Powder Diffraction

JCPDS

Volume 1 Number 3 September 1986

Powder Diffraction An international journal of materials characterization

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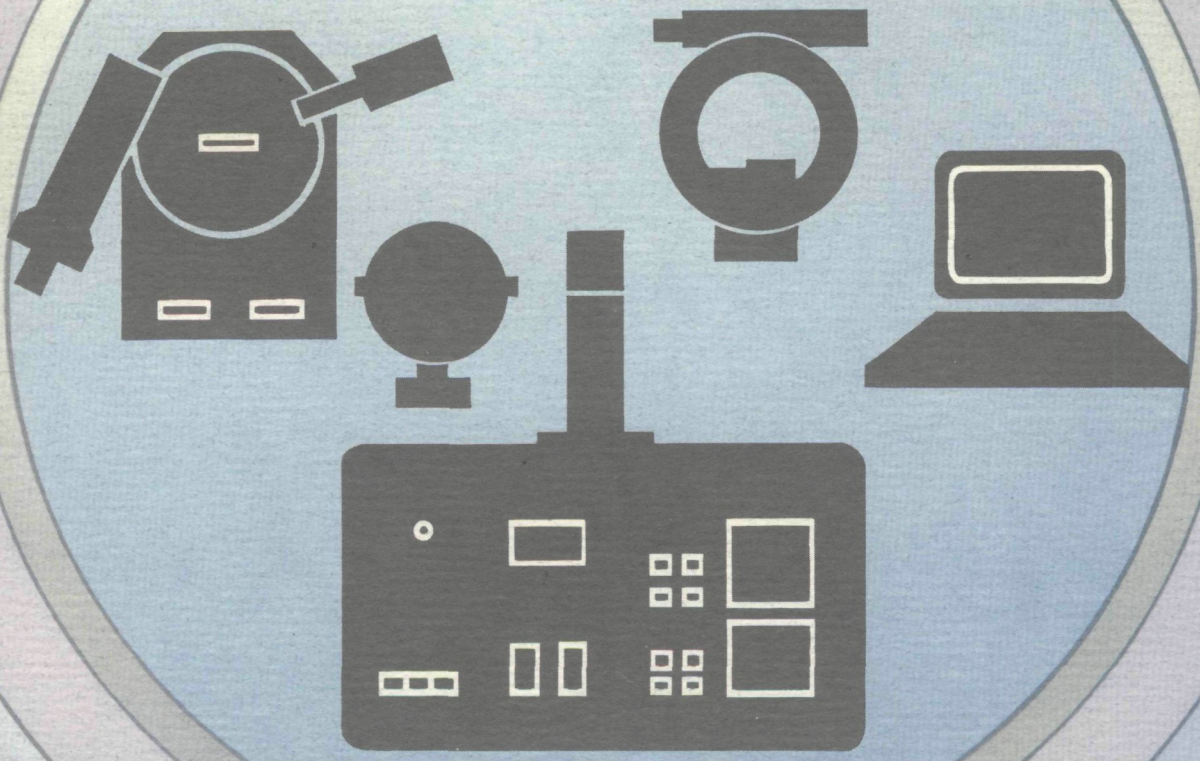

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Powder Diffraction

An International Journal of Materials Characterization

Publisher
JCPDS-International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, Pennsylvania 19081, U.S.A.

Powder Diffraction is a journal of practical technique, publishing articles relating to the widest range of application — from mineral analysis to epitactic growth of thin films and to the latest advances in software. Although practice will be emphasized, theory will not be neglected, especially as its discussion will relate to better understanding of technique.

Powder Diffraction is published four times annually by the JCPDS-International Centre for Diffraction Data.

Manuscript submissions. The Editors will consider all manuscripts received, but assume no responsibility regarding them. Materials will be returned only when accompanied by appropriate postage.

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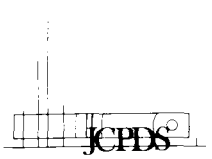

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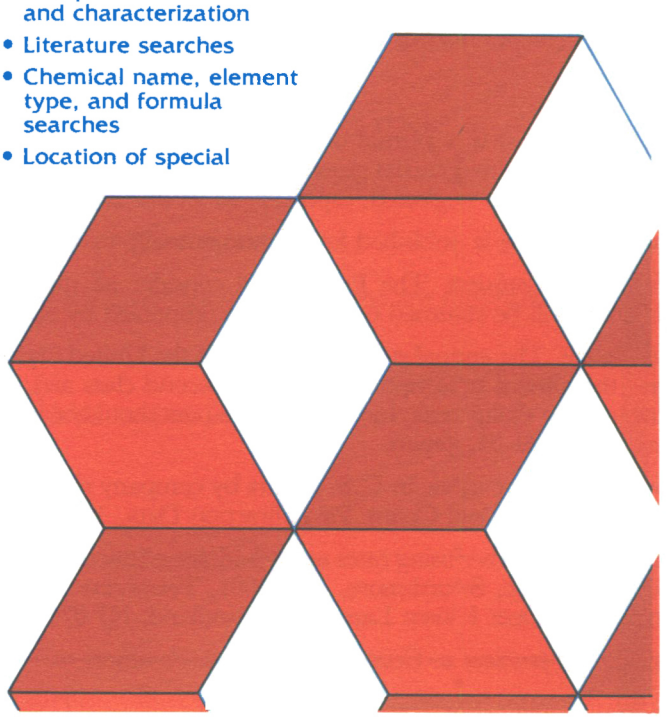

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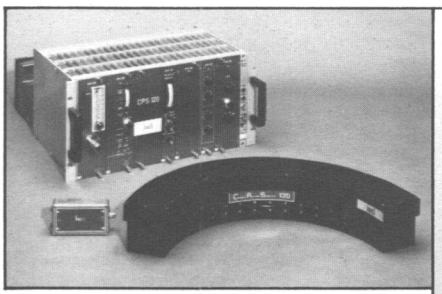

DETECTOR SYSTEM

Curved Position Sensitive Detector
American Instruments/
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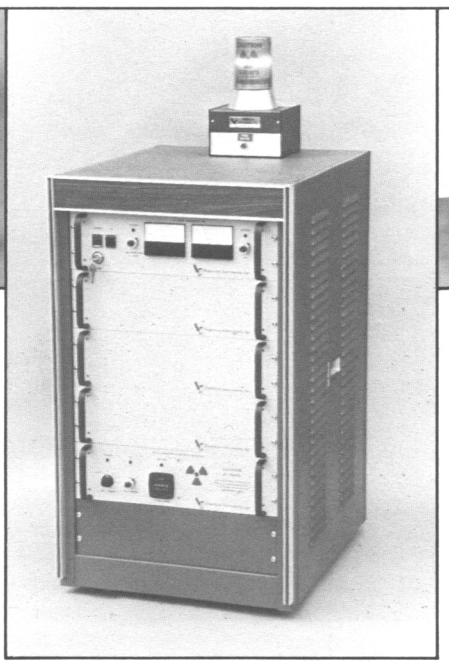
The CPS 120 is a curved position sensitive detector system with angular range of 120° two theta. It has the capability of giving a live display of the entire two theta diffractogram on a multi channel analyzer. The output from the multi channel analyzer can then be directed to a plotter or computer for data reduction. No movement of the sample or the detector is required. This detector system can be retrofitted to an existing diffractometer or purchased as a complete x-ray diffraction system. With a spacial resolution of better than .02° and high quantum efficiency, this detector system can be used for all phases of diffraction investigations, powder, texture, kinetic study, single crystal and stress.



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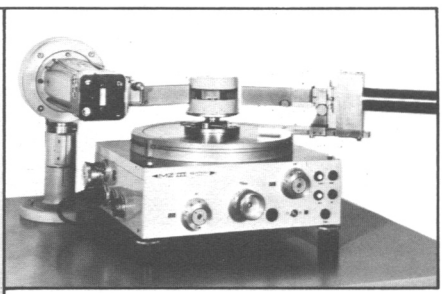

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Mineral
Powder Diffraction File
Data Book & Search Manual

850 *new* patterns

3400 patterns total
2700 species

Data Book
- Enlarged and revised for Sets 1–35
- Ordered alphabetically on mineral name

Search Manual contains sections on
- Chemical Name
- Hanawalt Numerical
- Fink Numerical
- Mineral Name

Since its inception almost 50 years ago, the Powder Diffraction File has always been well served in the area of mineral species. In 1974 the first special mineral based publication was produced, this being in the form of a book of minerals containing about 2,600 selected patterns in numerical sequence. A supplement to this edition was produced in 1981. In 1980 an alphabetically ordered data book was produced followed by a group data book in 1983. Each of these products has proven very popular both with the community of mineralogists as well as others involved in general qualitative phase identification.

The International Centre for Diffraction Data is now pleased to announce a new Mineral Powder Diffraction File containing about 2,700 species represented by 3,400 patterns. This selection includes about 850 new patterns added since 1980. This revision of the mineral file has been produced by the Editors of the International Centre for Diffraction Data in cooperation with the Minerals Subcommittee, and has been further guided by nomenclature recommendations of the International Mineralogical Association.

The Mineral Powder Diffraction File Data Book is ordered alphabetically on mineral name, thus grouping together patterns of the same mineral including hydrates, polytypes, order-disorder and chemical varieties, and obviating the need for an index. All data have been reedited with special reference to nomenclature, chemical formula, indexing and other crystallographic data. Physical data is also recorded including opaque optical data where available.

The Search Manual supplied with the new Data Book is based on the latest Hanawalt search/matching techniques including special provisions for finding patterns recorded using the Debye-Scherrer technique and data from highly oriented materials.

We feel that with the large number of new patterns, along with the improved quality of many of the older data, this new product should prove invaluable to both existing users of the Mineral Data products as well as to those new to the field.

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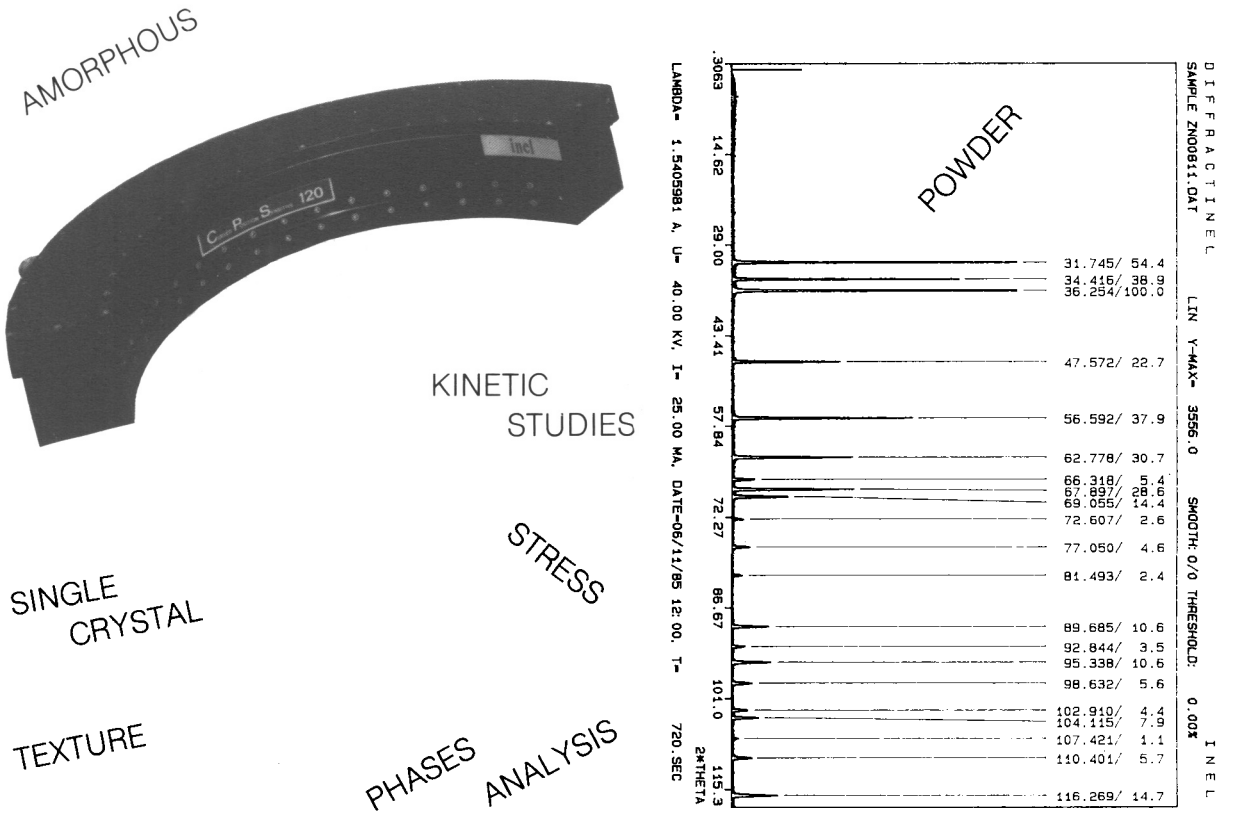

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Guest Editorial

The Status of Powder Diffraction Data

The characterization of materials and phenomena has historically been the principal limitation to the development of the various fields of engineering and science. Once what we are observing is well defined, theoretical descriptions rapidly follow. Modern theories of chemical bonding did not evolve until the methods of analytical chemistry and structural analysis had progressed to a point where the bulk stoichiometry of chemical compounds was firmly established. In fact, it is one of the fundamental tenets of the scientific method that we first carefully measure all properties of a system under study before attempting to develop a theory to explain them.

The advancement of both fundamental science and its engineering applications is critically dependent on our ability to characterize the phases in a material. For amorphous materials, where diffraction techniques do not apply and no other routine phase characterization method has been discovered, our understanding is at a very rudimentary level. For crystalline materials, where powder diffraction techniques apply, significant progress has been achieved. However, I believe that we usually overestimate the state of the art phase identification procedures by powder diffraction. The powder diffraction file (PDF) is only as good as the reference patterns on which it is based, i.e., those patterns published by researchers or sponsored by the International Centre for Diffraction Data. There are two aspects to what I mean by "good": the more obvious is the quality of the reference pattern (i.e. its metric and intensity accuracy), the less apparent but often more important aspect is the very presence of the pattern in the PDF.

It is of critical importance to the development of both science and engineering that the PDF contain patterns for the phases which researchers will encounter in their work. However, the dynamics of materials research and development often do not lead to the publication of patterns for new substances. There are a number of understandable pressures which lead to this situation, but the result often means large expenditure of time, money and wasted effort on the part of others. I recently learned of a company which spent over $200,000 investigating a material which would have been immediately rejected if two reference patterns had existed in the PDF. I suspect that many readers can think of similar instances. For example, the oxides of metals which can have more than one oxidation state usually show a complex series of phases depending on a number of factors such as thermal history and oxygen partial pressure; many of these phases, though commonly encountered in mixtures, have not been published and therefore are not represented in the PDF. Another example is the types of phases which devitrify from many of the hi-tech glasses. They are often not in the PDF in that they are stabilized by factors like particle size, nucleation agent, strain, etc.

The PDF is published by the International Centre which is a nonprofit corporation established for the purpose of collecting, editing, publishing and distributing diffraction data to serve as reference standards for the identification and characterization of crystalline materials. Obtaining PDF patterns for phases which occur in systems like those cited is one of the principal goals of the International Centre. Usually these phases can only be prepared by researchers who have both specialized equipment and knowledge. However, the phases will be encountered, as components of mixtures, on a routine basis by many characterization laboratories. Part of the rationale for the launching of *Powder Diffraction* was to try to encourage researchers to publish their powder patterns. A new Subcommittee of the Technical Committee of the International Centre has been created to identify those systems which should be targeted as our highest priorities for obtaining diffraction patterns.

In addition to encouraging workers to submit their patterns directly to the International Centre or to publish them in *Powder Diffraction* or elsewhere the International Centre has a grant-in-aid program which makes some limited funding available to support the collection of reference patterns for high interest materials. Researchers working with new materials who can use some funding to finish the preparation of diffraction patterns for publication are invited to submit proposals. The International Centre, will, however, where justified, consider proposals requiring higher levels of funding.

Robert L. Snyder
Chairman, Technical Committee
I.C.D.D.

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