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ARTIFICIAL INTELLIGENCE TECHNOLOGY AND ITS APPLICATION PROSPECT IN MATERIALS SCIENCE

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ABSTRACT

Artificial intelligence (AI) is an interdisciplinary research and it has been widely spread into many specific domains. In this paper, data engineering, knowledge engineering, innovation methodology and intelligent application technology of AI are mainly presented and their prospects in materials science are summarized after analyzing the intelligent service demands in nowadays materials engineering. The work of this paper will be helpful for new materials development and design and has reference value to the future research directions in materials informatics.

Keywords: *Data Engineering; Knowledge Engineering; Technical Innovation Method; New Materials Development and Design*

1. INTRODUCTION

Artificial intelligence (AI) is an arisen branch of computer science that aims to imitate and extend the intelligence of humans in theory, methodology, technique and application systems. The main research contents of AI involve knowledge representation, automatic reasoning and indexing methods, machine learning and knowledge acquisition, knowledge processing system, natural language understanding, computer vision, intelligent robots, automatic program design, and so on[1].With the development of computer science and internet technology, many engineering domains need intelligent informatics urgently [2,3,4,5]. According to the prediction of International Data Corporation (DIC), the demands of massive data and knowledge service market are going to increase 40% annually from 2010 to 2015[6]. The related techniques of AI, machine learning, data mining, knowledge engineering, etc, are widely needed. The industrial informatization process is especially important to materials domain since materials are the foundation and the pilot industry for the progress of the society and play a key supporting role in national economy and constructions.

In this paper, we prefer to aim at the new issues in materials domain focusing more on several research aspects of AI, including data engineering, knowledge engineering, innovation methodology and intelligent application technology, and discuss their prospects in materials science, especially in new material development and performance analysis.

2. INTELLIGENT SERVICE DEMANDS IN MATERIALS ENGINEERING

Materials engineering investigates the relationships among the preparation or processing technique of materials, the structure of materials at atomic or molecular scales and their macroscopic properties. With the rapid development of materials science, many new methods, new process and new materials are emerging, and the intelligent service demands in materials engineering are required consequently. The main representative demands for AI in new material development are summarized as shown in Fig1, including composition structure of high performance materials, nanostructure analysis and novel manufacturing techniques, material processing and control, etc. Associating the

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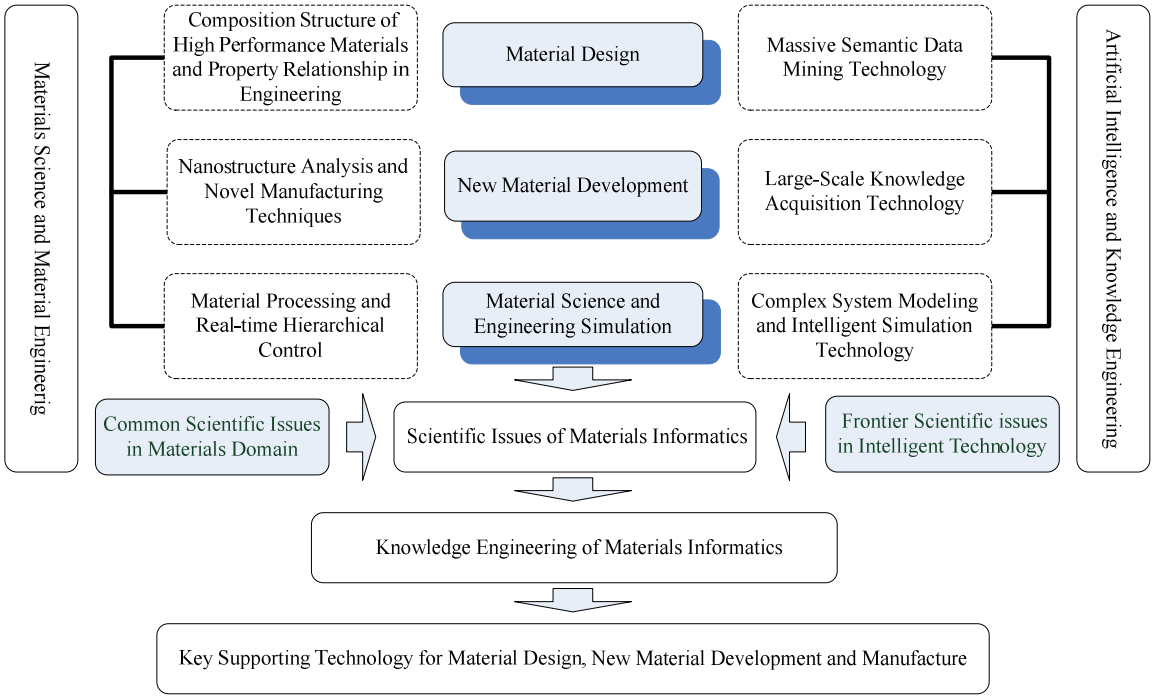

Figure. 1 Service Demands for Artificial Intelligence and Trends in Materials Science

materials science with artificial intelligence, knowledge engineering and other computer technology to form the supporting techniques for material design, experimental simulation and material manufactures, and to construct the knowledge engineering systems of materials field becomes the common key issues in materials engineering.

3. ARTIFICIAL INTELLIGENCE IN NEW MATERIALS DEVELOPMENT

The development of new materials refers to advanced materials exploration as represented by high-performance metal materials. It studies on the preparation and processing of new materials, the material forming process control and simulation, new technologies of plastic forming, material forming theory and microstructure control, metal solidification and control, advanced materials joining technology, crystal growth theory and control, etc [7]. Development of new materials cannot be separated from the existing data and knowledge, and also needs the support of innovative approaches which is the important guarantee for the realization of technical innovation since a methodology should go first if look forward to a sequence of innovations. In this section, the illustrations of AI in the related aspects for new material development are described as follows.

Data Engineering. The progress of materials science is closely depending on the basis of previous research results and experimental data. The research process of materials is also a process of generating material data. These data play more and more important roles and become the driven force in material scientific research. Moreover, with the convenience of the internet, the amount and the complexity of material data information are improved greatly. For example, the data amounts of combinatorial materials and generated in the high-throughput experiments are usually over a thousand times than those of conventional experiments [8]. How to manage the useful data and to discover the potential relationships among the massive data become close concerned matters in material design and development. Data engineering can provide a scientific resolution for handling these problems. It is mainly involved in the following aspects.

(1) Data Collection and Management.

Data collection and management is the first task in material informatics, in which all the data are suggested to be standardized and organized in uniform formats into the database. The effective data management is the foundation of the following analysis and applications.

(2) Data Mining.

The overall goal of data mining process is to

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extract useful information from an existing data set and transform the information into a human-understandable structure for further use [9]. The potential rules of previously unknown patterns can be found via data mining. The massive materials data mining is to solve the common issues on property prediction, data visualization, outlier detection and sequential analysis in the materials field. The researches on multi-relationship materials data mining and application techniques, real-time data mining in engineering environment of material processing, and knowledge-driven data mining in massive experimental materials are becoming more and more essential in materials engineering for solving the practical problems.

(3) Materials Data Sharing.

Materials data are very precious to the researchers since many of them were extracted from expensive experiments and long time accumulations. Data sharing is to make the users using different computers and different software in different places read other people's data and conducting various operations, computations and analysis. Materials data sharing can enable more people to fully use existing data resources, reduce the duplication work of data acquisition and the corresponding costs, and put more energy focusing on the development of the new applications and systems integration.

Knowledge Engineering. A higher level of using material data is to establish knowledge-based systems. Knowledge engineering is an engineering discipline that involves integrating knowledge into computer systems in order to solve complex problems normally requiring a high level of human expertise [10]. Normally, knowledge comes from books, human experience, observations and analysis via different ways, e.g. by data mining, and so on. How to acquire and represent the knowledge and how to infer the unknown from the known are the concerned problems which will exert huge effect on new material development if solved properly. The perspective researches of knowledge engineering in materials involve the following aspects.

(1) Cognitive-based Knowledge Discovery.

Knowledge discovery is developed out of the data mining domain. The mainstream of development in knowledge discovery pays more attention on new high-performance and highscalability mining algorithm. In fact, the research on process model and inner mechanism is more important [11]. Cognitive-based knowledge discovery concentrates on these aspects better. It is especially good at heuristic directional mining according to the cognitive psychology and dealing with nonlinear dynamic system. It is suitable for discovering the tacit knowledge in new material property analysis.

(2) Semantic-based Retrieval and Reasoning.

Retrieval and reasoning are the independent techniques in the knowledge system. They are also the foundations of an intelligent searching engine which is the link between the user and the knowledge base. Semantic technology [12] allows not only for the automatic comprehension of words, sentences, paragraphs and whole documents, but also for regularities searching in data and the application of these regularities for predictions. It is a good way to find, discover and create structured knowledge connections from the previously unstructured information sets. In the meanwhile, categorization, extraction, domain establishment, taxonomy and ontology creation are built upon the semantic backbone too. Combining semantic theory into the retrieval and reasoning process for new material design and analysis can provide more reasonable searching results.

(3) Construction of Knowledge Base Based on Ontology.

Knowledge base is different from traditional database. It not only contains a large number of simple facts, but also contains the rules and the process knowledge. During the construction of knowledge base, knowledge representation is a key process which can formalize and symbolize the knowledge. Knowledge processing can be deeply affected by different representation methods [13]. Among a number of successful applied representation methods of knowledge, e.g. logic, production rules, semantic networks, frame, script, ontology, etc, ontology-based method oriented to specific domains provides a basic structure for the construction of knowledge base. It can define the concepts of knowledge and their relationships more precisely and represent knowledge in lexical and semantic level more abundantly due to its description of objects with concepts, attributes, functions, axioms and instances. Therefore, an ontology-based knowledge base for materials domain can inherit these advantages to enhance efficiency of knowledge searching, accumulating and sharing.

Innovation Methodology. Technical innovation method [14] belongs to the scope of the scientific methodology. It refers to the problem solving methods, innovation cognition principles, and the knowledge and models adopted in the process of

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problem solving. How to break through the traditional material development method under the direction of scientific methodology is an emerging issue. The technical innovation in materials science and engineering area not only follows the general technical innovation principles, but also has its own domain-specifics due to its application background. The computer-aided innovation system for material development and design associating with database and knowledge base can be proposed as shown in Figure 2 Establishing technical innovation methodology system aims at materials field and its supporting technology will greatly shorten the development cycle and increase the effectiveness of new material design. It brings a new way of thinking for material development.

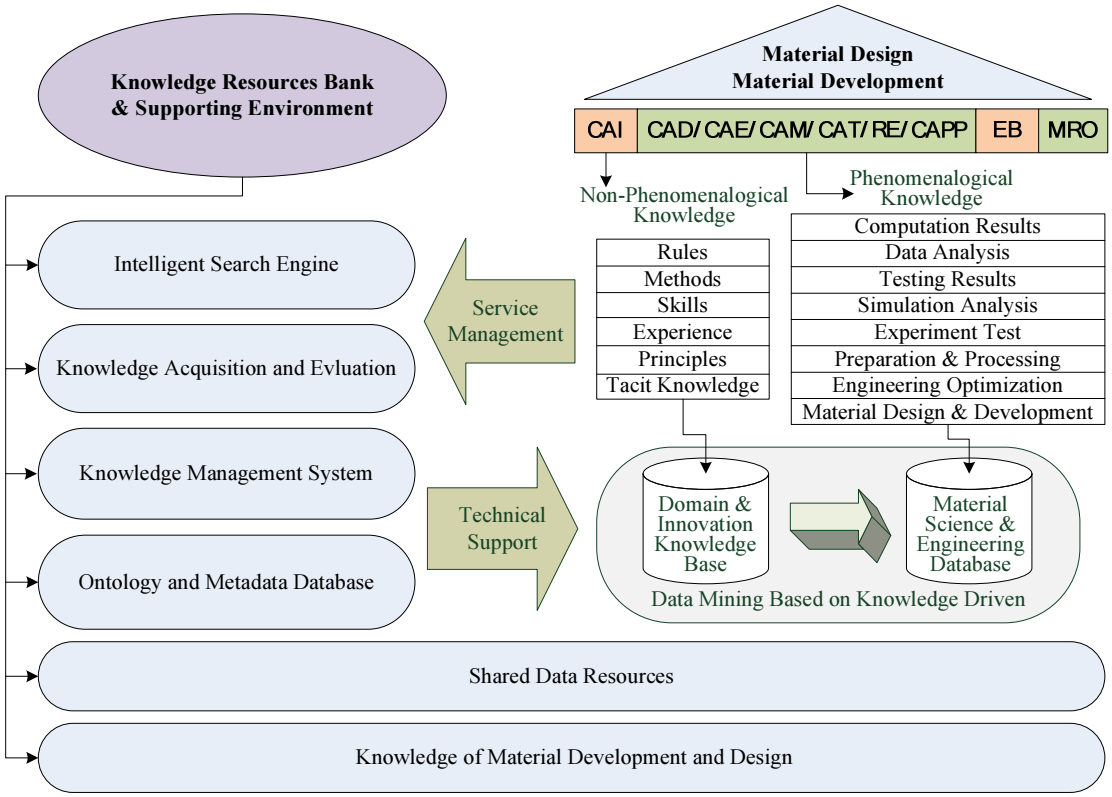

Figure. 2 The Computer-aided Innovation in New Material Development and Design

Intelligent Application. As for the level of applications, on the basis of material performance database, components database and technological process database, providing serviceable tools which apply the related intelligent techniques to form a computer aided design system is also the goal of materials informatics. The concrete forms of the tools could be as follows.

(1) Expert System.

An expert system is derived from the knowledge engineering, which is designed to solve complex problems by reasoning about knowledge [15]. As a science subject, the knowledge of material design is so diverse, integrative, and complex that it is necessary to combine with the artificial intelligence analysis into the design process. Expert system emulates the decision-making ability of a human expert. In new material development analysis, an expert system is expected to actively monitor computational and physical experiments, autonomously explore engineering design spaces and distinguish among theoretical explanations of observed phenomena.

(2) *Intelligent Simulator*.

During the process of material design, material model construction, visualized simulation, performance prediction and verification are very important to new material development and design besides data comparison and analysis. Intelligent simulation technology [16] is used to prepare computational experiments from high-level domain descriptions. It combines numerical, symbolic, and qualitative methods with computational formulations of mathematical or physical phenomena to present visualized results, such as 3D material structure, manufacture control process and

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so on, which can bring the greatest convenience of designing materials and analyzing material properties.

4. CONCLUSIONS

For today's materials sciences and engineering, data engineering, knowledge engineering, innovation methodology and intelligent application technology are broadly demanded and becoming the key techniques in new material development. These related aspects of artificial intelligence are presented and their prospects in materials science are indicated as well in this paper. The work of this paper provides a new train of thought for material development. It can also inspire some future research directions for materials informatics.

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