CUSTOMER NEWSLETTER OCTOBER 2010

Dear Customers and ICDD members,

Thank you for responding to the 2009 customer survey that we conducted in November and December of last year. Your feedback is important to us. We are already responding to information from the survey to guide product developments.

This newsletter is part of our commitment to customer service in providing you with some feedback on key results from the survey and responses to the common questions that you asked in the survey comments.

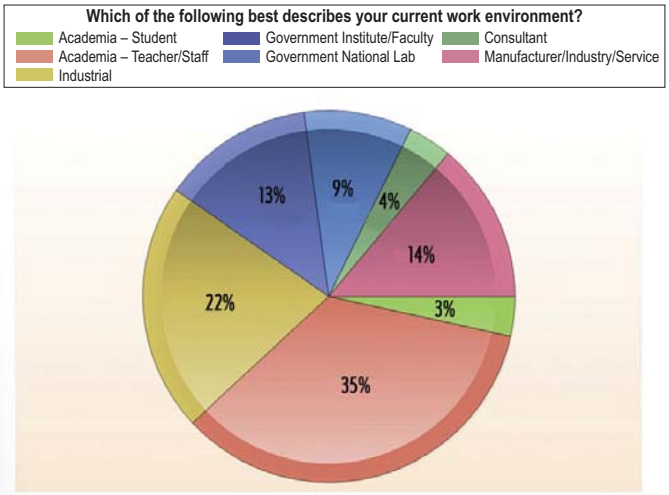
Key results

The ICDD received 811 responses to the 2009 survey. Eighty percent of the respondents perform material identification at least once a week, while 90% perform phase identification at least once a month.

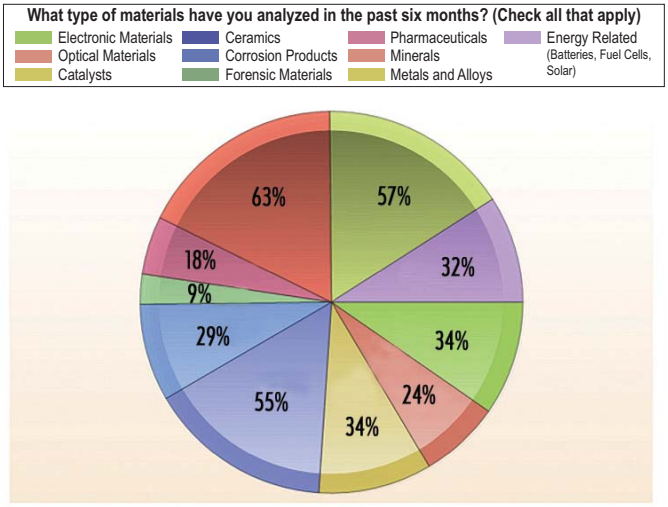
Within small variations, the survey responses (Questions 1 through 5) closely reflected the demographic distribution of our mailings, which was based on ICDD global sales and customer lists. We believe the following results to be representative of the larger materials analysis community.

As shown in the pie chart on the top right, there are large population groups of respondents from academia (38%), government (22%), and industry (36%). The large industrial segment distinguishes the ICDD customer and membership base from most other scientific societies. There was also broad participation from all major geographic regions of the world.

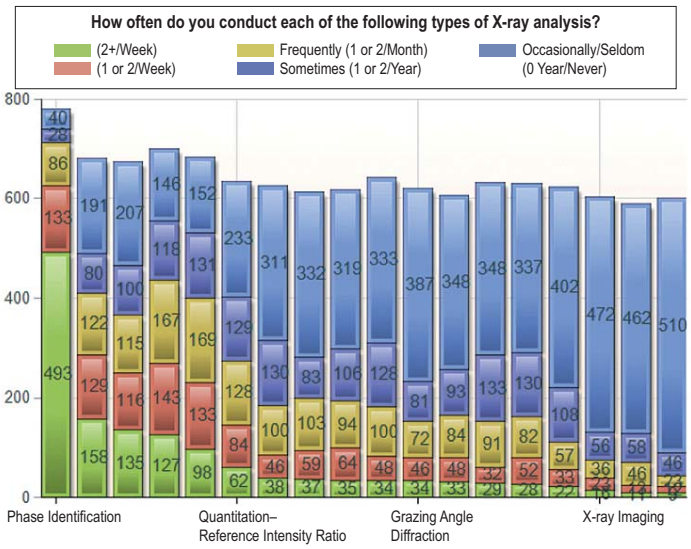
We had between 19–30% of the total participants from each region of Europe, North America and Asia, with smaller groups representing South America, Africa and the Middle East.



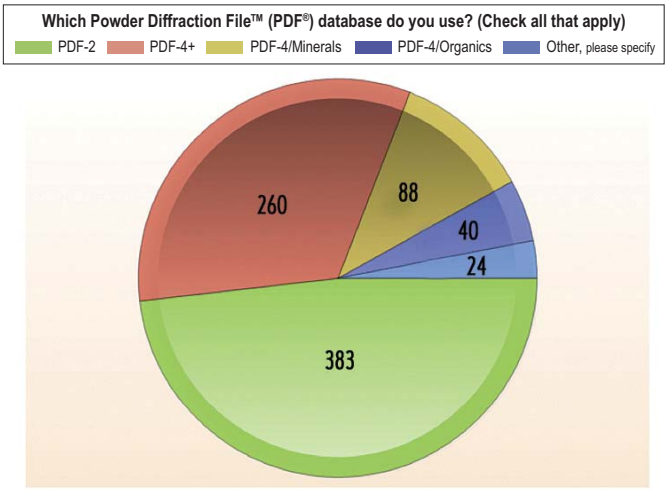
These percentages reflect commercial diffractometer sales' distributions, which are strong in industrialized countries and growing in emerging economies.



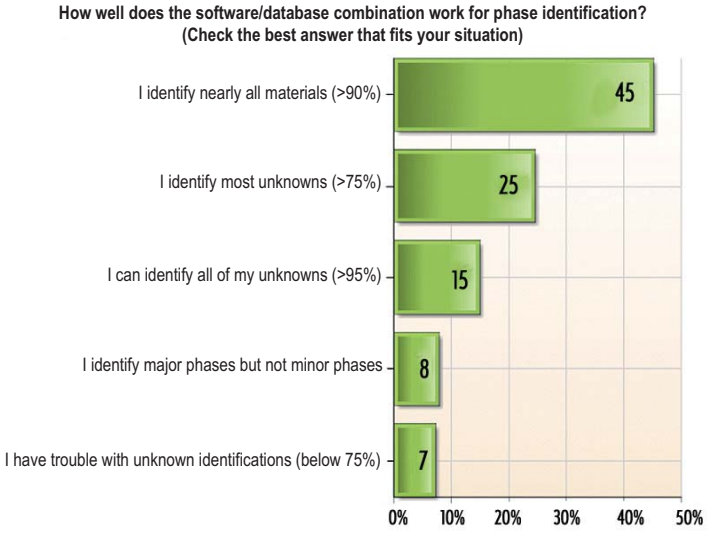
The pie chart directly above is from Question 9, demonstrating the wide range of materials being analyzed. The strongest responses for metals and alloys, ceramics and minerals reflect similar responses from decades of ICDD member surveys. The broad diversity is also characteristic of past surveys.



The results from Question 13, which asked about the frequency for several common types of analyses, is shown in the above bar graph. As expected phase identification was the dominate analysis. The most significant change was the increased frequency for several methods when compared to our 2006 survey and earlier member surveys. There were notable increases in Rietveld analyses (both structure and quantitation), RIR techniques, crystallite size and crystallinity measurements. The bar graph shows these were the next highest frequency of use after phase identification. We attribute this dramatic increase, in only 3 years, to the increased availability of automated software (Question 14) and international focus in the material science community on the analysis of nanomaterials (62% Question 27).



We asked users in Question 22 about what database(s) they were using and the answer is displayed in the above pie chart. There was nearly equal use of PDF-2 and PDF-4+ products. PDF-4 products were first introduced in 2005, hence this is the first customer survey with a significant PDF-4+ customer base. This result was also consistent with the answers to Question 14, which showed that 64% of the respondents' purchased a database within the last two years. In Question 24, we asked the critical question of whether the user's database/software combination solves their unknown identification problems. Seventy percent of those responding said they solved all, or nearly all, of their identification problems and 85% responded that they solve most of their problems.



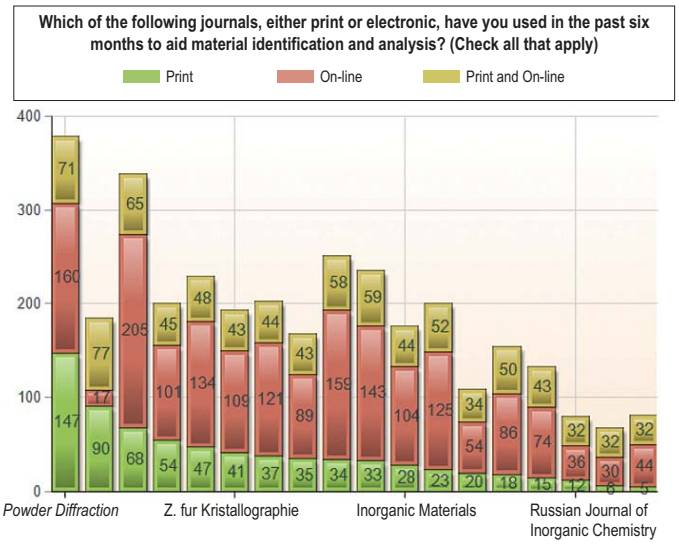
	Use Technique (>1 Mo.)		
Tool	Low Perf	Norm	High Perf.
Element Filter	52%	69%	75%
Subfile Filter	31%	52%	56%
Reference Quality	31%	40%	47%
GOM	28%	41%	51%
d-fit	25%	42%	40%
I-fit	37%	42%	42%
Seldom or Never Use	20%	23%	21%

Using the survey results, we can compare characteristics of a researcher that solves all their problems (high performance) with a researcher that has trouble (low performance) based on Question 24 as a survey filter.

In the table above, we see some of the differences between high performance and low performance groups. The high performance group used more analysis filters, utilized the quality system, and used statistical tools such as GOM, d, and I fits in their material identification assessments. The high performers were typically older and more experienced in the breadth of analysis techniques (Questions 2 and 13). A significant percentage of those who had difficulty were new to the field.

We also asked customers which journals they use to aid material identification and analysis. Seventeen materials' journals were compared and *Powder Diffraction* was the top

journal cited, which was also the top journal cited in the 2006 survey. *Acta Crystallography* was the second highest. Overall, 47% of those responding used *Powder Diffraction* with similar print and online usage.



Questions

The ICDD received over 220 comments from the last question in the survey. The comments could be classified into a few major groups:

- Positive feedback on ICDD products and services
- Questions about lower pricing
- Misconception on database capabilities
- Editorial and technical capability questions

Positive feedback: *"Very satisfied here, keep up the good work" …"Very useful database, I am in process to learn to use it as much as I can"…"An excellent product"... "I like all the areas done by ICDD".*

The largest category of responses was in the area of positive feedback, such as the comments above. We also had 63% of our database users state that they solve >90% of their material identification problems and 85% responded that they solve >75% of their problems. ICDD products are designed for material identification and the global user survey demonstrates that they work well in this application.

Pricing: *"I would like to see the price of PDF be lower… especially for developing countries".*

There are several mechanisms by which interested scientists can get access to the ICDD databases at low cost or no cost. These include academic discounts, site license discounts, and ICDD's Grant-in-Aid Program. These are summarized below and are also fully described on our web site **www.icdd.com/resources/academicservices.htm.** The web site also provides qualification criteria and application forms. For the past several years, the ICDD has also provided free-of-charge access to educational classes upon request. Contact information is provided on the web site.

Our grant program has been instrumental in financially supporting diffraction facilities in developing countries (all countries are eligible). We have a grant program where we offer cash to any laboratory in the world, on a competitive basis, in exchange for producing data that every user can use. **While this is a *competitive* grant program, we fund ~90% of all applicants.** Millions of dollars have been spent supporting grants in developing countries through ICDD's Grant-in-Aid Program.

Our pricing reflects the editorial work that is done on the database and the relatively small global market size. A very common misconception is that we could lower our prices by 50% and gain 50% more customers. Diffraction laboratories around the globe are measured in the thousands, they are enormous in impact, but small in numbers. For both ICDD and its distributors, costs cannot be spread over large markets or market segment sizes, so economics of scale are not achievable. The costs of products and services reflect the time and effort to produce the products and service. As a non-profit organization, the board of directors of the ICDD works constantly to maximize the value of the database by balancing the impact of pricing with the costs of providing the scientific community with a comprehensive, standardized database with significant technical capabilities.

The PDF databases are a combination of four international databases, which are standardized, edited and assessed for quality. The work involves a large number of employees, consultants, grantees and field experts from our scientific membership. In exchange for access to data we also provide funding to our database partners to support their database and editorial efforts.

We are very proud of the fact that we have not raised prices in the last five years. During this time we have been able to offer large increases in available data, higher quality data, and more analysis capability. In fact, in 17 of the last 24 years ICDD has kept prices constant while greatly increasing the size and capability of the database. Historically, the highest price for the database occurred in approximately 1986, when card files were the primary product with a price over $15,000 for a full card set. Today a PDF-2 database is over 500% larger at approximately 30% the cost for academic users.

In developing countries, most of our databases are purchased by Fortune 500 companies, government agencies, or through government-supported funding programs for universities. These are the same organizations that can afford

the price of a diffractometer, educated analysts, and supporting facilities to do materials research and development. Developing and emerging countries such as China, Russia and India have very large national budgets for materials development programs. ICDD sales in these countries have risen dramatically in the last few years in relation to increasing national investments in material science for infrastructure development. Our sales growth in these regions are a strong indication that pricing has not been a barrier to growth and development.

The database is actually one of the lowest priced components in a laboratory diffractometer system, especially if one considers that a product such as PDF-2 has a five year license term with an option for one five-year license extension at the end of the initial term. Additionally, a large portion of the databases sold by ICDD are through our site licenses. The renewals for the 2nd-10th copies in a site license are priced at $ 310-$ 400. For the size and capability of the PDF databases, this is an extraordinary value.

We have developed prices based on our non-profit principles and the needs of the overall community. This includes a 30% discount for all academic institutions, anywhere in the globe. All grant recipients also receive a 50% discount on all products in addition to grant funds. Finally, we should mention that there are tuition waivers available for attendees in need for all ICDD clinics. Application forms can be found at **www.icdd.com/education/clinics**.

Misconceptions on database capabilities: *"A search filter function for non-ambient conditions is highly recommended. Regularly we find non-ambient (e.g., high pressure) data as matches for unknown phases or in mixtures. It is very annoying to look into each hit to find out, if this is a valid one"… "Crystal size and quantitation of elements in compounds need to be added"… "Allow patterns with atom coordinates to be exported into CIF format file (useful for Rietveld analysis)"*

Actually, all the above capabilities are present in the current releases of PDF-4 products, and have been for several years. Filters for non-ambient conditions were added to the databases in 2005, crystallite size simulations were added in 2007, elemental compositions and searches were added 2006, and CIF file export with atomic coordinates was added in 2005. These filters and searches was added based on customer and member feedback from the past global surveys and our membership meetings. There are several reasons why customers perception and reality may not match the reality of current database capabilities.

The user may have a PDF-2 product that does not have atomic coordinates or the crystallite size simulation software that is present in PDF-4+ products. These are distinguishing features between these two product lines.

The user may be using distributor software to access and view the database. Most distributor software uses 40–50% of the available searches in the PDF-4+ database. We frequently get comments on temperature and pressure filters despite the fact that these have been in place for over five years. To use the filter, the user would have to open the embedded PDF-4+ software. In another example, most vendors allow for a periodic table type elemental search, but the database actually has weight and atomic % formulas that can be precisely searched through the PDF-4+ software.

Tutorials on how to export CIFs, use the crystallite size module, apply composition filters or temperature and pressure filters can be found at **www.icdd.com/resources/tutorials**.

Most software developers only use a fraction of the provided database capability in order to facilitate high-speed phase identification and batch processing. By reducing the available tables and searches, significant gains can be made in processing speeds and with most software "speed sells". ICDD software is designed to maximize data mining capability, sometimes with a speed penalty, particularly if complex calculations are involved (simulations of crystallite for example) in large data arrays. Because of these two design differences, embedded ICDD software can be very complimentary to the high throughput phase identification process supplied by software developers. Examples are shown in the many "data mining" tutorials on our web site.

There can also be major differences between older software systems and more recent releases of both the ICDD database and your distributor software. Software developers in both organizations continuously look for ways to improve performance and increase speed. This has resulted in the oddity that while the database has been dramatically increasing in size and complexity, the speed of most functions and analyses has actually significantly improved in the last few years.

Editorial and Technical Capabilities: *"Please include a database related to nanomaterials"… "I would like to see more structure data files for clay minerals, especially swelling clays and particularly mixed layer clays. Someone has this data but it is hard to perform Rietveld without good structural data. Mixed layer clays are very important in geological analysis"… "The polymer database in PDF4+ is still poor, so it would be great if it was expanded… There is an urgent need to develop a standard pattern of MOF (metal organic framework) type materials though it is a tedious job"… "Chemical names and chemical formulas that better reflect*

phase structure or composition. Consistent use of "common" and more structurally relevant "chemical" naming".

All the above ideas are represented in active database development projects being conducted by ICDD member task groups of our Technical Committee or by editorial projects being conducted by ICDD staff. We agree with the comments above that there is work to be done and we will be doing it. The exact methods of how to analyze clays, polymers, metal-organic framework and tackling the current maze of international nomenclatures is the subject of many debates among ICDD member scientists.

If you want to join the debate, think about becoming a member:
www.icdd.com/membership/register.htm
If you want to see the discussion you can access the ICDD subcommittee minutes at:
www.icdd.com/membership/minutes/index.htm

Polymers: Actually, the polymer database in the Powder Diffraction File is the most extensive in the world, with over 1,000 polymer materials characterized. Historically, the database has included known crystalline polymers but not polymers of mixed amorphous /crystalline state and non-crystalline materials. This has changed starting with Release 2009. We are now adding full digital experimental patterns of polymers that show the mixed states of matter in these materials. We are also adding digital patterns of amorphous materials, allowing the users to assess at crystallinity and amorphous content.

Clays: Our approach is to obtain higher quality experimental clay powder patterns that are natural materials. This means that the materials have to be well characterized elementally to account for substitution and absorption effects. High-quality digitial data can be used in many pattern fitting methods, often in combination with Rietveld refinement.

In Release 2008, we published 40 digital patterns from the historical clay mineral collection from the Pennsylvania State University. They show montmorillonites and several other clays in the dry state, swollen state and as oriented dry mounts. We will continue to add digitial clay material patterns in subsequent releases, but these will be a few at a time based on the amount of work it takes to prepare and analyze these materials for use as reference materials. We are seeing more Rietveld refinements of clays in the public literature. Although the quality is highly variable, we will publish these materials as we receive them with an editorial quality review to give users an idea of reliability.

Nanomaterials: Almost by definition, the pattern of a nanomaterial contains mixed states of crystalline and amorphous components. The latter is a consequence of the fact that small nanoparticles have a high surface area and that surface represents a bulk property. This is challenging our editors to define these mixed states of order so that experimental patterns can be used as reference materials and they need to be described both in terms of scattering and diffraction. The diffraction component can be simulated. This was the concept behind the crystallite size module added in 2007, which is described by the authors in an online tutorial. We currently have two projects, one with a member scientist and another with a grantee, where we are collecting experimental nanomaterial data for inclusion in the database. The first patterns of nanocrystalline cellulose will be published in Release 2010.

Metal-organic frameworks: Our member task groups for inorganic materials and zeolites both strongly agree with you. Approximately two years ago, this technical subcommittee and the zeolite editorial task group decided to expand their effort into a wider range of porous materials and framework materials. They have worked on providing technical definitions of these materials to ICDD editors so that they can be flagged and studied in the database. Under ICDD's ISO quality system, a material group needs to be analytically defined and then populated before it becomes a subfile or subclass in the database. The definition is being provided, and now, a combination of task group member field experts and ICDD editors are populating the subclass with MOF materials. The classification and identification of MOF materials can often be tedious, but the work is well underway.

The work is being organized under the newly formed "Micro and Meso Subcommittee". Scott Speakman, from MIT, is the subcommittee chair. More information can be found in the subcommittee notes, which are posted on ICDD's web site.
www.icdd.com/membership/minutes/pdf/2009-MicroMeso.pdf

This subcommittee is always looking for volunteer experts to help with the process of definition and classification. If you are interested, please contact the ICDD.

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