

Brief Analysis of Application of Computer Software in Materials Science

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Abstract : With the development of science, materials science has developed to a new level. In order to make it continue to develop towards more integrity and refinement, the application of computer software is particularly important in materials science. For different material forms, computer software and simulation technology can be widely used. With the continuous progress of science, the application of computer software in materials science has a broad growth prospect, and can further promote the complementarity between computer software and materials science.

Keywords : Materials Science; Application; Computer

1. Introduction

Computer, as a basic tool in the electronic information age, with the use of various software, plays a very important role in all fields of our life. At the same time, it also plays a very important role in the research of material science. At present, the simulation technology of computer software can be widely used to guide the material design, the precise control of preparation parameters, design and reduce the research and development cost and cycle. It is not difficult to see that the application of computer in materials science has broad prospects. As relevant personnel, in addition to having a full understanding of computer software, materials science and the relationship between them, they should seriously explore and analyze the application direction of computer software in materials science.

2. Data storage application of materials science software

2.1 Integrating resources and establish material database

As we all know, material science has a powerful feature, that is, a huge amount of data. There are more than 100000 kinds of engineering materials in the world, as well as millions of compound data. There are complex and huge databases on the function and composition structure of materials. If only a single manual collection, it is impossible to complete the storage of such large data. At the same time, it will be more prone to errors and cause inevitable scientific losses. Taking Baidu network disk, office and other storage software as an example, at present, various computer software blessings have stored more than 10 kinds of data, including but not limited to alloy phase diagram database, raw material corrosion database, mechanics database and so on. With the popularization of computer software in materials science, the material database is further refined. At the same time, it has been applied in research, testing and product manufacturing. Materials science will obtain relevant experimental data during research. At this time, it can borrow the storage function of computer software, easily retain relevant data, and carry out these data, including but not limited to calculation, drawing, analysis, rapid query and other functions. Optical microscopy and electron microscopy are generally used to study the relationship between the properties of materials and their condensed structure. These technologies can use the image analysis and processing effect of computer software to study the material structure more easily. Finally, the relevant structure information, such as the distribution, aggregation and size of different crystals, can be obtained from the image. The computer software can integrate the information and use researchers to guide the relevant structure of material structure.

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2. 2 Facilitate inquiry and knowledge communication

In addition to the advantages of fast access to information, large amount of stored information, flexible use and wide application, convenient query is also a major feature of computer software in the application of materials science. By using the query function of computer network software, researchers can query the material information they need in time, pay attention to the latest developments in material science research in real time and the development direction of material science research, and correct the deficiencies of the studied materials in time. Relevant researchers can also publish their own achievements through computer software and communicate with researchers in different fields, so as to promote the development and research process of material science.

3. Development and processing of computer software for materials science

3. 1 Material science requires physical simulation of computer software

In the research process of materials science, it is inevitable to establish the simulation experiment of physical model in advance in order to ensure the further development of follow-up projects. Although materials science requires physical simulation of computer software, this application is no longer a problem. However, the physical model that can be established by simulation is still quite different from the actual situation. Taking the atomic arrangement in the structure of infinite solid solution as an example, it can generally be divided into absolute order, long-range order and short-range order, and the reality will be much more refined than the above classification. Relatively speaking, it is more important to establish the physical model. If it is not appropriate to create the physical model, even if the previous calculation program is written in detail, it will lead to a large deviation in the simulation structure. With the use of computer software, the simulation field can be created in the direction of heat transfer, internal atomic change and mechanics during joint material processing. Taking the computer software materials studio as an example, in the research of superconducting materials, Bi superconducting materials can be prepared by sol-gel method. The corresponding modeling process of the precursor complex of Bi superconducting materials is processed by software, and the understanding of the process of obtaining the superconductor by the former drive is increased. The development of follow-up research also has an ideal foundation. In this way, the establishment of the above model also plays a very important role in scientific research: There is another difficulty in creating the model, that is, because the model with complex structure is easy to change in the differentiated environment, it is difficult to study the thermodynamic stability through experiments. Therefore, based on the established model and specific environment, a variety of calculation modules built in materials study software can be used to obtain research data while carrying out the thermodynamic stability research of relevant models, so as to better promote research progress and harvest relevant research results.

3. 2 Application of computer software in numerical model analysis

In addition to the necessary physical simulation, the application of computer software in materials science is often in the analysis and research of materials. After the real simulation operation of the real operating system by the computer software, the data obtained in the simulation process also has important achievements. The analysis and application of all the obtained data models is a very important application of computer software in the development of materials science. By comparing the data simulated by computer software with the data obtained by actual operation, the accuracy of the data model can be verified more effectively. For example, in the study of thermodynamics, it is necessary to use the phase diagram describing the main geometry of the phase equilibrium system to obtain some thermodynamic data. The software developed by the Royal Institute of Technology of Sweden and FACT software system developed by Montreal University of Technology of Canada are relatively representative material integrated thermochemical database and phase diagram computer software.

Taking the calculation of the vertical section of Fe-8% Cr-C ternary system as an example, first select the calculation database TER 98 in the TCW MATERIAL window, select the elements Cr, Fe and C, and then use the conditions window to judge the temperature and composition. The THERMO-CALC calculation result window appears. Relevant thermodynamic data can be viewed from the calculation result window. Finally, the corresponding window is selected to draw the parameters of the calculated phase diagram, so as to draw the phase diagram.

Similar professional computer software has the same feature, that is, it integrates self consistent thermochemical data and excellent calculation data, which can be applied to different types of phase diagram calculation. Computer software plays a very important role in the whole process of the application of materials science. Accurate simulation and data integration can effectively promote the research and growth of materials science.

4. Crossing application of computer software and materials science

4.1 Complementarity between computer software and materials science

Generally, there is no clear boundary for the application of computer software in materials science. In other words, it is also necessary to carry out gap learning on the relevant knowledge of computer software in the time of learning materials science. The use of computer software and the research of materials science are integrated with each other. The two complement each other, mainly through the assistance of computer software or even guiding technical means to carry out the properties and development of materials. In the whole research of materials science, it is natural to use computer software, and it plays a particularly important role. In a word, computer software and materials science can jointly promote each other's research on the way of scientific development.

4.2 Calculation software is indispensable in material science

In the whole process of material science research, in addition to basic knowledge, it is essential to analyze the properties of materials, analysis of material composition, as well as research and development of new materials, preparation methods, processing technology and other aspects need to use computer related software to complete. Every field of materials science research would probably be impossible without the support of computer software. Therefore, material science needs the support of computer software, computer software has an unshakable position, so as to master the application of computer software, and make material science research more tend to automation and integration.

5. Conclusion

Materials science, as a multi-disciplinary emerging science, is relatively not mature. At present, the research on materials science still depends on the accumulation of life facts and experience to a large extent. If it needs to be systematically studied, it is still a long process. In today's world of gradual progress in various fields, in the process of increasing development, the use of computer software is indispensable, computer software has already gradually infiltrated into the research of material science and daily life. And all kinds of computer software as a very important tool in daily life, and in the application of material science are also a major reason for the rapid growth of material science.

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