Baikov Institute of Metallurgy and Materials Science of Russian Academy of Sciences, leading engineer, P.O.Box: 119991 GSP-1, 49, Leninskii Prospect, Moscow, Russia, e-mail: eldream@e-music.ru

Valentin V.Khorbenko – A.A.Baikov Institute of Metallurgy and Materials Science of Russian Academy of Sciences, programmer, P.O.Box: 119991 GSP-1, 49, Leninskii Prospect, Moscow, Russia, e-mail: Khorbenko_v@mail.ru

Andrey V.Stolyarenko – Moscow Institute of Electronics and Mathematics (Technical University), post-graduate student, P.O.Box: 109028, B.Trehsvjatitelsky per. 3/12, Moscow, Russia, e-mail: stol-drew@yandex.ru

Dmitriy P.Murat – Moscow Institute of Electronics and Mathematics (Technical University), post-graduate student, P.O.Box: 109028, B.Trehsvjatitelsky per. 3/12, Moscow, Russia, e-mail: mr_wire@mail.ru

Victor S.Zemskov – A.A.Baikov Institute of Metallurgy and Materials Science of Russian Academy of Sciences, head of Laboratory of Semiconducting Materials, P.O.Box: 119991 GSP-1, 49, Leninskii Prospect, Moscow, Russia, e-mail: zemskov@ultra.imet.ac.ru

TRAINING A LINEAR NEURAL NETWORK WITH A STABLE LSP SOLUTION FOR JAMMING CANCELLATION

Elena Revunova, Dmitri Rachkovskij

Abstract: Two jamming cancellation algorithms are developed based on a stable solution of least squares problem (LSP) provided by regularization. They are based on filtered singular value decomposition (SVD) and modifications of the Greville formula. Both algorithms allow an efficient hardware implementation. Testing results on artificial data modeling difficult real-world situations are also provided

Keywords: jamming cancellation, approximation, least squares problem, stable solution, recurrent solution, neural networks, incremental training, filtered SVD, Greville formula

ACM Classification Keywords: I.5.4 Signal processing, G.1.2 Least squares approximation, I.5.1 Neural nets