The history of the International Centre for Diffraction Data

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The International Centre for Diffraction Data has a colorful history, starting as a small task group of involved and interested scientists and progressing through a number of evolutionary steps that were required to deliver scientific products and services globally. The results of these efforts can be found in numerous scientific publications that focus on basic physics, method development, and analyses of the material identification of solid-state materials. This article examines the evolution of the organization through its members and employees. © *2012 International Centre for Diffraction Data.*
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I. INTRODUCTION

Julian Messick started as an employee of the International Centre for Diffraction Data (ICDD) in 1966 and eventually became General Manager in 1984. J. Messick's work as an employee, general manager, and eventually member of the board of directors brought him in regular contact with most of the founding members of the organization. He was personally involved with the key members, employees, and directors who shaped the organization for several decades. Indeed, J. Messick is considered an important contributor in the evolution of the ICDD as he organized the construction and design of the current ICDD facility, was in management during the critical transitions from paper to electronic products, wisely managed ICDD finances for decades, and hired and developed many employees who work at the ICDD today. In 2007, Tom Blanton, the ICDD Chairman of the Board of Directors, asked J. Messick to write about the history of the ICDD, focusing on the people and organizations that shaped it. This article is the result.

II. THE ICDD

The International Centre for Diffraction Data (1978–current)

The Joint Committee on Powder Diffraction Standards (1970–1978)

The Joint Committee on Chemical Analysis by X-ray Diffraction Methods (1941–1970)

The ICDD adopted several names over a span of many years. In each case, the name change clearly reflected the ICDD's expanding mission as it constantly worked to satisfy the growing needs of the X-ray diffraction community. At present, the ICDD clearly states that its mission shall be "to continue to be the world center for quality diffraction and related data to meet the needs of the technical community. The ICDD promotes the application of materials characterization methods in science and technology by providing forums for the exchange of ideas and information."

III. FOUNDING YEARS: 1930s TO 1940s

In the early twentieth century, many scientists including G.L. Clark (1932), F. Halla and H. Mark (1937), A. W. Hull (1919), Ewald and Herman (1931), and Wheeler P. Davey (1934) studied the aspects and utility of X-ray analysis (Hanawalt, 1986; Hanawalt and Rinn, 1986). All of these scientists made great contributions to the field of X-ray analysis, but little was done in establishing standards for general use. In 1937, the American Society for Testing and Materials (ASTM) conducted a symposium on radiology and X-ray diffraction methods (Hanawalt *et al.*, 1938) where the importance of generating and producing adequate standards was brought forth and a joint subcommittee was established to address this issue. The membership of this subcommittee was drawn from the Committee on X-ray and Electron Diffraction, Division of Chemistry and Chemical Technology of the National Research Council; ASTM Committee E-3 on Chemical Analysis of Metals; ASTM Committee E-4, Subcommittee VI, on Metallography, and ASTM Committee E-7 on Radiographic Testing (Davey, 1941).

W.P. Davey of the General Electric Company was designated as Chairman of the Joint Committee, and other members included:

H.A. Bartrom, American Institute of Physics.
H.W. Pickett, ASTM E4 and General Electric Company.
W.L. Fink, Aluminum Company of America (ALCOA).
M.L. Fuller, New Jersey Zinc Company.
J.D. Hanawalt, the Dow Chemical Company.
V. Hicks, Navy Department.
M.L. Huggins, Eastman Kodak Company.
P.F. Kerr, Columbia University.
J. Magos, Crane Co.
H.R. Nelson, Battelle Memorial Institute.
W.E. Richmond, U.S. Geological Survey.
L.L. Wyman, General Electric Company.

It is highly probable that this first meeting of the newly formed Joint Committee was the beginning of the Joint Committee on Chemical Analysis by X-ray Diffraction Methods. "The initial role of the Joint Committee was to approach industrial and scientific organizations for support and to initiate a structure for overseeing this activity" (Smith, 1986). About this time, it was becoming known that several individuals were working with or constructing limited,

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smaller files of diffraction data to satisfy their specific work requirements. Through the efforts of this Committee, "contributed data was solicited from workers in various laboratories in advance or in lieu of publication." William L. Fink and K. Van Horn of ALCOA, M.L. Fuller of the New Jersey Zinc Company, and C.H. Hogg of the Pennsylvania State University were generous contributors (Davey, 1941). A substantial amount of the card data for the first ASTM data card set was from J. Donald Hanawalt, Harold W. Rinn, and Ludo K. Frevel of The Dow Chemical Company and reproduced from Dow's original card set (Hanawalt *et al.*, 1938).

Until 1938, and well after, diffraction films were retained as the permanent record of X-ray pattern characteristics (Blanton, 2003). With the publication of the classic article, "Chemical analysis by X-ray diffraction" (Hanawalt *et al.*, 1938), a new presentation of data, in table form, was introduced, along with a method of searching the file to retrieve data. "Reprints of the publication were quickly exhausted and the General Electric Company sponsored a second printing of 500 copies. Even this printing was insufficient. In 1941, the ASTM issued the data sets on 3×5 cards. This issue became Set 1 of the Powder Diffraction File" (Davey, 1941). This publication has long been considered the official beginning of the Powder Diffraction File (PDF, 1941) and the ICDD. The year 1942 marked the first appearance of an Alphabetical Index. The index was contributed to the ASTM by two organizations: the F.P. Hochgesang, Research and Development Division of Socony-Vacuum Oil Co., Inc., and M. Stevens and J.B. Reed of the Frankford Arsenal (Davey *et al.*, 1942).

In 1944, a Supplemental Card Set was published by the ASTM. Mineralogical data were furnished by F.A. Bannister of the Department of Natural History of the British Museum and by the Crystallographic Laboratory of the Cambridge University. The work of the British Institute of Physics, through Sir Lawrence Bragg and A.J.C. Wilson, was extremely valuable. Considerable use was made of the resumes of G.S. Harcourt, *American Mineralogist*, Vol. 27, and A.K. Boldyrev *et al.*, *Annales del Institute des Mines Leningrad*, Vol. 11 (Davey, 1944).

W.P. Davey conducted years of scientific research at the General Electric Company, and, in later years, he joined the staff of the School of Chemistry and Physics at the Pennsylvania State College. W.P. Davey carried on his efforts to establish a file of X-ray diffraction standards while serving as Chairman of the Joint Committee. It has been reported that significant financial support by the General Electric Company was provided to the Pennsylvania State University as a grant so that W.P. Davey could continue this work (Wyman, 1966). W.P. Davey retired from Pennsylvania State College (now renamed Pennsylvania State University) in 1949, but retained his office and continued his contributions to the X-ray community. His assistant, Art S. Beward, assumed increasing responsibility and moved the production of the PDF (using hand-cut paper strips) to a house on Heister Street in State College, Pennsylvania, where it remained until the organization introduced computers in about 1963.

The collaborators in publishing Set 1 of the Card File, in addition to the Joint Committee of the ASTM, were the Committee on X-ray and Electron Diffraction of the Division of Chemistry and Chemical Technology of the (USA) National Research Council and the British Institute of Physics. The British Institute of Physics, which had previously proposed a similar activity, polled its work with that of the Joint Committee. In practice, the application of this Card File proved somewhat cumbersome. There were no "Search Manuals" as we became accustomed to in later years. Searching the file was accomplished using data cards. The three strongest lines of a diffraction pattern were also listed on two other cards on which the second and third strongest lines, respectively, were listed first. "This arrangement was devised to use the search scheme proposed by J.D. Hanawalt, H.W. Rinn, and L. Frevel (Hanawalt *et al.*, 1938). By placing the cards in a drawer in 'Hanawalt' order, the user could thumb through the cards examining index lines to find a match. As the number of cards increased with Set 2 (1944) and Set 3 (1949), the stack of cards became quite large. The larger number of entries in the Card File made it more useful because of increased coverage, but it was cumbersome to use for the identification of unknown materials" (Jenkins and Smith, 1996). In the preface of the first Card File, a note appeared stating, "The Hanawalt Method is described rather fully in Industrial and Engineering Chemistry, Analytical Edition, 1938." Subcommittee VI of ASTM Committee E-4 has issued a Tentative Recommended Practice for the Identification of Crystalline Materials by the Hanawalt X-ray Diffraction Method. It should be studied by all users of this Card File.

The article by Hanawalt *et al.* (1938) did not take long to revolutionize the efforts in building a file of X-ray diffraction standards and a method of data retrieval. *Industrial and Engineering Chemistry* stated that it "considers itself fortunate in being able to present a complete, new workable system of analysis, for it is not often that this is possible in a single issue of any journal. Several qualified reviewers assure us that the authors present here a method that is not only workable but so clearly described that their scheme of chemical analysis will be readily understood by all those familiar with X-ray diffraction. The reader does not need to be skilled in crystal analysis; only to be familiar with the bare principle of diffraction. There is reason to believe that this publication, which is made possible in this form by the generous financial assistance of the Dow Chemical Company, will serve to bring this method of analysis into general use in industrial and consulting analytical laboratories" (Hanawalt *et al.*, 1938).

Hanawalt *et al.* (1938) wrote, "This paper supplies tabulated data on the diffraction patterns of 1000 chemical substances and gives a scheme of classification which makes possible a routine and valuable use in the chemical laboratory". In 1919, Hull emphasized the experimental simplicity of obtaining the diffraction pattern of a substance and the fact that it requires only a minute amount of material. He stated that, "every crystalline substance gives a pattern; that the same substance always gives the same pattern; and that in a mixture of substances, each produces its pattern independently of the other." The author states, "However, as yet, no extensive use has been made of X-ray diffraction. Probably one of the most important circumstances, which at present handicap the general use of the method, is that an adequate file of standard patterns is not available for reference. The method being empirical, standards are necessary." The author also stated, "The use of the X-ray method of analysis would be greatly extended if crystal structure workers, after they have taken

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care to get a pure material, would publish the powder data of the material in the same or equivalent form" (Hull, 1919).

Hanawalt *et al.* (1938) also discussed an index book currently in use at the Dow Chemical Company. Lines that lie between 20 Å and 0.5 Å for indexing are grouped into 77 suitable divisions. Each of the divisions of the index is followed by a section called the Supplementary Group Index in which all patterns whose strongest line falls in the major group have their three strongest lines listed in the order 1, 2, 3. All patterns whose second strongest line falls in the major group have their three strongest lines listed in the order 2, 1, 3; and all patterns whose third strongest line falls in the major group have their three strongest lines listed in the order 3, 1, 2. In 1942, W.P. Davey introduced an Alphabetical and Formula Index that listed, in a modified alphabetical order, the chemical names of substances represented in the first set of data cards. Each name was followed by its chemical formula and by a statement of the strongest line in the X-ray pattern. In 1945, in the second release of the Alphabetical Index, the second card set was included, and the index was modified with the three strongest lines in accordance with the Hanawalt Method (Davey, 1945). By the 1950s, an Alphabetical Index, a Grouped Numerical Index (Davey, 1952), and a Mineral Listing were published with the fourth set of cards. "There were three sections to the Alphabetical Index. The first and largest section listed the Inorganic compounds and elements; the second listed Organics and the third listed Minerals. In the Numerical section, for every data card in the File, the entry in the Index consisted of the three strongest lines of the pattern, their intensities, the chemical name and formula of the substance and the numerical sequence number of the data card. Each data card would have three entries in the index depending on the three strongest lines." The indexes, because of their size, were now published as hardcover books.

This was truly the beginning of the PDF as we know it today or, at least until the onset of the computer age. The preparation and production of the PDF, soon after the format for data cards and index books was agreed upon by the (ASTM) Joint Committee, proved to be laborious, expensive, and time consuming. Initially, the first few sets of data cards were handwritten and no index books were available. The Alphabetical Index was prepared by typing strips of one-line entries with the three strongest lines, the chemical formula, and the PDF number for each compound. The Hanawalt Numerical Index provided for the permutation of the three strongest lines. The typed strips were then ordered in a Termitrex holder and then photographed for printing. The Termitrex holder was a metal frame about 15 inches by 20 inches that permitted the insertion of typed strips of data in slots that were provided in the back of the frame assembly. Each time a page was complete, it was photographed for printing and the next page assembled in the same manner.

IV. BECOMING A BUSINESS: 1950 TO 1970

Until this time, the editorial work on the PDF was accomplished under the direction of W.P. Davey at the Pennsylvania State University. By the late 1950s, G.W. Brindley of the Pennsylvania State University was assigned the role of Editor. Somewhere around 1960, L.G. Berry of the Department of Mineralogy, Queen's University, Kingston, Ontario, Canada, was designated Editor of the PDF. H.W. Rinn was Chairman of the Joint Committee, having served in this capacity since 1956. The PDF was becoming self-supporting through its sales and soon, under the direction of A.S. Beward, the offices of the Joint Committee, including the technical and data acquisition activities, moved from the Pennsylvania State University to Heister Street in downtown State College, Pennsylvania. By the early1960s, the entire activity was moved to the ASTM Headquarters at 1916 Race Street in Philadelphia, Pennsylvania, initially under the direction of A.S. Beward and later J. Caum and Sam Etris. As gathered from conversations with a few of the early members of the Joint Committee, the move was probably required since the Joint Committee appeared to be a viable business activity with increasing business and production demands. A.S. Beward played a vital role in the activities of the Joint Committee at the Pennsylvania State University, the office in downtown State College, and, for a few years, at the location at ASTM Headquarters. Joseph V. Smith of the Department of Mineralogy at the Pennsylvania State University soon assumed the duties of Editor of the PDF. A unique feature of the Joint Committee was that it was a quasi-independent organization. The Joint Committee managed and directed all activities concerned with the PDF and always retained the proceeds from its sale. The ASTM furnished accounting and logistical support, provided office space, hired employees, marketed the product, and arranged for printing of the Joint Committee's products. In other words, the ASTM provided all the services necessary to operate a business. The Joint Committee, naturally, on a monthly basis, reimbursed the ASTM for all costs incurred.

As the PDF began to gain recognition, the scientific community requested regular, more frequent issues of the sets of data and the publication of better quality data. To meet this challenge, data acquisition activities had to be increased. Mary Lotz became Bibliographer of the Joint Committee and took on the task of searching the scientific literature. This activity was conducted at the Pennsylvania State University because of their excellent library facility and extensive collection of scientific journals. To improve the overall quality of data, a "type" of grant-in-aid program was established through the effort of A.J.C. Wilson of the University of Birmingham, Birmingham, England. It was agreed upon by the Joint Committee that, in lieu of actual cash funding to support the production of high-quality X-ray patterns for inclusion in the PDF, printed sets of the PDF would be supplied for sale in the United Kingdom. The proceeds from the sale were then used to support the generation of high-quality patterns at cooperating universities. (The author believes that after World War II, it was very difficult to get British pounds out of the country, and this was a solution to that problem.) A few of the participants included: University College, Cardiff, Wales; University of Leeds, Leeds, England; University of Durham, Durham, England; ARC Unit of Structural Chemistry, London, England; Rothamsted Experimental Station, Harpenden, Hertz, U.K.; and the University of Aberdeen, Old Aberdeen, Scotland.

An Associateship was established in 1953, under the direction of Howard F. McMurdie, at the National Bureau of Standards (NBS), Gaithersburg, Maryland (Mighell *et al.*, 2004). The mission of the Associateship was "to collect data under controlled and reproducible conditions, to provide *d–I* data on common important compounds, to replace multiple

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entries in the earlier sets, and to improve the overall accuracy of the PDF" (Jenkins and Smith, 1996). Following H.F. McMurdie as Director, this activity was carried on for many years by Stanley Block and Camden Hubbard. Members of the Associateship included Eloise Evans, Marlene Morris, Johan De Groot, Winnie Wong-Ng, and Boris Paretskin. Through the years, the powder patterns produced by the Associateship were regarded as being of the "highest quality." The NBS, in conjunction with the Associateship, also published the *NBS Monograph Series* that included most of this work from 1953 to 1985. In Release 2011 of the PDF-4 + , 493 reference patterns were published through the *Circular 539 series* (Swanson and Tatge, 1953) and another 1473 patterns were published through the *NBS Monograph 25 series*. Even under 2011 quality standards, and more than 25 years after they were produced, 57% of these patterns are still receiving ICDD's highest-quality designation (Kabekkodu, 2011).

In 1961, W.L. Fink assumed the duties of Chairman of the Joint Committee. Under the direction of W.L. Fink and J.V. Smith, the Joint Committee made outstanding progress over the intervening years. Through the effort of W.L. Fink and Professor Y. Takeuchi of the University of Tokyo, the Japanese Powder Data Commission was established. This program paralleled the activities of the Associateship at the NBS in producing high-quality data for inclusion in the PDF. Pieter M. DeWolff and Jan Visser, Technisch Physische Dienst, TNO-TH, Delft, Netherlands, are also recognized for being outstanding contributors of quality data to the PDF through the ICDD Grant-in-Aid Program. Over the last 10 years, the ICDD through its Grant-in-Aid Program has disbursed over $3 million to numerous universities and colleges worldwide. This program must be considered one of the best investments the Joint Committee has ever made. Grantees, once established, improve with experience and have an excellent record for producing the highest-quality data sets. Professor Shao-Fan Lin from the People's Republic of China recently became the second grantee to publish over 1000 material data sets in the PDF, joining Larry Calvert of the National Research Council of Canada.

In the 1960s, to process the increasing influx of data that was being acquired and to maintain high-quality data for publication, the Joint Committee realized the need for additional editorial assistance. Benjamin Post of the Polytechnic Institute of Brooklyn and Sigmund Weissmann of Rutgers University were engaged as Associate Editors of the PDF. B. Post reviewed inorganic and organic materials and S. Weissmann reviewed metals and alloys. J.V. Smith reviewed all mineral data. L.G. Berry, Deane K. Smith, Peter Bayliss, and Mary Mrose also served as Mineral Editors during this period. To supervise the day-to-day operations at the ASTM (with about 10 staff) and to serve as liaison with the ASTM management and the Joint Committee members, Rodger G. Simard was hired as Corporate Secretary and General Manager.

Soon after the move to the ASTM Headquarters, work commenced on revising the original five sets of data. With an editorial staff now established, and the need to update data in the original publications, this project was considered absolutely necessary. The project was completed in the early 1960s and plans were formulated to eventually revise Sets 6–10. In addition to the data cards, the 1960s introduced the PDF in "keysort cards." These cards consisted of holes representing "*d*" values in which long needles were inserted to obtain data of interest. This product was eventually discontinued because of exorbitant production costs. The Matthew Index was also discontinued at this time because it had reached the maximum number of patterns it could accommodate. In the 1960s, the data sets approached and exceeded 10,000 entries, making several manual methods impractical (taking too much time), especially those like the Matthew Index that required many pieces of information to perform a search. In today's world, with the computing power of modern PCs, some of these limitations have become advantages and multivariable searches are often combined into data mining algorithms.

There were very few total members, and actually fewer than 10 people did the work of the organization. When the various committees met, the same people simply changed chairs and rehashed the same topics! Many of the Joint Committee Annual Meetings were held concurrent with the Pittsburgh Diffraction Conference in 1960–1970 (when A.S. Beward was the principal worker at State College, Pennsylvania). In the 1965 annual meeting, held concurrent with the Gatlinburg ACA, Bill Parish, another Pennsylvania State University graduate, questioned the Treasurer about finances. The Treasurer did not like being questioned, and walked out! The organization had no budget that year! When the organization moved to the ASTM Headquarters in Philadelphia, some new members and workers helped to improve the organization (Fred Van Atta, Joe Smith, Andy Danko, L.G. Berry, Ben Post, Sig Weissmann, and Gerald G. Johnson).

Professor Wilbur (Will) Bigelow, a graduate of the Pennsylvania State University, addressed the identification problem of not using intensities for the construction of a search index. Will was using electron diffraction where the diffraction intensities were not as meaningful as with X-ray diffraction. His work was the basis for the Fink Index. Over the years, Prof. Hanawalt would claim that the Hanawalt method of identification could do everything that the Fink Index used. Hanawalt simple said; "It just takes more work." They were both at the University of Michigan and did not interact; G.G. Johnson was the channel between them. The Fink and Hanawalt indexes are still used in manual methods and have been adopted in computer-automated searches; both methods can excel with certain classes of materials. The Fink method works best with materials having larger unit cells and "long" *d*-spacings.

Another solution to the Matthew Index was proposed by Dr. Jan Visser of Delft, Netherlands. For several years, Dr. Visser's group in Delft attempted research funding using holographic techniques. Although nothing came of this research for the Joint Committee on Powder Diffraction Standards (JCPDS), many other funded projects formed the basis of other scientific diffraction activities.

Starting in the mid-1960s, computer technology made great advancements in data processing and retrieval techniques. Vladimir Vand and Gerald G. Johnson, Jr., of the Pennsylvania State University soon began to investigate the application of data processing for the PDF. Not only were search/match programs being developed, but also the master copy of the book index was printed at the Pennsylvania State University. The final pages were then carefully shipped to professional print shops to produce the various search manuals! The JCPDS had special print trains cast by IBM so that Greek, superscript, subscript, and italic fonts could appear in

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the search manuals. This work was of vital interest to the Joint Committee because the Hanawalt Numerical Index and the Davey Alphabetical Index were distributed with each set of the PDF. As mentioned previously, both indexes were produced manually, resulting in lengthy production times and considerable expense. The research by V. Vand (who died in 1968) and G.G. Johnson was eventually supported by the Joint Committee Grant-in-Aid Program and continued for many years under the direction of G.G. Johnson. A great interest was developing in the scientific field for automated searching of chemical databases Johnson and Vand (1967) also directed their efforts in this area. At the 1965 Pittsburgh Diffraction Conference, Dr. Ludo Frevel of the Dow Chemical Company (Frevel, 1965), Mr. Monte Nichols of Lawrence Livermore Laboratories (Nichols, 1966), and G.G. Johnson of the Pennsylvania State University each presented a different computer search match program for the identification of multiphase powder diffraction patterns. The Joint Committee distributed the mainframe software, written by G.G. Johnson, without change until the PC appeared. G.G. Johnson rewrote the mainframe software for IBM, UNIVAC, CDC, and Honeywell-type computers over the next 15–20 years.

The entire set of *d–I* pairs in the data sets were independently keyed by the personnel at the Pennsylvania State University, and, unknowingly, also at 3M (under the supervision of Dr. Byron T. Gorres). This allowed a computerized comparison of the two independent data set entries to reduce data entry errors.

At the 1974 Berkeley American Crystallographic Association (ACA) meeting, the scientific community asked for the magnetic tape to be reorganized from two separate files (the first with chemical names and formulae and the second with *d–I* pairs) into a single file with the merged information available in a linear manner. It should be remembered that magnetic tapes were the principal storage media for computers; the massive high-speed disks of today were only available at national data centers.

The tasks at hand were not simple considering that the starting point for this work was to create a computer-readable file from the existing PDF, to write the computer programs to produce the indexes, and to write programs to search the PDF for the identification of unknown materials. All of this work started with the tremendous task of keypunching the PDF on "IBM" cards. Over time, the difficulties were overcome and the first computer-generated indexes appeared in 1964. Soon thereafter, V.V and and G.G. Johnson developed the PDF on magnetic tape, with associated search programs. To satisfy copyright concerns, the product was only made available on lease. This work was eventually transferred from the Pennsylvania State University to the staff at the ASTM Headquarters. G.G. Johnson continued working for the Joint Committee at the Pennsylvania State University as a computer consultant. The creation of a computer-readable database not only led to the development of other products, such as the PDF on "IBM" cards, 2dTS, a computer time-sharing system, the Fink Graphical Index and the Fink Numerical Index, but also paved the way for the development of products that we know today and provided the impetus to remain "state-of-the-art" in this activity.

The early computer programs were very different from those in use today. Several limitations were fundamentally based on the small storage capacity and limited processors of existing computers. Many automated indexes were developed that use small portions of the data files to automatically process data sets. In fact, one of the early programs designed for a laboratory computer, instead of a company mainframe (Frevel *et al.*, 1976), was designed for single peak search on a small number of 298 common phases. This number was selected from the historical records of phases that were important to the Dow Chemical Company.

J. Messick joined the staff at the ASTM Headquarters in 1966 as Assistant to the General Manager, and, in a few years, W. Frank McClune joined the staff as Manager of the Diffraction Data Department. A governing group was established, with W.L. Fink serving as Chairman of the Joint Committee. Other members included R.G. Simard, L.L. Wyman, J.D. Hanawalt, J.V. Smith, and A.W. Danko. L.L. Wyman served as Treasurer and, for the most part, J.V. Smith organized and managed the technical activities. Over the next several years, the overall administration of the Joint Committee improved dramatically.

During this period, the editorial, bibliographic, and publication functions began progressing favorably and the annual updates to the PDF consisted of 2000 patterns per set. As more and more individuals and industrial concerns became familiar with the Joint Committee, the membership steadily increased. Around 1940, there were perhaps 15 members; by 1950, at least 25 members, and in the 1960s, the membership increased to approximately 70 members. With increasing membership, the organization required at least one meeting a year to discuss technical and editorial issues. Financial issues were discussed to a lesser degree. Three committees were eventually established—the Editorial Committee, the Technical Committee, and the Finance Committee.

In 1969, Tom Marshall, Executive Director of the ASTM, passed away and William Cavanaugh was recruited to serve as the ASTM's new Executive Director. From the onset, Cavanaugh objected to the quasi-independent status of the Joint Committee while operating at the ASTM Headquarters. At the same time, the Joint Committee was in the process of being incorporated as a nonprofit corporation in the Commonwealth of Pennsylvania. In December 1969, the incorporation was approved by the Pennsylvania Department of State and the Joint Committee became a "Nonprofit Corporation in the Commonwealth of Pennsylvania," exempt from taxation under section 501(c)3 of the Internal Revenue Code. The incorporators were W.L. Fink, J.D. Hanawalt, R.G. Simard, Morris R. Brooke, and L.L. Wyman. The first directors, who were collectively designated as the Board of Directors and served at the first annual meeting, were A.W. Danko, W.L. Fink, J.D. Hanawalt, H.W. Rinn, R.G. Simard, D.A. Vaughan, and L.L. Wyman. Naturally, the incorporation of the Joint Committee required appropriate organizational changes. Of primary importance was the establishment of a set of bylaws to officially describe the organization's mission and outline how the organization would conduct its affairs. Topics such as Membership, Meeting of Members, Election of Officers and Directors, Committees and Subcommittees, Proxies, Quorums and Voting Requirements, and many additional areas had to be addressed. M.R. Brooke, while serving as the Joint Committee's legal consultant, prepared the first set of bylaws. Through the years, numerous revisions of the bylaws have

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been required to accommodate the ever-changing activities of the Joint Committee.

V. INTERNATIONAL GROWTH: 1970 TO 1990

By 1970, the objections of the Joint Committee's status and other issues raised by W. Cavanaugh necessitated decisive action by the relatively new Joint Committee Board of Directors. The Board of Directors announced that the Joint Committee would vacate the ASTM Headquarters located at 1916 Race Street, Philadelphia, Pennsylvania, and conduct operations at the Mutual Benefit Life Building, 1845 Walnut Street, Philadelphia, Pennsylvania. The new office facilities were located on the 20th floor, overlooking Rittenhouse Square. In less than two years, the Joint Committee acquired a new building in Swarthmore, Pennsylvania. Soon after the move to the "permanent" Headquarters in Swarthmore, J.D. Hanawalt proposed that the organization's name be changed to the "Joint Committee on Powder Diffraction Standards" (JCPDS) in order to more accurately reflect the mission and purpose of the organization. The proposal was unanimously approved by the Board of Directors. In 1978, J.D. Hanawalt, again, proposed that the name of the corporation be changed. The JCPDS–ICDD was approved and adopted to better reflect the international scope of operations.

At J.D. Hanawalt's insistence, new members were brought into the organization. One of these new members was Walter Eysel, a visiting professor at the Pennsylvania State University, who was eventually a key figure in the German diffraction community and worked at the historic Heidelberg University. G.G. Johnson introduced the following distinguished members of the organization:

Herb Goebel, winner of the 1998 Hanawalt Award.

Shao-Fan Lin, chief scientific liaison in China, Distinguished Grantee 2004.

Sergei Kirik, Distinguished Grantee 2007, from Krasnoyarsk, Russia.

In 1968, D.K. Smith left Lawrence Radiation Laboratory and joined the Pennsylvania State University faculty. He spent well over half of his time on efforts for the Joint Committee, until the time of his death in 2001. D.K. Smith and G.G. Johnson worked together for more than 40 years on computer software for powder diffraction.

With the increasing membership participation in business and technical activities, the growing user base, and the need to continue to produce the best products possible, it soon became apparent that the internal operating procedures at the Headquarters had to be further developed. Through the efforts of G.G. Johnson, consultant for computer activities, Mark Holomany was recruited and joined the ICDD's staff as Manager of the Computer Department with the primary mission to adapt editorial activities to the newly acquired "VAX" computer. Up to this point, the search indexes were computer-generated, but data cards continued to be typed onto 6 × 9-inch formatted sheets using IBM Selectric typewriters. Typing a single card required changing the symbol head numerous times, and proved to be time-consuming and inefficient. Through the guidance and expertise of Camden Hubbard, the Diffraction Data Department became equipped with Hewlett Packard terminals, which permitted input of data directly to the computer. Shortly thereafter, software was obtained to automate the sales, finance, and accounting activities. Within a few years of the introduction of the personal computer, the entire Headquarters' operation was considered state-of-the-art, a level of operation that continues to be maintained today.

In 1973, with the closing of the Westinghouse Astronuclear Laboratory in Pittsburgh, Pennsylvania, A.W. Danko, through the influence of L.L. Wyman, was added to the staff of Joint Committee as Special Consultant to the General Manger. With the decreasing employment at the U.S. Steel Corporation, Leo Zwell, also through the influence of L.L. Wyman, was added to the Headquarters' staff as Assistant Bibliographer.

W.L. Fink relinquished his position as Chairman of the Joint Committee in 1974 and L.L. Wyman was elected Chairman and served for a year. R.G. Simard, Corporate Secretary and General Manager since 1964, retired and A.W. Danko was selected to fill the position. With the passing of L.L. Wyman in 1975, Jesse W. Caum, formerly Technical Director at the ASTM, was appointed to fill the unexpired term of L.L. Wyman. At the next scheduled election in 1976, J.D. Hanawalt was elected Chairman and was followed by D.K. Smith in 1978. Shortly after A.W. Danko passed away, J.W. Caum was appointed Corporate Secretary and General Manager. W.F. McClune was appointed Editor of the PDF. To assist with the increasing editorial workload, Theresa Maguire was added to the staff in 1977 as Assistant Managing Editor, Donna Barry in 1979 as an accountant, and Terry Kahmer in data entry in 1981; all three are department managers today.

In 1973, Gregory J. McCarthy of the Pennsylvania State University, and later of the North Dakota State University, was elected as Member-at-Large of the Board of Directors and while serving on the Board, was appointed Chairman of the Technical Committee. Over the next 14 years, G.J. McCarthy served on the Board in various positions under the W.L. Fink, L.L. Wyman, J.W. Caum, J.D. Hanawalt, and D.K. Smith administrations. He was elected as Chairman in 1982. In 1975, database sales first exceeded one million dollars and sales steadily grew during the decade. J. Messick was appointed as Corporate Secretary and General Manger in 1984, and, approximately a year later, Ron Jenkins joined the staff as Principal Scientist. G.J. McCarthy's organizational and management skills were put to use to establish a new sense of direction for the ICDD in all areas of operation. As Chairman of the Technical Committee, he focused on new areas of interest and products by establishing subcommittees whose members were selected relative to their fields of interest. Early on, only a few subcommittees existed, but over time it was standard practice to take advantage of the membership's expertise and willingness to volunteer. With the considerable growth in membership interest and participation, the number of subcommittees increased dramatically. The list of active subcommittees is constantly being updated to satisfy the ever-changing activities within the ICDD.

Also, during G.J. McCarthy's term as Chairman, a similar program of extending the activities of the Board of Directors was completed. The Awards, Employee Benefits, and the Long-Range Planning Committees were established. The Finance Committee also added the Budget Review Committee and the Marketing Subcommittee. It now appeared that the ICDD was a well-administered organization and, for

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the most part, many of the programs, policies, and procedures developed at this time are still practiced today. Several outstanding contributors to G.J. McCarthy's administration were R. Anderson, J. Edmonds, W. Eysel, T. Fawcett, G. Fischer, C.M. Foris, G.P. Hamill, H.D. Hitchcock, C.R. Hubbard, R. Jenkins, G.G. Johnson, H.F. McMurdie, B. Post, M.C. Nichols, D.K. Smith, R.L. Snyder, L. Frevel, and J.W. Visser.

The G.J. McCarthy era is best defined as a period of necessary growth. In addition to essentially restructuring the ICDD, he greatly expanded the scope of activity by instituting a program of tutorials and workshops that were an immediate success. One of the first programs presented was at the Denver X-ray Conference (DXC) at the University of Denver. "The organization and sponsorship of the Conference was administered by the University of Denver until 1997. Beginning in 1998, the ICDD assumed ownership of the Conference from the University of Denver. Each year, the technical program of the DXC is created and monitored by the Denver X-ray Conference Organizing Committee (DXCOC). The Committee consists of specialists from various fields of X-ray analysis, each of whom contribute[s] their expertise to the technical program. Today, this activity is conducted worldwide. While exhibits have become a large attraction at the Conference, DXCOC maintains a commercial-free, vendor-neutral program. Working in partnership with the DXCOC, [the] ICDD manages the financial aspects of the Conference and its administration, including the exhibition of X-ray products and publication of the conference proceedings, *Advances in X-ray Analysis*" (Maguire, 2010). The ICDD was also a major participant in the annual meeting, technical presentations, and exhibits of the Australian X-ray Analytical Association. ICDD member Brian O'Connor of the Curtin University of Technology was among the early organizers of this conference. The ICDD also participates in the European Powder Diffraction Conference (EPDIC). ICDD members, Herbert Goebel, W. Eysel, J.W. Visser, and R.L. Snyder, were among the first EPDIC organizing committee. Similarly, ICDD members have been influential in the organization the South American X-ray Conference (SARX). Each conference promotes materials analysis and provides educational workshops to both novices and experts. The ICDD continues to provide both technical assistance in the form of workshops and financial assistance to these organizations.

G.J. McCarthy stepped down as Chairman in 1986 and D. K. Smith was elected, once again, as Chairman. Note that with the exception of the first three chairmen, D.K. Smith is the only one to have served as Chairman on two different occasions for a total of eight years. One of the highlights of the D.K. Smith administration was the introduction of the NBS*AIDS83 review program. The potentially acceptable *d–I* data were keyed into computer-readable form and both the data and the NBS*AIDS83 output were supplied to Associate Editors. The NBS*AIDS83 program provided the editors with sufficient information to make a final decision on the appropriateness of the new data for the PDF and to assign the quality mark of the pattern. D.K. Smith also solicited the cooperation from other database organizations such as Fachinformationszentrum Karlsruhe (FIZ), to obtain additional information on existing patterns in the PDF and to explore other sources of data availability. The POWD program, developed by D.K. Smith, has been used to calculate hundreds of thousands of powder patterns for the PDF.

For several years, computer-readable versions of the PDF, known as PDF-1, were available and contained *d–I*s, chemical formulae, and PDF numbers on magnetic tape. However, most laboratories used manual methods with indexes and card files. In 1985, PDF-2 was introduced, displaying all the data that appeared on a card image in computer-readable form. X-ray manufacturers were greatly interested in computer searching the PDF and most of the manufacturers of X-ray equipment were introducing automated systems. The early major suppliers of APD systems included Philips Electronics, the Diano Corporation, Siemens, and the Rigaku Corporation. The APD brought the electronic search process from a mainframe computer and into the laboratory. Material Data, Inc. (MDI) was a major supplier of software for automated systems incorporating the PDF. Over the next few years, the cooperation between the ICDD and equipment manufacturers and software developers proved to be very rewarding and the cooperation continues today as new products are produced. Sanyo Shuppan Book Company, and, in later years, Sanyo Information Systems, under the direction of Toshimichi Matsukura, proved to be an exceptional distributor of ICDD products in Japan and the Far East. During the second term of the D.K. Smith administration, he and R. Jenkins collaborated to produce and publish, *Powder Diffraction*, an international journal of materials characterization. The journal has proved to be a valuable source of information to all working in the field of X-ray diffraction. Ting Huang has been Editor-in-Chief of *Powder Diffraction* since 1999.

In 1985, R. Jenkins, a world-renowned expert in XRD and XRF, long-time ICDD member, and development scientist at Philips Electronics in North America, joined the ICDD staff. This coincided with the closure of Philips research facilities in the United States. R. Jenkins was aware of an exciting new technology being developed by Philips at their main research facilities in the Netherlands, the CD-ROM. He was very influential in convincing the ICDD's Board of Directors to investigate this new technology and then adapted it as a database media. He had a very able partner in Editor-In-Chief Frank McClune and they quickly adapted the PDF on a CD-ROM at the critical period when APD's were transitioning to personal computers. Initially, both the ICDD and Philips (Netherlands) developed the concept of placing the total PDF on a single read-only media. For approximately three years in the mid-1980s, the ICDD not only sold the database but also distributed the CD-ROM drive and instructions on how to use both the CD-ROM drive and the database. Eventually, CD-ROM drives became common on PCs and the ICDD produced the database exclusively. The convenience of this new technology was quickly adapted and, within a few years, CD-ROM sales supplanted sales from all other media: books, cards, VAX tape, and microfiche. Because of the drop in sales and expense of manufacturing, in 1987 the production of cards was stopped, but a book in card format continues to be produced today. Over the next 10 years, global sales doubled from US $2 million to $4 million.

VI. COLLABORATIONS: 1990 and beyond

L. Frevel was elected Chairman in 1990 and the ICDD continued to experience growing acceptance of its products.

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In 1991, L. Frevel made a significant financial contribution to the ICDD for the establishment of a Crystallography Scholarship Fund to "encourage promising graduate students to pursue crystallographically-oriented research." For many years, he continued his guidance over the program and today, to honor this pioneer in the science of X-ray diffraction, this fund is known as the Ludo Frevel Scholarship Fund. From 1991 until 2011, with the additional financial assistance from the private and industrial sectors, the ICDD has awarded 122 scholarships totaling over US $282,550.

All scholarships are funded from the principal and today the fund is sufficient to award 13 scholarships annually. All donations to the fund go toward the scholarships.

L. Frevel served only two years as Chairman and, by 1992, the Headquarters staff had increased considerably to meet the demands of the rapidly growing product line, the increasing membership, and increasing marketing and technical activities. This business growth led to the demand for an expansion in office space. Shortly before the completion of his term as Chairman, L. Frevel suggested that the ICDD investigate the possibility of obtaining a larger office facility. L. Frevel appointed a committee of J. Messick, G.G. Johnson, G. Hamill, and G. Fischer to conduct the search. G.G. Johnson was elected Chairman in 1992 and, in a short period of time, property was acquired in Newtown Square, Pennsylvania. Over the next year, the facility at 12 Campus Boulevard was designed and constructed and became the new Headquarters for the ICDD. J. Messick retired in 1994 and Dan Richardson was employed as Secretary and General Manager.

In 1996, R.L. Snyder was elected Chairman of the ICDD and R. Jenkins was appointed Secretary and Executive Director. Over the intervening years, John Faber joined the Headquarters staff as Principal Scientist as the ICDD made remarkable progress in database management and product development. C.R. Hubbard served as Chairman of the ICDD from 2000 to 2004 and James A. Kaduk from 2004 to 2008. In 2009, Tom Blanton became Chairman of the ICDD. As chairmen, they all played a major role in the advances of the ICDD. As a group of chairmen and scientists, they were all personally involved in the generation and evaluation of computer-enhanced analyses of powder diffraction data. During this period, the concept of "Total Pattern Analysis" was put forward in many presentations by the chairmen, where all aspects of diffraction and scattering can be extracted from the patterns of materials (Hubbard, 2000, 2001). The scope of the ICDD was expanded beyond crystalline materials to all materials.

The 1990s began a period of international collaborations as the PDF grew with the additions of powder patterns and physical property data calculated from single-crystal crystallographic experiments. Between 1998 and 2001, the ICDD negotiated data access agreements with Fachinformationszentrum Karlsruhe (FIZ), the Cambridge Crystallographic Data Centre (CCDC), and the National Institute of Standards and Technology (NIST). In 2003, the ICDD negotiated a collaboration agreement with the Material Phases Data System. The PDF was modified to include the use of powder patterns and physical property data calculated from single-crystal diffraction data (using the POWD program developed by D.K. Smith). A tremendous amount of editorial effort went into standardizing the formats from the different database organizations, categorizing the data and reviewing the quality of the data, independent of whether it came from a powder diffraction or single-crystal experiment. The fundamental structure of the database was changed to accommodate the large increase in data as the database was put into a relational database housing. Today, the PDF includes 750,000 material data sets published in several database products. The PDF is growing rapidly as over 50,000 new data sets are processed each year. The workshops and tutorials started in the 1980s have now expanded to a global network of workshops, clinics, and symposia that are sponsored by the ICDD and include many ICDD members and staff as instructors.

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