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THE CONCEPTION AND ARCHITECTURE OF THE INTERNET PORTAL FOR THE STUDY OF THERMOPHYSICAL PROPERTIES OF MATERIALS

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Abstract We consider the Internet knowledge portal that provides intelligent analysis and integration of knowledge and information resources for the study of thermal properties of materials, including organic and inorganic materials in a wide temperature range. The portal provides a systematization and integration of available information resources in a single information space. The use of ontology to describe the domain of the portal allows to structure its content semantically and organize it for navigation and meaningful information search. For the development of this portal a technology oriented to a subject domain experts is used. The portal includes a system to import data from files to a database (DB) which can be local or remote. Resources developed on the basis of free software products are used to display the data as interactive graphs using smoothing algorithms, interpolation and approximation.

Key words: Knowledge portal, thermophysical properties of materials, information resources, ontology, meaningful search, ontology-driven navigation.

AMS Mathematics Subject Classification: 68T30, 68Q55, 97R50

1 Introduction

Recently, specialized commercial software packages that allow to obtain data on thermophysical properties for certain classes of substances and materials are actively developed and used in the world. An experience of a practical use of these programs revealed their significant drawbacks. They do not give access to a tables of primary experimental data, do not allow to select the model for a data processing. The models used are not physically based, which does not allow for extrapolation of data, there is also no real possibility of predicting a properties, etc. All this makes them suitable only for engineering calculations rather than research. The information system that could combine the advantages of existing software and eliminate the above disadvantages would be an important tool for the development of theories of substance properties and phase transformations.

Integration of information resources into a single information environment and providing access to computing resources is also one of the main directions of development of modern information technologies. Addressing the creation and integration of information resources and products is becoming a prerequisite for development in many countries, including Russia.

2 The current state of the problem.

Existing scientific databases contain information about the properties of the objects under study and are either purely factographic or even contain bibliographical and textual information.

Among the most famous documentaries EC Science-direct [1], Wiley [2], American Chemical Society [3], Chemical Abstract Service [4], VINITI [5], e-library [6]. According to the total volume of data they are superior to factual IP. The National Institute of Standards and Technology (National Institute of Standards and Technology - NIST) developed a resource "NIST Chemistry WebBook" - http://webbook.nist.gov/ [7].

It provides access to data collected and distributed by NIST the program reference data. The Institute of High Temperatures, Russian Academy of Sciences and the Moscow Energy Institute created, created a resource http://thermophysics.ru/triptych/ - "Information triptych thermal properties of substances: a guide to the Internet, a knowledge base and an electronic reference" [8]. This resource is an information and analytical system for the storage and distribution of bibliographic and numerical data on the thermal properties of substances. For the exchange of heterogeneous data of differing formats and structure developed Thermodynamic Research Center of the US exchange standard thermodynamic data, COSTAT (Codata STAndard Thermodynamics), was developed Thermodynamic Research Center of the United States for several years under the auspices of the International Commission on numerical data (CODATA) [9]. The most advanced in the creation of such ICs are researchers from the National Institute of Standards and Technology, USA [10] and the National Institute for Materials Science, Japan. [11] These organizations have created and are actively developing material science complex information systems. Successful work is carried out in Russia - in the High Temperatures Institute for High Temperatures [12]. The current state of Thermal Physics, as a science, accompanied by the enormous scale of the new data, published in the journal Physical, chemical and engineering profiles. Among them, the demand Journal of Chemical and Engineering Data [13], Journal of Chemical Thermodynamics [14], Fluid Phase Equilibria [15].

That is why the creation of online databases that allow to collect, organize scientific information and make it accessible to a wide range of researchers, is an urgent task. At the present stage it is through the development and creation of a network database based on WWW-technology it is possible to make the collected information available to the widest possible range of users and thus significantly improve the efficiency of research.

2.1 Justification of the work. Goals and objectives.

The need of many researchers in reliable information on the state diagrams of multicomponent systems and thermodynamic properties is extremely high. A factual material on these issues existing in literature is scattered over a huge number of periodicals many of which are not available because of their absence in a libraries of a city, a region and even the country. Also a reference material is often poorly accessible or outdated. Suffice it to say that in the libraries of such major scientific center like Yekaterinburg there are reference books on state diagrams issued merely 30-40 years ago generally. There is no even the famous reference book of R.Haltgrena et al (R.Hultgren, P.D.Desai, D.T.Hamkins, M.Gleiser, K.K.Kelley. Selected values of the thermodynamic properties of binary alloys. ASM. Metal Park. Ohio. 1973), not to mention later editions. Specialized magazines, for example Bull. of Phase Diagrams, CALPHAD, are unavailable. That is why the creation of online databases allowing to collect, organize scientific information and make it accessible to a wide range of researchers is a task of current interest. Until recently database created by different groups were available only to a limited number of users. It concerns ACTPA.OWN databank supported by Institute of Metallurgy of Ural Branch of Russian Academy of Sciences (UB RAS). However, at the present stage it is the development and creation of a network database based on WWW-technology that makes the collected information available to the widest possible range of users and thus significantly improve the efficiency of research.

2.2 Ontological approach.

Thermal physics is one of the disciplines in which work with numerical data takes center stage. When working with them one must take into account that several standard forms namely tabular, graphical and mathematical (in the form of stored formulas or programming code) are used in publications and databases. Graphic format illustrates the nature of dependency, scattering of experimental points, etc. The tabular form is the most reliable on data transmission, easily controllable with in regard to omissions, errors in the sign or the order of magnitude, etc. The mathematical form eliminates the need for interpolation but requires increased thoroughness in error detection. A prevalent form in experimental studies and references is a tabular form.

To provide the possibility described above for users, the knowledge portal developing must not only have flexible means of providing diverse information and meaningful accessing to it but also to provide the operational management of its information content. The information model of the knowledge portal that describes the subject area serves all of this goals.

A promising approach in the design of information system is a simulation of subject area using ontology [16]. The classic definition of term "ontology" was given by Gruber [17] and modified by Borst [18]: "Ontology is a formal specification of a shared conceptualization". Conceptualization refers to strict description of domain concepts and semantic relations between them, including one by means of natural language. Conceptualization should be shared, that is it should commit common knowledge recognized by some group and not the private knowledge of a particular individual. Formal specification refers to a knowledge (concepts) representation in a certain formal format, for example in terms of a language understood by a machine.

Thus, the ontology allows us to describe the subject area in a formal language that allows us to operate the concepts of the domain within the information system [19]. This is the approach we use to interact with data on thermal properties of substances and materials [20-21]. The ontology developed must adequately describe a given subject area. It should be the basis for the information systems working with thermal properties of substances and materials.

One of the most popular and appropriate formal systems for describing ontologies is OWL (Web Ontology Language) based on Description Logics (DL). Around the OWL community is formed, application programming interfaces (API), reasoners, applications are developed.

Domain knowledge can be divided into two types: the first is more stable and permanent and the latter is more prone to modifications. In accordance with this division, knowledge written in the OWL is divided into a set of terminological axioms (TBox, terminological box) and a set of assertion axioms (ABox, assertion box). The union of both these axiom sets makes up of knowledge base (ontology).

The objects of research in thermal physics are materials, including substances. Material is an object whose properties can be appreciably defined by area of production: the manufacturer, brand, technology, storage conditions and so on. The substance is an object whose properties are defined by its nature: the stoichiometric formula, composition, phase and other. Figure 1 shows the basic concepts related to data on the properties of substances.

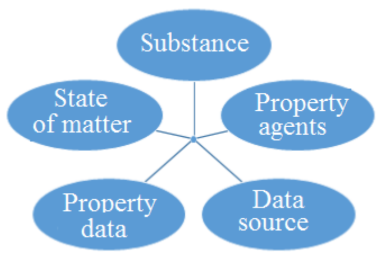

Figure 1: Basic Concepts in thermal physics.

Then the master record of the thermal data is the following: "A given substance in a given state has a given property with a given value obtained from a given source".

2.2.1 Substance.

There are several methods of identifying a substance:

1. CAS (Chemical Abstracts Service) number.
2. Name.
3. Chemical formula.
4. Composition (for mixtures).

2.2.2 State.

A substance may exist in different states:

1. Single–phase state.
   Phase.
   - Solids (different orientational and translational order).
   - Liquids (different orientational order).

   - Gas.
   - Plasma.

2. Two–phase state.
   Interphase boundary (equilibrium line).

   - "liquid-gas" - boiling/evaporation curve;
   - "solid-gas" - sublimation curve;
   - "solid-liquid" - melting curve;
   - "solid-solid";
   - "liquid-liquid".

3. Three–phase state. Special point (equilibrium point).

   - triple points;
   - critical point.

2.2.3 Data.

A value of substance property may be:

1. Constant.

2. Single variable function:

   - analytical;
   - tabular (one-dimensional).

3. Two variables function:

- analytical

- tabular (two-dimensional).

In most cases, a property dependent on the temperature and is measured in an experiment at different temperatures. The result is a one-dimensional table. If a property also depends on the pressure and is measured at different pressures, we get a two-dimensional table.

2.2.4 Source.

A data source in thermal physics may be:

1. Databases.

2. Articles.

3. Own experiments.

3 Architecture of the information system.

Multilevel client-server architecture is used for information system (IS) implementation. According to the separation of concerns (SoC) principle business logic is taken out into a separate module. The graphical Web user interface (Web UI) communicates with the main application (server) via the Application Program Interface (API) over HTTP. JSON is chosen as the requests and responses format. Other applications may also interact with the server via the API.

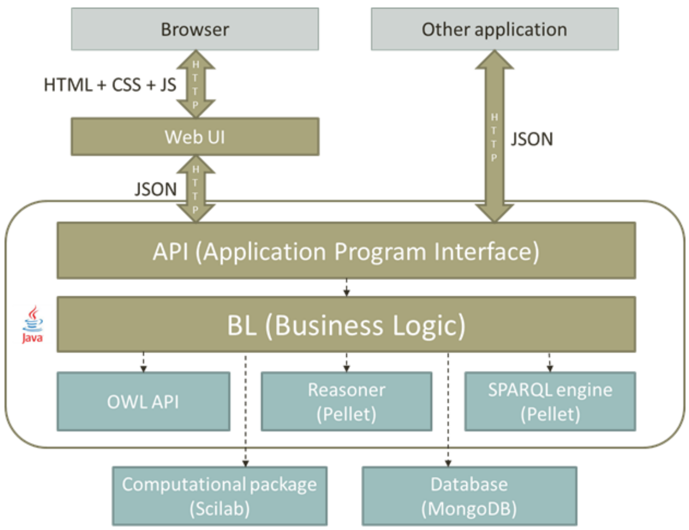

Figure 2: Architecture of the IS.

All numerical data describing the properties of materials are stored in non-relational database MongoDB. Numerical data processing may require both simple and complex mathematical calculations. Integration with a numerical computational package is needed for this purpose. This information system is integrated with the Scilab [22].

3.1 Functionality of the IS.

An important component of the information system is the graphical user interface. So with its help materials classification is displayed (Fig.3).

Figure 4 shows the phase diagram of water. It is built automatically, based on the data available.

Figure 5 shows the result of the processing of the experimental data on the Nickel density depending on the temperature. Two phases of substance (solid and liquid) were investigated, including the phase transition (melting) between them. We can not process the entire set of data (due to the presence of a phase transition), so we process data portions with smooth curves in a single state. For each data portion approximation is calculated and displayed.

The following can be displayed on the same plot:

- all available data on the property (from all sources);
- specific data from a single source;

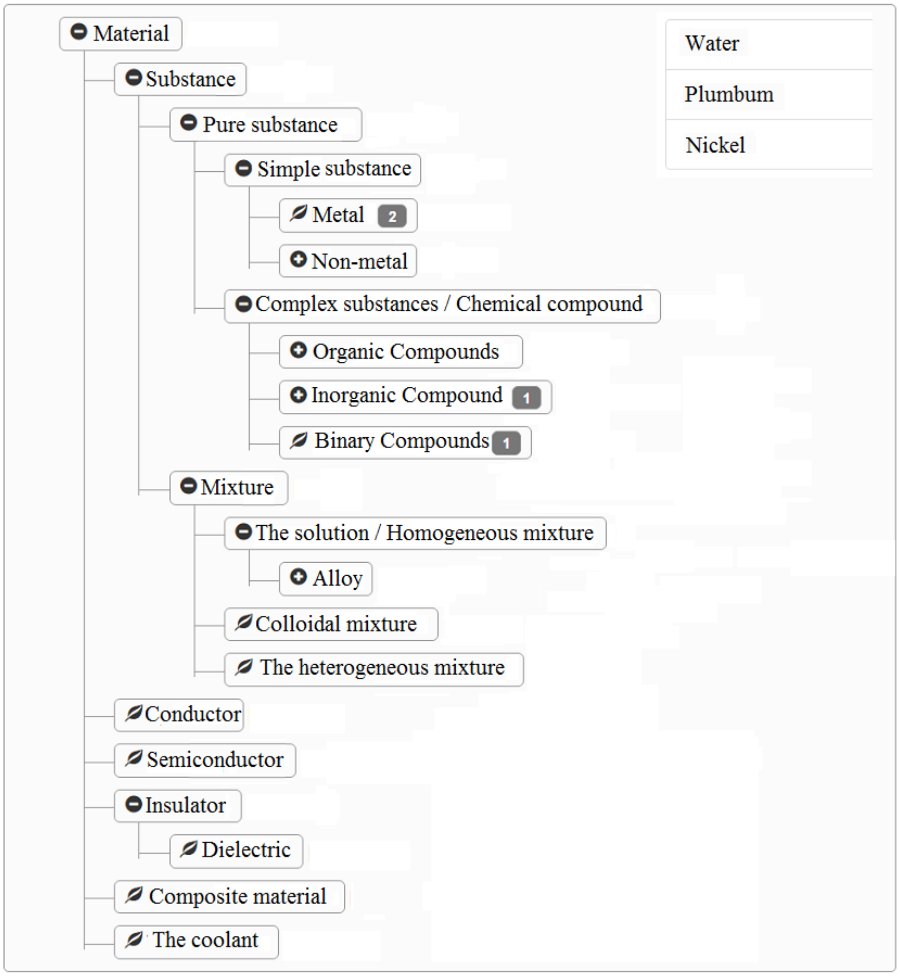

Figure 3: Materials classification.

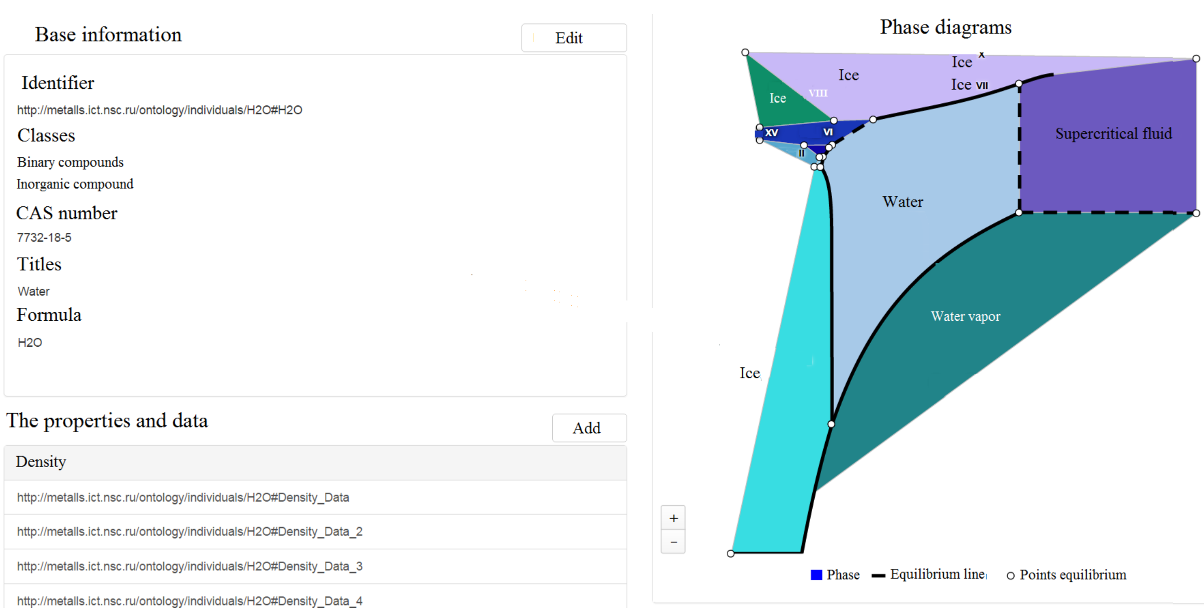

Figure 4: Phase diagram of water

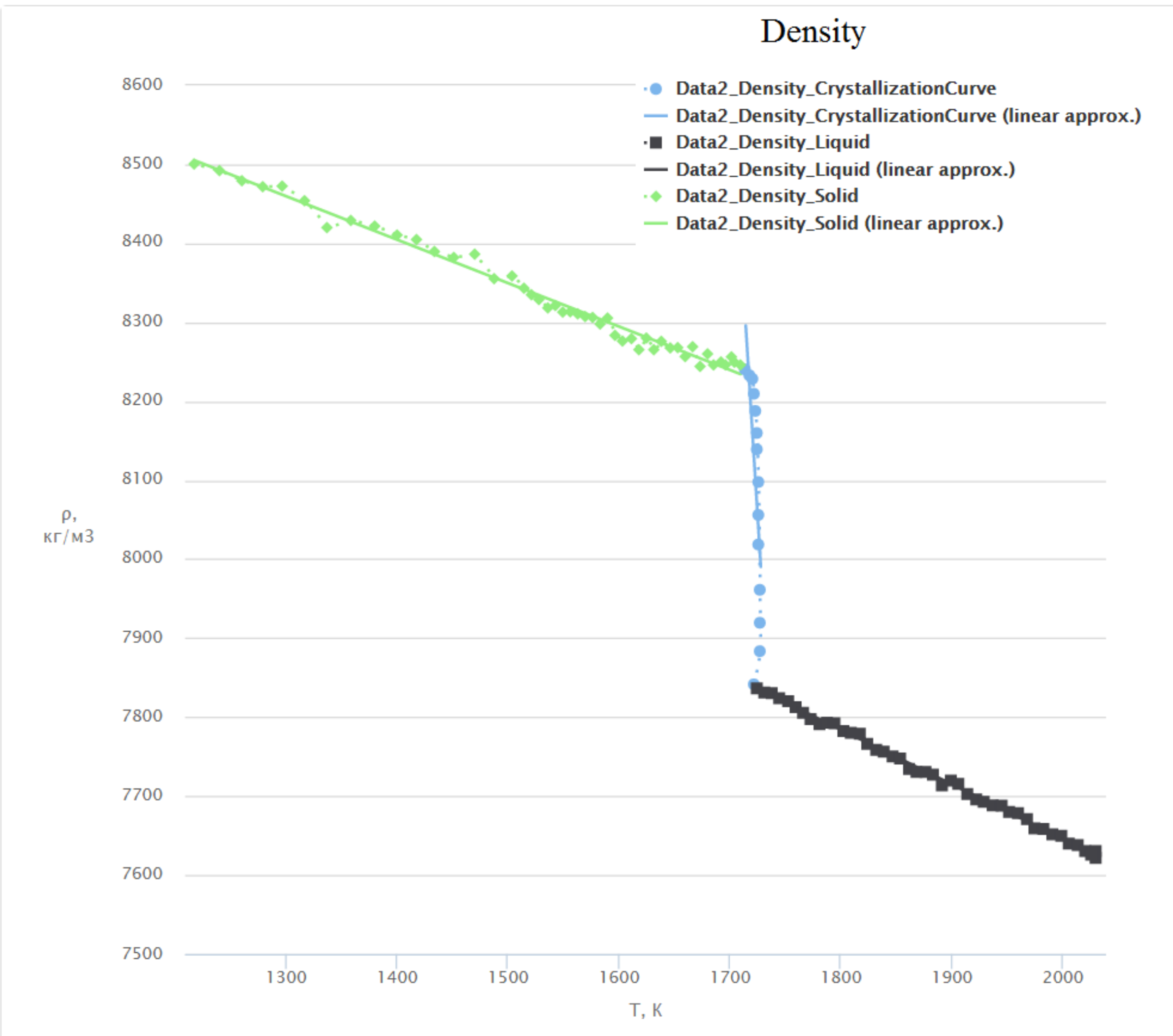

Figure 5: Changes in the density of Ni depending on the temperature.

- part of the data from a single source related to a single substance state.

4 Conclusion.

The knowledge portal considered provides a systematization and integration of knowledge, primary experimental data and research data presented in scientific literature related to a study of materials properties into a single information space and meaningful access to them.

The ability to import data from files, view and edit it is implemented. The result of data processing may be presented both in tabular and graphical form using approximation algorithms.

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