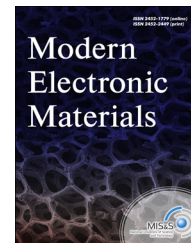




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Object-relational architecture of information support of the multi-circuit calculation multilayer semiconductor nanostructures

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Database;
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Abstract

The article examines the object-relational approach to the creation of a database designed to provide informational support to the multiscale computational scheme of multilayer semiconductor nanostructures. The MSNS computational scheme developed earlier by our group uses a hierarchic representation of computational data obtained by various computational modules. Each layer of MSNS is treated separately. In contrast to well-known materials databases which serve for storing and retrieving of information on existing structures and their properties the database described in this paper is the central unit of the MSNS computational scheme. The database provides data interchange between various computational units. In this paper we describe the modern approach to material database design. More specifically, a data storage relational model which applies to solving resource-intensive and different-scale problems is proposed. An object-relational scheduler architecture is used in our work. It provides for high-speed data exchange between various computational units of the MSNS computational scheme. We introduce a simple and user-friendly interface allowing criteria-based data retrieving as well as creation of input files for computational modules. These approaches can be applied in various branches of science, including the aviation and space industry, in particular in control systems of engineering (materials science) data.

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1. Introduction

The use of imitation modeling for the development of new technologies of multilayered semiconductor nanostructures with desired properties is an important task of modern science.

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There are a wide range of materials science databases, but each of deals with the problem from a specific viewpoint. One can separate several groups.

1. Databases of physical properties of various materials.
These databases contain information on physical properties of materials but most of them contain no information on the crystalline structure of the compounds. Such databases are, for example, Chemical Abstracts Service, Cambridge Scientific Abstracts METADEX, MIT Material Properties Database [1] and semiconductors database of the A.F. Ioffe PTI, RAS [2].
2. Crystallographic databases.
The databases of this group contain information on the structure of a wide range of chemical compounds but only little information on the required physical properties. Such databases are, for example, Crystallography Open Database, Inorganic Crystal Structure Data, and NIST Structural Database.
3. Databases of articles on materials science.

An advantage of these databases is a wide choice of information on various properties of materials. Their disadvantages, however, include the following: the data contained therein are often poorly systematized, this being a large hinder to the search and further work with them. Example of such databases is Ulrich's Periodical Directory.

The aim of this work is to design software providing for information support of calculation experiments aimed at prediction modeling of new multilayered semiconductor nanostructures with desired parameters and predictable properties.

2. Specific features of the information support architecture for multilayered semiconductor nanostructure calculation

A multilayered semiconductor nanostructure (MSNS) is an inhomogeneous structure grown on a substrate and consisting of multiple semiconductor layers having specific thicknesses (measured in nm), chemical compositions and generally differing in band gap and crystalline structure parameters. During the synthesis of these structures a heterojunction forms between two different layers that may contain higher carrier concentration. Following the hierarchic representation of multilayered semiconductor nanostructures suggested earlier [3] one can separate the following components of MSNS:

1. the substrate which is a crystalline basis onto which semiconductor layers are applied;
2. the crystalline semiconductor matrix which is a layer having specific chemical composition and crystalline structure;
3. the interfaces which are interlayer boundaries;
4. the subsurface and superficial crystalline matrices adjacent to the interface (subsurface layers containing 1 to 3 atomic layers).

The database (DB) designed in this work is component of the multiscale computational scheme (MSCS) for the calculation of

the structure and properties of MSNS reported earlier [3]. This scheme also includes units based on the static and dynamic models of solids. The unit consisting of software modules relying upon a statistical model is used for the theoretical calculation of the equilibrium properties of semiconductor crystalline structures and MSNS on their basis. It includes different software modules, for example, the software module for close packing of single crystals based on the ionic-atomic radii model [4,5] allows determining the metrical parameters, including basis atom coordinates and unit sizes, for individual crystalline layers of MSNS on the basis of crystallochemical information. The software module based on quantum-mechanical calculations used for the modeling of the atomic crystalline and electronic structure as well as several properties of MSNS includes methods of first-principles molecular dynamics within the electron density functional theory with the use of plane wave basis and PAW potentials (the VASP [6] and PWsef [7] software complexes) [8,9]. The dynamic unit includes software models for the modeling of MSNS structural changes in time, for example, to study early stages of MSNS growth, analyze structures that contain defect, including linear ones, etc.. These computational modules are based on the use of molecular dynamics methods (with the atomic interaction potential parameters being chosen on the basis of first-principles calculation DB), kinetic Monte-Carlo method etc.. The DB reported in this work contains calculated and experimental data on the crystalline structures and chemical compositions of both individual MSNS layers and entire structures. Furthermore, it provides for the storage of intermediate calculation results and data exchange between computational modules. The DB will be used for the storage of calculation results on different physical properties of semiconductors and data on the synthesis methods of specific semiconductor nanostructures.

Figure 1 shows examples of the hierarchic representation for the GaN/Si (InN/Si) semiconductor nanostructure and for the GaN/AlGaN/AlN multilayered semiconductor nanostructure on an Al₂O₃ substrate. Data on each individual layer are stored in the DB separately. For example, the DB stores information on the Si crystalline matrix, the subsurface Si layer, the interface, the subsurface GaN layer and the GaN crystalline matrix (Figure 1a). A similar information storage method is used for the GaN/AlGaN/AlN/Al₂O₃ structure shown in Figure 1b.

Based on data operation descriptions and information flow specifications, the scheduler should provide for interaction between the computational modules of the multiscale computational scheme (input data of one module are output data of another module) [3].

For the creation of the MSCS we used a hierarchic sequence of computational algorithms. The MSCS consists of two main units each of which corresponds to the static and dynamic models and the respective database scheme. The MSCS units contain computational modules. Each computational module is intended for the solution of specific tasks and can be treated as a separate application with specific functionality. For designing the information support we used a sequential hierarchic representation and storage of data with the support of the respective structure-property relationships at different structure hierarchy levels. For a specific MSNS, source and calculated data are collected for each crystalline matrix of the substrate, each

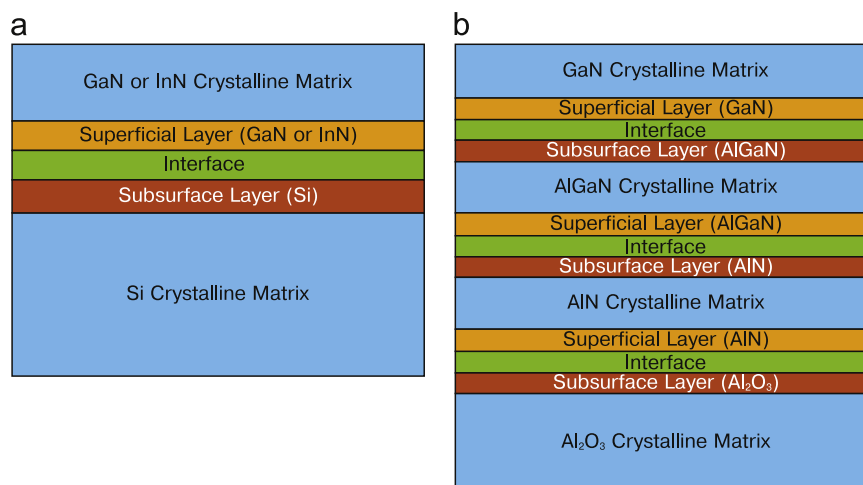


Figure 1 (a) GaN/AlGaIn/AlN/Si and (b) GaN/AlGaIn/AlN/Al₂O₃ semiconductor nanostructures.

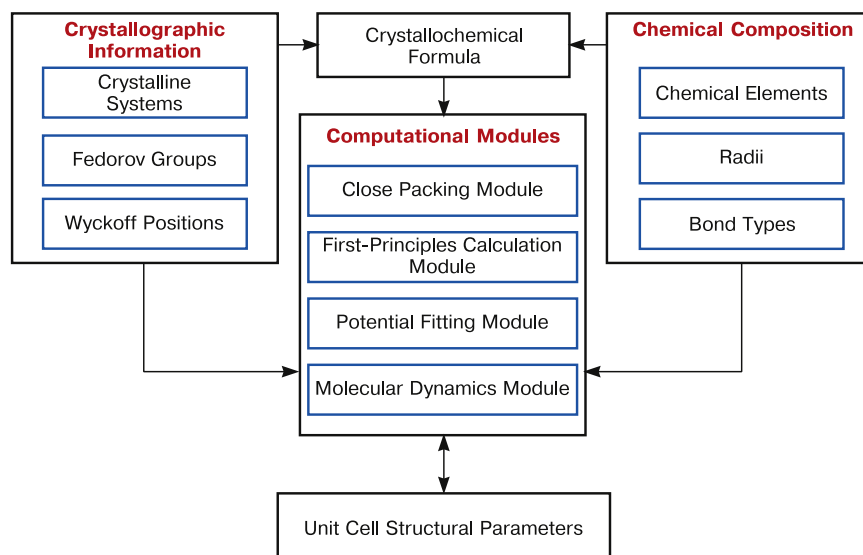


Figure 2 Database flowchart.

subsurface and superficial layer and each interface in tabular form. Then the resultant data are integrated and compared with available experimental data or MSCS-calculated macroscopic properties of the entire multi-layered semiconductor nanostructure.

Our work resulted in the creation of a relational data storage model [10] and the development of an object-relational scheduler architecture. Figure 2 shows flowchart of the designed DB.

According to the above flowchart, each single layer (the Crystallochemical Formula Module) is associated with parameters obtained using various computational modules (the many-to-one relation), its chemical composition (the one-to-many relation) and compound geometry (the many-to-one relation).

The chemical formula of the composition (the Chemical Composition Module) and the Mendeleev Table elements are in the many-to-many relation. It is implemented using the associative nature. The chemical elements and radius types are also in the many-to-many relation (because each

chemical element may correspond to multiple radii for different bond types). This relation is implemented by introducing the associative nature which includes the values of radii and a reference to a table containing additional information, i.e. charge and coordination number of the specific atom.

The Fedorov group (the Crystallographic Information Module) pertains to a specific crystallographic system (the many-to-one relation). For each Fedorov group, a set of Wyckoff positions are determined that refer to it through an external key (the one-to-many relation). The Wyckoff positions pertain to a specific type that in turn is determined by the table of Wyckoff position types. The condition of an atom's pertinence to a specific Wyckoff position means that the center of the atom is within a certain space, lies in a plane or on a line etc.. In other words this condition limits the range of the atom's coordinates.

The unit cell (the Unit Cell Structural Parameters Module) corresponding to the single layer in question is represented both by its own parameters and by the set of its constituent

atoms as well as the bonds between them (the one-to-many relation). The atoms and the bonds refer to the containing cell through an external key. Furthermore, each bond refers to the pair of atoms it links (two one-to-many relations).

The single layer in question is described by its chemical composition (formula) and crystalline structure. Also, an important factor for determining the chemical formula is the number of components and the type of the chemical bond (ionic, covalent etc.).

The geometry of the compound is determined by the Fedorov group (which pertains to a specific crystalline system). Each chemical component constituting the chemical composition is associated with its atomic radius (depending on the type of the bond in the compound) and the Wyckoff position (depending on the Fedorov group selected and taking into account the order of each specific atom constituting the chemical formula). In case of the ionic bond type, the coordination number and charge of the atom are also important for the selection of the atomic radius.

The single layer with preset chemical formula and crystalline structure is associated with computation results that can be obtained using different computational modules (the Close Packing Module, the First-Principle Calculation Module, the Potential Fitting Module and the Molecular Dynamics Module).

The result are the physical properties (closeness of packing, full energy, distribution of electron densities etc.) and the structural parameters (lattice constants, angles and atom coordinates). Data obtained using one module can be used as input data for another module.

We used the application that implements the scheduler functions to plot a map of the relational model in the object model and implemented the user interface (Figure 3) allowing data sampling based on the preset criterion and save the query processing result in a text file for further importing into a chain of computational modules.

The implementation of the object-relational mapping (ORM) was based on the NHibernate technology [11,12]. Its important characteristic is the abstract invariant data mapping model that can be easily adapted to the user interface layer (the mapping mechanism) and to the DBMS environment (the connection mechanism). In the course of this work we used a C# code and the respective Fluent NHibernate library for mapping.

By way of example we will show how the scheduler forms maps and imported working files in the DB for the computational software modules of the MSCS. In the user-friendly graphic interface (Figure 3) the user sets the number of components constituting the required chemical formula, enters the names of the constituent chemical elements (the basis atoms) and their coefficients in the chemical formula. Depending on the type of the chemical bond in the material (ionic, covalent etc.) the user can choose the radii of the basis atoms taking into account the respective coordination numbers [4]. Then the geometry of the structure in question should be set. From the list of all the possible Fedorov symmetry groups and the corresponding sets of possible Wyckoff positions that determine the ranges of coordinates for the basis atoms constituting the chemical formula, the user chooses a specific geometrical representation of the chemical formula. The work of this module results in a file containing data on the chemical composition and the atomic radii of the chemical elements of which the material in question consists. Thus, the DB forms maps and working files for the computational modules that can be modified by the user if necessary. Results of the work of other MSCS computational modules are also saved in the special subsystem of the DB [13].

For creating information support for the storage and management of properties of multilayered semiconductor nanostructures we used the following software and technology:

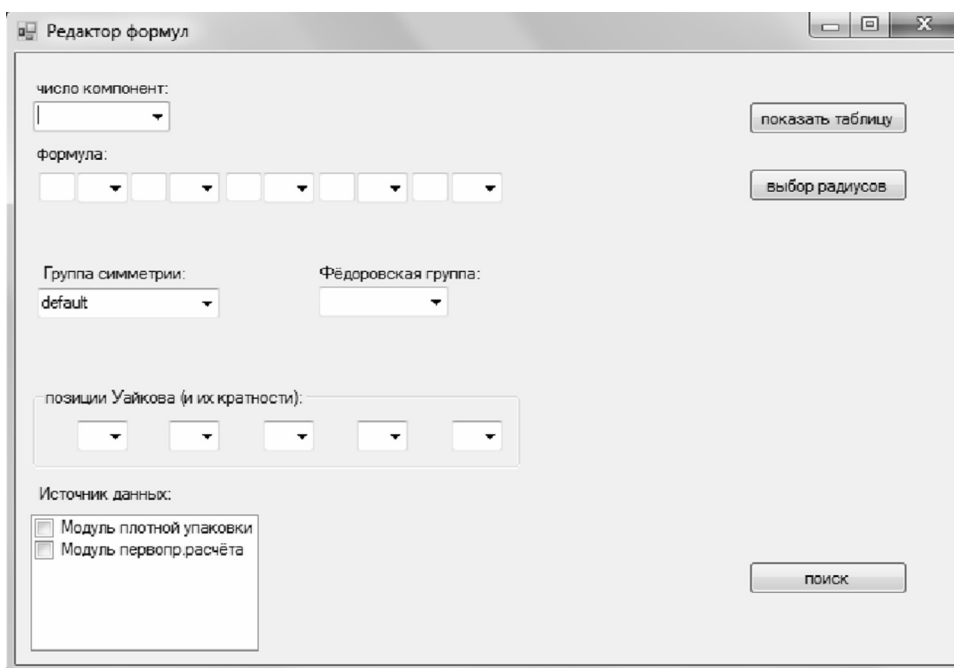


Figure 3 Information support user interface.

1. Microsoft SQL Server 2008, a target DBMS.
2. NHibernate, and ORM library.
3. NET Framework 3.5, a software platform.
4. Microsoft Visual Studio 9.0, a development environment (the C# language).

3. Summary

Subject domain data have been classified and systematized and functional requirements have been summarized for project implementation. Information support for a computational experiment has been developed that includes a DB flowchart, integrity limitations, data aggregation rules and a user interface prototype. Furthermore, the relational model has been mapped in the object model and a scheduler has been developed for data supply to applications. The multiscale computational model has been tested for computer modeling of the synthesis of promising multilayered heterostructures and the assessment of their main parameters.

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