

The Importance of Numeric Databases to Materials Science

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Scientific numeric databases are important research tools for materials scientists. In distinction to bibliographic databases, these numeric databases are useful primarily to provide direct, immediate access to data, often evaluated data. Examples showing the application of crystallographic databases are given, including determining candidate materials for certain applications. Thermochemical data useful for optimizing optical fiber processing are discussed

showing the importance of high-quality data. In addition, these databases are an important tool that can be utilized in the graduate education of the next generation of materials scientists.

Key words: CRYSTDAT; industrial use of numeric databases; lattice matching; materials science; numeric databases; on-line searching; prediction of ferroelectricity; superconductivity.

Introduction

In this introduction, I would like to briefly point out some aspects of the importance of numerical databases to materials sciences, specifically the importance of good data and the quick dissemination of numeric data to a wide audience. All the examples that are mentioned come from the work at AT&T Bell Laboratories.

If one were to claim that numeric databases were the most important development in materials science, that would clearly be an overstatement. On the other hand, if one were to claim that they are of no value to materials science, that would be understating their importance. The importance lies in between and can be expected to increase as knowledge of them becomes more widely known. Many of these databases, specifically in the crystallographic area, have developed from print products that existed for decades and putting them into numeric databases is a shift in content and in means of

access. But it's more than that, much more than that. As with many new technologies, there are uses that are unanticipated when a new technology first appears. The usual advantages of having data in numeric form include the following: they're easy to update, there's a potentially faster delivery of information to the user, and there's a potentially large audience of scientists and engineers that can be reached by having the data in the electronic form, because these people can access this data by their personal computer or microcomputer in the laboratory, the office, or even at home.

I want to point to several examples. First, I'll discuss one of the main processes for making optical fibers, which I'll spend the most time on, and which will illustrate the need for good data. Other examples I will mention are the prediction of ferroelectricity, lattice matching, and high-T_c superconductivity. I'll close with a lesson from history.

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