COMPUTER SIMULATION OF COMPOSITION COATINGS WITH SET PROPERTIES

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ABSTRACT

The main purpose of this scientific work is to review the current methods of multifunctional material design, and to establish approaches based on multiscale non-deterministic analyzes that can be used to model composite coatings. Analyzing of the literature data showed that methods of computer modeling of materials can be classified by the following. The first group represents approaches in which for selected values of functional properties the process of selecting materials is based on a combinatorial search in the experimental database. The second one is a computer simulation based on computational methods and the theoretical foundations of physical materials science, where a bottom-up approach, including quantum and molecular modeling, is used to accelerate the discovery of new materials. The third is the method of modeling materials, based on the integration of computational stimulation, system engineering, production and design. It is established that all the listed approaches are designed for bulk materials and are not adapted for protective coatings. Therefore, the creation of methods for modeling computer design of composite coatings with given functional properties is an important task in the field of information systems.

Keywords: composition coatings, computer simulation, mathematical model, set properties, calculation methods

INTRODUCTION

The process of selecting protective coatings in the field of materials science was based on the use of tabular data on mechanical, physical and other properties [1]. The modern trend has shifted towards the composition of materials and the connection of the microstructure and properties of the system components. The purpose of the creation of composite coatings with various special, sometimes contradictory, properties [2]. In the past, development of new composite coatings took a lot of time and with a large amount of effort: experimenters obtained protective coatings under various regimes, studied

their properties, and out of hundreds of specimens selected the best one [3-7]. Then there was tries to design the technique of development compositions with set properties. This process could take decades and frequently had big material cost. The need of development of technique that could give prediction with no error revealed itself. Meaning that not experimenting in laboratories but give a task to computer to make prediction, which coating with certain composition construction and microstructure will have certain required properties under certain operating conditions [8-10].

Over the past decade, several new areas of material development have emerged. The process of selecting materials for composite coatings focuses on the design and combinatorial search in the database of properties and characteristics that are most suitable for selected values of functional properties. Another class suitable for computer design of coatings is based on computational methods and the theoretical foundations of physical materials science.

To accelerate the discovery of new materials, a computational structure and a bottom-up approach is used, including quantum and molecular modeling. The purpose of this paper is to review the current methods of multifunctional material design, and to establish approaches based on multiscale non-deterministic analyzes that can be used to simulate composite coatings.

TECHNOLOGY OF COMPUTER PREDICTION OF COATING PROPERTIES

According to the authors [11-12] the main task is to predict the crystal structure of composite coatings, which determines the mechanical properties, thermal and electrical conductivity. The technique consists in step-by-step testing of crystal structures, starting with a small random sample. Next, various solutions are ranked, the worst of which are discarded, and the best ones are produced by different variants of recombinations and mutations. The most profitable ones are selected and combined, producing the next generation. After an assessment on physical properties being held like chemical composition and stability. So step by step approaching the optimal material in standpoint of particular physical property. This evolution method was patented by A.Oganov and currently is broadly being used by companies like «Intel», «Toyota» и «Fujitsu» for development of new materials. The main conclusion of evolution method is statement that either in computation or in the nature new material can be created only from two sources not three, four or more. But this method is not adapted for composite coatings.

Using the evolutionary optimization algorithm implemented in the USPEX crystal predictor program, and the first principles for calculating the total energy, phase composition diagrams were calculated for Al-Sc and Al-Ta systems of alloys at zero temperature and pressure. In addition to the known binary intermetallic phases, new potentially stable $AlSc_3$ and $AlTa_7$ alloys were found in the Al-poor phase diagram. The dynamic and thermal stability of their lattices was confirmed from the calculated spectra of vibrational normal modes in the harmonic approximation. Figures 1 and 2 present examples of studies of the thermodynamically stable binary phases of the Al alloy with Sc and Al with Ta.

The author [13] describes a material modeling approach based on the integration of computational stimulation, system engineering, production, and design. This idea is developed in the hierarchical concept of Olson (Figure 3), and is also considered in [13]. The advantages of this approach are the use of modeling and stimulation, which ensures the design of stable structures of materials with desired properties. The disadvantages include the lack of development for composite metal-based protective coatings.

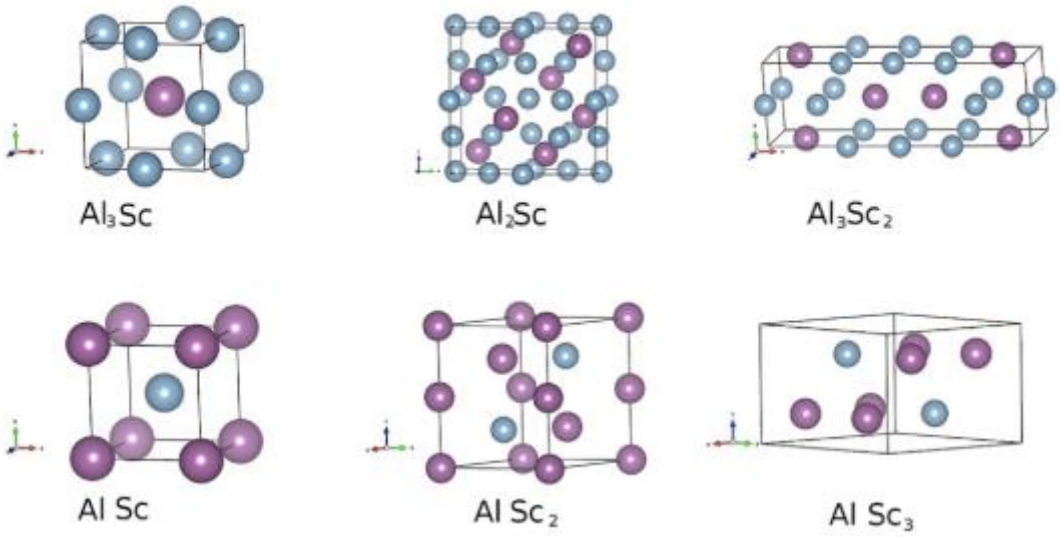

Figure 1 - Assessment of the stability of new intermetallic alloys Al-Sc [12]

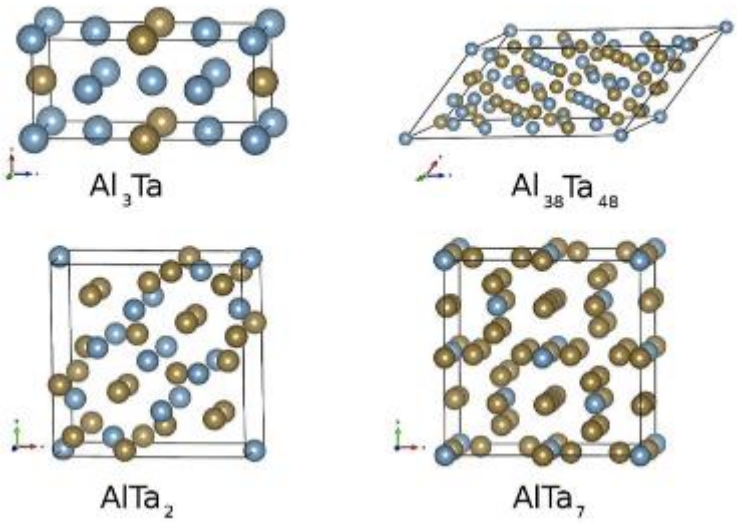

Figure 2 - Evaluation of the stability of new intermetallic alloys

Al with Ta [12]

Large-scale databases is traditionally used to search for experimental and theoretical data. In article [13], three different cases are considered to illustrate the application of statistical methods. In the first, a complete large-scale database of molten salts is visualized for sample retrieval. In the second case, a virtual combinatorial library of chalcopyrite semiconductors was developed from an experimental and theoretical database. This method involves the selection of statistically relevant parameters based on the physics of materials. In the third case, "secondary" descriptors were developed for the base of zeolites in order to more fully understand the topology of mesoporous structures in the design of materials. These examples serve to demonstrate how databases can be used to determine important combinations of parameters related to combinatorial experimentation.

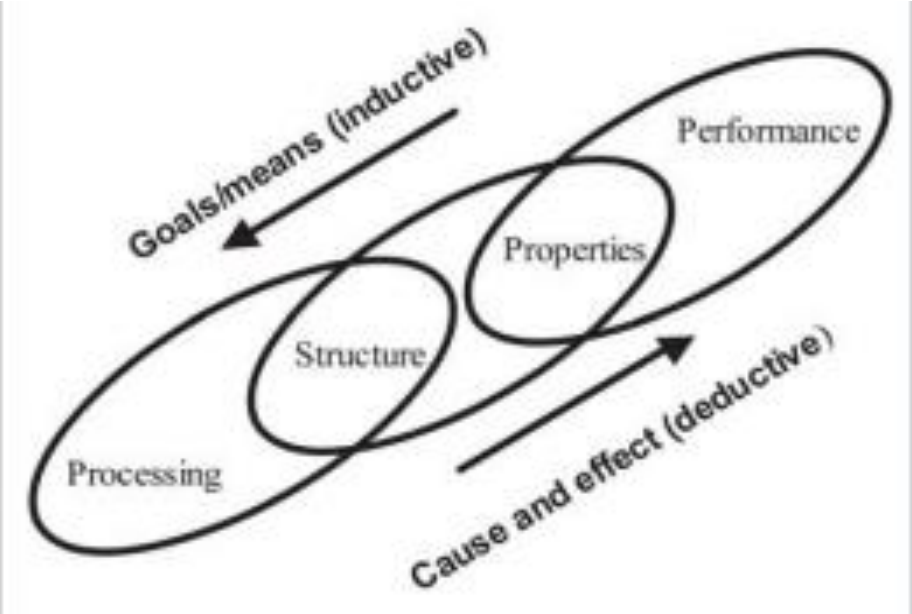

Figure 3. Olson's hierarchical concept [13]

The relationship between clearly separated data sets is a critical component of interpreting the behavior of materials, especially in terms of assessing the influence of the microscopic characteristics of materials on their macroscopic or engineering behavior. In [14] demonstrates the importance of analyzing the main components of these properties associated with high-temperature superconductivity for studying the statistical effect of the intrinsic characteristics of materials on high-temperature superconducting behavior. The authors of [15] consider the relationship between the microscopic characteristics of materials and their macroscopic properties. This article demonstrates the analysis of the basic properties associated with high-temperature superconductivity. In works [12-15] the approach of software development is

considered, allowing to select a material by functional properties. The procedure itself uses experimentally obtained graphics and optimization methods for the instantaneous selection of both material and form.

CONCLUSION

Analysis of the literature data showed that methods of computer modeling of materials can be divided into 3 main groups.

1. Approaches in which for selected values of functional properties the process of selecting materials is based on a combinatorial search in the experimental database.

2. Computer modeling based on computational methods and the theoretical foundations of physical materials science, where a "bottom-up" approach, including quantum and molecular modeling, is used to accelerate the discovery of new materials.

3. Methods for modeling materials, based on the integration of computational stimulation, system engineering, production and design.

At the same time, all the listed approaches are designed for bulk materials and are not adapted for protective coatings. Therefore, the creation of methods for modeling computer design of composite coatings with given functional properties is an urgent task in the field of information systems.

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