Application of Computer Simulation Technology in Material Science

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Abstract. With the development of modern society, science and technology, information technology and computer technology have been developing rapidly. The computer simulation technology is mainly to use the electronic computer to carry out simulation work, which is expected to provide new research work for the research and production of material science and to raise the development of material science to a new level. Therefore, the author mainly analyzes the application of computer simulation technology in material science, and hopes to provide some suggestions and references for the development of material science through the author’s elaboration.

1. Introduction
With the development of modern society, material science is becoming more and more popular in people's life and work, especially in industrial production. The research on material science is getting deeper and deeper. in the process of the study of material science, because of the numerous parameters of the system in many cases and complex relative environment, the mathematical formula obtained is only approximate, and we have no way to know how certain systems will react when the external conditions may change. However, if we apply the computer simulation technology in the process of material science research, the experimental conditions will be improved greatly, mainly because the computer simulation technology that had accurate experimental data, can analyze and feed back the data in time, and provide timely guidance to the site, so that we can provide new tools for the research and production of material science, and raise the research work of material science to a new height.

2. An Overview of Computer Simulation
The computer simulation is mainly dynamic simulation of the behavior of a complex system on a digital computer, or the repetition, so that we can get quantitative indicators of the characteristics of the system, providing some bases for our decision making. The generation of computer simulation technology is relatively late, and it appears after the electromechanical computer. In the 40s of last century, it was first introduced by American Von Neumann and Uram in the study of the atomic bomb. Computers mainly used to simulate some probability calculations of random diffusion of neutrons in fission products. In order to use computer simulation, the corresponding mathematical model of the system is needed to established that we want to study and the environment of computer work, so that a system model is easily sent into the computer.

Computer simulation is being used in material science. According to the scale of its simulation, it can be divided into three kinds of simulation methods. The first is the simulation computation of atomic scale, mainly including molecular dynamics and Monte Carlo method. It mainly calculates the structure of the multi particle system, the structure of a variety of systems and various properties according to the
interaction potential between particles. The second is the microscale simulation calculation. This kind of computer is mainly based on the concept of continuous medium, and the method of computer simulation is used to calculate the thermal stress distribution of the material in the complex existence of the basic gradient material, which can provide a basis to find reasonable material structure. Moreover, the thermodynamics method can predict phase transition and microstructure of phase transition products, which is also the research area of this method. The third is the simulation calculation of the macro size. The use of this method is related to the engineering production of general materials or material components, for example, the amorphous alloys are formed by quenching. Computer simulation is used to calculate the heat and mass transfer process of fast cooling of liquid alloy, which has a very important role in the design of reasonable equipment and technology, greatly ensuring the quality of the product. The correlation is mainly shown in Table 1 as follows.

Table 1 The simulation level, spatial scale and simulation object of the computer

| Simulation level       | Spatial scale | Simulation object                                           |
|------------------------|---------------|------------------------------------------------------------|
| Electronic level       | 0.1nm~1nm     | Electronic structure                                        |
| Atomic and molecular   | 1nm~10nm      | Structure, mechanical properties, thermodynamic properties and kinetic properties |
| Micro level            | ~1μm          | Grain growth, sintering, dislocation network, coarsening and texture |
| Macro level            | >1μm          | Casting, welding, forging and chemical vapor deposition     |

3. Advantage Analysis

Computer simulation technology is being used in the research of materials science. It uses new algorithms and combines the powerful computing function of the computer in this process, so when people study the material science, the meticulous and precise degree of research is greatly improved, therefore, the use of computer simulation technology is becoming more and more popular in the process of material science research. And on this basis, a new branch of material research—computer science is produced. It mainly studies the material science with the advantage of computer simulation technology. It can not only simulate the process of various experiments, but also understand the microscopic properties of the material and the macroscopic mechanical behavior. Even when these materials were not be produced, the properties of these materials can be predicted, which will provide us with favorable theoretical guidance for the design of excellent new materials. In addition, in the process of material science research, simulated experiments are often more economical and practical than physical experiments, and reduce the influence of human errors on the experimental results in experiments. For example, if the object is used to do the experiment, it is easy to make mistakes when people are very sleepy, and if computer simulation experiments were did, people can still carry out simulation experiments when they are very sleepy. Even when the micro state and process were understood, the simulation experiment has an irreplaceable role.

4. Analysis of Computer Simulation Technology

4.1. The First Principle Simulation Technology

In the process of material science research, the electronic structure of materials and the relative physical properties are closely related to the macroscopic properties. Therefore, the electronic structure and related physical properties of the materials were needed to study in the process of research. The
macroscopic deformation of the materials and the essence of fracture mechanics behavior were needed to understood from the microscopic angle, which is of great value and significance, and can also provide effective guidance for improving the mechanical properties of materials.

4.2. Atomic Simulation Technology
The atomic simulation technology is mainly based on the method of obtaining the atomic position or the microscopic state. The following simulation methods are used to study the complete or noncomplete crystal structure, dynamics and thermodynamics properties, such as the molecular dynamics method, Monte Carlo method and minimum energy method. The method of molecular dynamics is to solve the equation of motion, which is mainly by analyzing the force of each particle in the system, and using classical method or wave quantum method to solve the position and speed of each particle in the system at a certain time, so that the state of each particle movement can be determined. The Monte Carlo method is mainly to create an appropriate probability model artificially according to the law of development and change of the problem to be solved, and then carry out a lot of statistical experiments according to this probability model. In the process of experiment, some statistical parameters are exactly the solution of the problem to be solved. The minimum energy method uses the computer to calculate the energy of the crystal, mainly by adjusting the position of the atom and the chemical bond length and the bond angle between atoms to get the most possible structure, so that the energy of the system can be continuously reduced. When the energy reaches the minimum, the energy value calculated is compared with the experimental results, so that we can meet the requirement of accuracy.

4.3. Simulation Method of ContinuousMedium Model
The use of the simulation method of continuous medium model is mainly to solve the macro problems. The commonly used methods mainly include the following, namely, the traditional finite difference method, the finite element method, the boundary element method and so on. In the process of material research, these methods can be used to solve problems such as heat transfer temperature field, and mass transfer diffusion. In addition, for the evolution of the microphysics of some continuous materials, certain algorithms are used to simulate the data on the basis of space and discretization processing, which has great advantages.

4.4. Integrated Simulation Method
The integrated simulation method appears late, which is a new technology that has emerged in recent years. The integration is mainly manifested in two aspects, namely, the research method and the spatial scale of the research object. In addition to the development of new technology, the research method mainly includes the simulation technology which combines the original atomic simulation technology based on the interaction potential function, various computing techniques based on the first principle, continuous medium model and discrete numerical calculation. For the spatial scale of the object, the structure and performance of the intermediate scale material are directly studied between the atomic scale and the macro scale, or the material behavior of different scales are connected together as a unified object to make the research. Especially, for research links at different levels, it has become the focus and difficulty in the field of material simulation.

4.5. Artificial Intelligence Simulation Technology
In the course of material research, experience are still used to solve problems in many fields. Even if there is a theoretical algorithm for the problem to be studied, these algorithms are very complex, and there are many problems in the actual application process, so it is difficult to achieve. In view of the existing problems, the emergence of artificial intelligence simulation technology provides an effective tool to solve these problems. Artificial intelligence simulation technology mainly includes clustering simulation recognition technology, expert system, artificial neural network technology and so on. With the development of science and technology and computer technology in modern society, its application in material science is more and more common.
5. Application of Computer Simulation in Material Science

5.1. Synthesis and Preparation of Materials and Computer Simulation
In the process of synthesizing or preparing materials, whether the improvement of the existing materials or the study of new materials, the experience is still needed in the synthesis and preparation of the existing materials to a great extent. Therefore, data is needed to establish for all kinds of materials, especially the establishment of the database of chemical and physicochemical properties of various materials. In this process, if computer simulation technology is used, people can greatly reduce the blindness in work and reduce workload. For example, in the process of material research, the research institutes in various countries have established many different types of databases, such as phase diagram of alloy system, crystal structure parameters and physical properties, and mechanical properties diagram of the phase and microstructure, which provide great convenience for the research of materials. Material design is one of the ultimate goals of studying the synthesis and preparation of materials. Many chemists, physicists and materials scientists are working tirelessly in this direction. They have accumulated a large amount of data and experience in materials, and formed a large and small expert system on the basis of the database, and some work has achieved good results, as shown in Fig.1.

![Figure 1. Flow chart of expert system for material design](image)

5.2. Composition and Structure of Materials and Computer Simulation
At present, in the study of the composition and structure of materials, a variety of large analytical equipment is mainly used, such as scanning electron microscopy (SEM), transmission electron microscopy (TEM), analytical electron microscopy (AEM), scanning probe microscope (SPM). The use of these large devices is under the control of computers, which provides different analytical simulation software and corresponding databases. The function of these analytical simulation software is very powerful, so it greatly reduces the amount of work and reduces the error in the process of data processing. Not only that, these analysis simulation software is also used to make various charts directly used for publication, which is very convenient.

5.3. Performance Testing and Analysis of Materials and Computer Simulation
In the course of the study of materials, the determination of most material properties requires special testing equipment and instruments. Even at the time of determination, in order to determine some specific performance, some general testing equipment and instruments are also used to make up a more complex system for testing. In building a more complex testing system, if the computer is used to control the test system, it will help the test system run. In this process, data collection and processing are also carried out, which improves the function of the test system. For example, computerized material performance testing system (CAT system) is an important tool to improve the research level. This is mainly because the computer can carry on the flexible programming and process the data, has the powerful computation speed, and can do a lot of work that people can’t do, which greatly improves the accuracy of our test experiment.

5.4. Automatic Control of Material Processing
In the process of studying materials, materials are needed to process, which is not only an important means of industrial manufacturing, but also an important part of processing materials. The processing of materials mainly includes the following steps: casting, forging, pressure processing, heat treatment, powder metallurgy, and so on. All the steps in the processing of materials can be automatically controlled by the computer, which not only saves manpower, but also reduces the loss caused by staff error in the course of processing, so as to achieve better results.

6. Conclusions
This paper mainly analyzes and studies the application of computer simulation technology in the material science, and puts forward the author’s own views. It is hoped that the author’s exploration can provide some suggestions for the development of material science.

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