2012 ICDD Annual Spring Meetings

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Members of the International Centre for Diffraction Data met during the week of 19 March 2012 for the Annual Spring Meetings. Members from 12 countries gathered, along with staff and guests, at ICDD headquarters, Newtown Square, PA, to learn about ICDD's educational events, database, and product development over the past year, and to reconnect with one another. Throughout the week, various committees, subcommittees, and task groups met for special-interest discussions. For the second year in a row, the ICDD successfully offered a live, online broadcast of the Technical Committee Meeting and the Annual Meeting, which took place on Thursday, 22 March.

All were in attendance for the plenary session, which was held on Tuesday, 20 March. This year's plenary featured four international speakers: Dr Masatomo Yashima, Tokyo Institute of Technology, Japan, gave a talk titled, *Precise Structure Analysis of Inorganic Crystalline Materials through Neutron and Synchrotron Powder Diffractometry up to 1830 K*; Dr Timothy Fawcett, International Centre for Diffraction Data, U.S.A., spoke on *Database Tools for the Study of Nanomaterials;* Dr Chan Park, Seoul National University, South Korea, gave a talk titled, *The Crystal Structure and the Thermoelectric Properties of* $(Ca_2CoO_3)_xCoO_2$; and Dr. Jeffrey Deschamps, Naval Research Laboratory, U.S.A., gave a talk titled, *Chitin Preparation and Characterization.*

After the plenary session, members, staff, and guests traveled to Philadelphia for an informative afternoon at the Mütter Museum. The Mütter Museum is America's finest museum of medical history and is housed by the College of Physicians of Philadelphia. Guests enjoyed an afternoon viewing the preserved collections of anatomical specimens, models and medical instruments in a 19th century "cabinet museum" setting. Besides touring the museum, a Mütter Lesson: Bone Detectives, allowed guests to learn what happens when a human skeleton is discovered, and the role of forensic anthropology in a criminal investigation.

The day concluded with a poster session, in which 27 posters were on display, followed by a reception in the Gold Ballroom at the Concordville Inn. The evening gave ICDD members and staff the opportunity to display their research and discuss with one another their studies and findings.

This year also served as an election year for the ICDD Officers and Board of Directors. In accordance with the bylaws, the following were duly elected: Chairman (2012–2014), Scott Misture; Vice-Chairman (2012–2014), Davor Balzar; Chairman, Technical Committee (2012–2014), Matteo Leoni; Directors-at-Large (2012–2016), John Anzelmo, Vanessa Peterson and Jordi Rius. The ICDD congratulates all the newly elected Board members, and thanks earlier officers and directors who served the organization well.

The week's end brought to conclusion another successful and productive Annual Spring Meeting for all who were in attendance.

Full details of the ICDD meetings are available at www.icdd.com.

Below, please find the abstracts submitted for the Poster session. Further information about each abstract can be obtained by contacting the author whose name is underlined.

SYNCHROTRON X-RAY SCATTERING INVESTIGATION OF THIN-FILM INTERFACE KINETICS

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Nano metric films of pure Cu continue to attract attention because of their widespread use as the interconnect material in the semiconductor community. Among the various engineering and scientific challenges posed by the continued use of Cu is its high surface mobility, which is well known to result in both electromigration and stress-induced void formation resulting in eventual device failure. The use of barrier layers greatly improves the reliability of Cu interconnects. Nonetheless, the diffusion of Cu along the Cu/barrier interface is not well understood. Addressing the thermal stability and morphological evolution of Cu/barrier interfaces with the intent of quantifying interfacial diffusivities is the ultimate goal of this research.

Synchrotron X-ray scattering was used to study the evolution of interface roughness with annealing for a series of Cu thin films. The films were encapsulated in SiO_2 or Ta/SiO_2 and prepared by sputter deposition. Specular X-ray reflectivity was used to determine the root mean square roughness for both the upper and the lower Cu/SiO_2 (or Cu/Ta) interfaces. The lateral roughness was studied by diffuse X-ray reflectivity. Annealing the films at 600 °C resulted in a smoothing of only the upper interface for the Cu/SiO_2 samples, while the lower Cu/SiO_2 interfaces and both interfaces for the Ta-encapsulated films did not evolve significantly. As a function of roughness wavelength, the upper Cu/SiO_2 interfaces exhibited a roughness decay with annealing that was only 12.5% of that expected for classical capillarity-driven smoothening of a free surface.

Ongoing work is focusing on further quantifying the interface kinetics for Cu/barrier systems. Using e-beam lithography methods, we have patterned a grating onto the surface

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of Cu thin films. Subsequent encapsulation and annealing will be carried out to study the effects of time and temperature on the patterned interface. Transmission electron microscopy will be used in addition to specular and diffuse X-ray reflectivity methods to quantify the decay of the corrugated interface.

CHARACTERIZATION OF X-RAY-IRRADIATED GRAPHENE OXIDE COATINGS USING X-RAY DIFFRACTION, X-RAY PHOTOELECTRON SPECTROSCOPY, AND ATOMIC FORCE MICROSCOPY

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Graphene is a single-layer planar sheet of sp2-bonded carbon atoms that are packed in a two-dimensional honeycomb lattice. Intrinsic graphene behaves like a semi-metal or zero-gap semiconductor. One problem with graphene is that it cannot be dispersed in water, preventing any practical applications that use aqueous coating or deposition technology.

Graphene oxide, GO, is generated by treating graphite with strong oxidizers. GO retains the layer structure of graphite but with a larger and irregular basal plane spacing. The name graphene oxide is not correct chemically. Besides oxygen epoxide groups, other functional groups observed to be present are carbonyl, phenol, and hydroxyl groups. It is the presence of the hydroxyl groups that allows GO to be dispersed in water. However, GO does not possess any of the electrical properties observed in graphene. Methods have been developed that convert GO to graphene but this transformed graphene retains defects seen in the original GO, resulting in a graphene that has a reduced conductivity and charge mobility compared to pristine graphene.

In an effort to study an alternative approach to make graphene from GO, exposure of GO to high-energy X-ray radiation has been performed. X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and atomic force microscopy (AFM) have been used to characterize GO before and after irradiation. Results will be presented that indicate GO exposed to high-energy radiation is converted to an amorphous carbon phase that is conductive.

STRUCTURE FUNCTION RELATIONSHIP OF ENERGY STORAGE MATERIALS

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Sustainability is where society overlaps with the environment and the economy. With concerns over the future availability of fossil fuels and climate change Scientist and Engineers from all disciplines are focusing their research on materials for a sustainable future. Examples of areas where crystallographers are taking up the charge include Li-ion batteries for electric cars, new solar materials, and thermoelectric materials. This is also reflected in the user research that is carried out at the POWGEN diffractometer, the recently built general purpose neutron powder diffraction instrument at the Spallation Neutron Source. Some of this research on energy-related materials with regard to structure–function relationship will be presented.

INTERACTION OF CARBON NANOTUBES WITH SOME POLYMERS

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Microscopical, differential scanning colorimetry (DSC), and X-ray structural investigations of solution-crystallized carbon nanotube (CNT) composites with linear polyethylene (LPE), isotactic polypropylene (iPP), polybutene-1 (PB-1), and nylon 6 (PA6) disclosed varying degrees of surface interaction and nucleation effect of CNT in these polymers and formation of oriented shish-kebab overgrowths on the CNT ropes in LPE and PA6. The character of the attraction and orientation forces at the CNT–polymer interface is discussed.

Key words: carbon tube–polymer interaction, polymer overgrowth on carbon nanotubes, crystallization, melting of some polymers on carbon nanotubes

STRUCTURE AND MORPHOLOGY OF ORIENTED ISOTACTIC POLYPROPYLENE SHEETS

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Sheets of isotactic polypropylene (iPP) uniaxially oriented to the draw ratio 5, 8, and 11 were annealed at temperatures 120–172 °C. The sample structure and morphology were examined by X-ray diffraction, electron microscopy, DSC and mechanical testing. The structure characteristics were related to mechanical property measurements. The oriented samples are characterized by a system of parallel-oriented fibrils, where orientation degree, crystal size, crystallinity, and melting behavior depend on draw ratio and annealing temperature.

Key words: oriented iPP, X-ray diffraction, electron microscopy, DSC, mechanical testing

FOX.GRID ENHANCEMENT FOR SPEEDING UP THE GLOBAL OPTIMIZATION METHODS BY GRID COMPUTING

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Solution of the phase problem from powder diffraction data remains, in many cases, a challenging task. The

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one-dimensional character of the powder diffraction record necessarily leads to overlaps of reflections, which complicate the task considered as routine ones in single-crystal diffraction. For these reasons, development of new methods and algorithms designed especially for powders still continues. Alongside with the direct methods, which unfortunately often fail for powder diffraction data, there is another wide family of solution methods based on the direct space.

Direct space methods such as simulated annealing or parallel tempering try to find the correct crystal structure by modifying the starting model until the global minimum represented by low values of profile *R* values is found. The probability of reaching the global minimum decreases with the complexity of the investigated crystal structure, thus require many optimization runs and correspondingly long computing time. The issue of computing time can be solved by the parallelization using a grid computing approach.

We decided to modify the existing code of FOX (Favre-Nicolin and Černý, 2002), the well-known software for *ab initio* crystal structure solution from powder diffraction data by direct space methods. The resulting program named FOX.Grid enhances the 'brute force' approach of direct-space global optimization methods by distributing optimization jobs on multiple cores or CPU's on a single computer or on several networked computers. The time necessary for solving more complicated structures is therefore significantly reduced and more complex solution strategies are therefore tested. The distribution of computing jobs to the slave computers or processors is fully automated as well as completing the results from the partial calculations. The usage of FOX.Grid on several real crystal structures will be presented.

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SUBFILE POPULATION IN 2012 PDF® RELEASES

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Keeping in view the huge number of yearly additions to the database, the classification of entries into various important subfiles is vital in enhancing the effectiveness of search/match using the Powder Diffraction File™. The identification and assignment of subfiles are done in two ways: (i) Manually by the ICDD's editorial team and task group members, and (ii) semi-automatically by query-based assignment that compares entries with matching chemistry and similar crystallographic parameters (with a user-defined tolerance factor). New subfile entries are reviewed by various editors and task group members for consistency. This poster is a report on the subfile population in the upcoming 2012 releases.

A NEW DATA SUBMISSION PROCESS

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With the increasing difficulty of finding useful *quality* experimental data in today's literature, the ICDD is exploring alternative methods for acquiring such data. Given the hectic, über-busy lifestyle of many, any such method must prove to be a quick and simple process. Furthermore, the method must be cost effective for both the submitter of the data and the ICDD. Today most labs have access to the internet and data transfer via the internet is often a quick and reliable process; therefore, the ICDD has developed a web submission program. This program, which employs Java WebStart technology, is designed to enable the user to submit key experimental data directly to the ICDD by compiling their data into a CIF and directly uploading it to our server. The purpose of this poster is to describe the new web submission program to our members and to raise awareness of its existence in hopes of receiving necessary and valued feedback.

ICDD PDF-4 PRODUCT DEVELOPMENTS FOR RELEASE 2012

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For Release 2012, ICDD has incorporated many new PDF-4 product developments that have a focus on faster and more accurate total pattern analysis. The similarity index (a numerical value that represents how well a simulated pattern matches the user's experimental data) has been enhanced to allow the user to select which overlapping region is used for comparison. This "local" or "global" compared region in 2θ is then displayed to the user, allowing for more realistic similarity indexes. Additionally, the user can now obtain similarity indexes by comparing their experimental data to PD3 patterns (high-quality raw experimental data in the PDF-4 databases). These PD3 patterns will be converted internally to match the wavelength of the user's experimental data. Lastly, numerous internal routines have been translated from C + +/Fortran to Java, increasing the overall performance and maintainability of using similarity indexes with simulated patterns.

Also for Release 2012, many developments have been made to improve the functionality and visual clarity of the search-index plug-in SIeve+. We have added "Pharmaceuticals and Excipients" as a common match filter when importing experimental data. We also now calculate an estimated weight percent of all found phases if all have I/Ic value. This is a semi-quantitative analysis using the reference intensity ratio (RIR) method. For the SIeve+ graph, the experimental data are now plotted as individual points instead of a continuous line. This distinguishes the experimental data from the identified phases better. The user now also has the option of graphing these identified phases as simulated profiles, PD3 patterns (new option), or stick patterns (new option). Finally, the tick markers that represent the peaks for the experimental data and all identified phases are now displayed in a separate subplot, allowing the main graph to be independently controlled.

These are just some of the many value-added developments designed to make the ICDD PDF-4 products more functional and powerful for 2012.

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IMIPENEM MONOHYDRATE X-RAY POWDER DIFFRACTION

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This is the first reported experimental X-ray powder diffraction pattern for imipenem monohydrate. Imipenem monohydrate, $C_{12}H_{17}N_3O_4S{\cdot}H_2O$ [6-(1-Hydroxyethyl)-3-(2-(iminiomethylamino)ethylthio)-7-oxo-1-azabicyclo(3.2.0)hept-2-ene-2-carboxylate monohydrate] has been used in combination with cilastatin sodium as an antimicrobial injection. The experiment used shallow-cavity zero-background holders to minimize transparency problems. The zero-background configuration also works well when limited amounts of sample are available.

The experimental data were analyzed and refined using the SQL Aids for indexing, Mercury crystal calculation/display software for three-dimensional visualization, and GSAS Rietveld refinement program to resolve heavily overlapping peaks at lower angles, typical for organic compounds. It was found that imipenem monohydrate has an orthorhombic crystal system with reduced cell parameters of $a = 8.2534(3)$ Å, $b = 11.1293(4)$ Å, and $c = 15.4609(6)$ Å. The resulting unit-cell volume, 1420.15(15) Å^3 indicates four formula units per unit cell. Observed peaks are consistent with the $P2_12_12_1$ space group. The aforementioned data are consistent with data calculated from the reported single-crystal structure. The compound includes a number of electronegative atoms, such as oxygen, nitrogen, and sulfur, in the forms of carboxyl, hydroxyl, imino, amino, and sulfide groups. The molecule also includes water which, along with the electronegative atoms, contributes to intra-molecular and inter-molecular hydrogen bonding. This hydrogen bonding network greatly influences the packing arrangement of the crystal structure.

FEASIBILITY OF *AB INITIO* STRUCTURE SOLUTION FOR METAL–ORGANIC FRAMEWORK MATERIALS FROM X-RAY POWDER DIFFRACTION DATA: THE KEY ROLE OF SIMULATION

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Discovered in the early 1990s, metal–organic framework (MOF) compounds have become an important class of materials scientifically and also industrially [Chem. Soc. Rev. (2009) **38,** issue 5]. They are crystalline compounds consisting of metal ions or ionic clusters [e.g., Cu(II), In (III), etc.] most commonly, though not exclusively coordinated to rigid organic molecules (e.g., pyrazine). When suitable organic linkers are chosen, a variety of structures can result with 1D, 2D or 3D connectivity; most importantly, then may be microporous. As such, they can be used to store industrially important gases such as H_2 and CO_2, but also have applications in catalysis as well as in gas separations and purification.

Similar to pharmaceuticals and other compounds, newly synthesized MOFs are often available in powder form much sooner than in single-crystal form. Yet, their crystal structures are mostly determined using single-crystal X-ray diffraction (SXD) owing to the apparent complexity of the associated unit cells (e.g., Samanamu and Richards, 2007).

In this work, we argue that at least in some cases, the presence of heavy atoms (the metal ions) or nearly rigid bonding environments (surrounding the metal ions) composing the MOFs can lead to their successful *ab initio* structure determination from synchrotron powder data. Additionally, when a new MOF is obtained as modification of one with a known structure by the replacement of the organic linker or alternatively by the replacement of the metal ion by a chemically equivalent one, the chances of success are then even greater since the parent structure can be used to predict the local geometry of a large fragment surrounding the metal ion. This portion of the structure can be treated as a super heavy atom which aids in structure solution.

We demonstrate the structure solution process using GSAS to simulate high-resolution powder data for the In(III) Cl3 (pyrazine) MOF (C6H6Cl3InN3), where the structure is known from SXD (Samanamu & Richards, 2007), We use (i) DICVOL06 or/and NTREOR-09 to index the latter, (ii) direct methods from EXPO2009 or/and simulated annealing from FOX to locate the metal ion coordination fragment (super heavy atom) including and surrounding the metal ion and (iii) an appropriate difference Fourier synthesis to complete the MOF structure. Since no *ad hoc* hypothesis is made in the data analysis regarding the organic linker, we feel entitled to infer from our simulation that a real high-resolution synchrotron diffraction experiment, such as at the APS 11-BM beamline, structure solution involving a new linker of similar complexity to the former linker is likely to be met with success… provided that a stable single-phase powder sample can indeed be synthesized.

FORTY YEARS OF POWDER-DIFFRACTION-PATTERN INDEXING WITH THE DICHOTOMY ALGORITHM

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The successive dichotomy method for indexing powder diffraction patterns was devised in 1972 by Louër and Louër. The method has been used extensively in the group of powder crystallography at the University of Rennes for the identification and characterization of newly synthesized compounds and, also, in more than 50 *ab initio* structure determinations from laboratory powder diffraction data. The more recent reported computer program is DICVOL06. Some improvements have been done during the last few years. They are presented and illustrated by many examples (most of them from literature) and a few peculiarities in powder pattern indexing are discussed.

Among changes, some filters used to avoid too close solutions in the course of the tree-type strategy have been optimized, some limits in triclinic linear parameters have been increased, in the review of the whole input dataset all calculated lines are presented as an aid to space groups selection,

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the standard uncertainty on volume cells has been added, a more stable zero-point shift analysis has been implemented.

General methodological aspects are discussed, such as the absolute error on peak positions, input in the dichotomy program, with a particular emphasis on ultra-high resolution and precision obtained with modern synchrotron X-ray sources, as well as the role of the input error on the results with regard to the crystalline systems. Many datasets have been used with the modified version, they include standard X-ray diffraction powder patterns reported in the NBS monograph 25 (1953–1985), ICDD-PDF2, Rennes powder data collected with monochromatic laboratory X-rays. Additional cases with long or short axes, mixtures of phases and lattice metric singularity are discussed.

HIGH-TEMPERATURE EXPANSION AND TRANSPORT PROPERTIES OF THE LAYERED CUPRATES LN_2CUO_4 (LN = PR, ND AND SM) WITH T′-STRUCTURE

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Solid oxide fuel cells (SOFCs) are considered as one of the alternatives to traditional hydrocarbon sources of energy because of their high efficiency and excellent fuel flexibility Ralph et al. 2001). They are operating at high temperature up to 1273 K and this creates numerous problems such as chemical stability, matching of the thermal expansion coefficients (TEC) between the components of the SOFC etc. (Soorie and Skinner, 2006). Therefore, efforts are directed to the creation of the so-called intermediate temperature SOFC (IT-SOFC) with operation temperatures down to 773 K(Steele and Heinzel, 2001). Recently layered cuprates have attracted attention for the application in high-temperature electrochemical devices. Although the high-temperature properties of the La_2 CuO_4 are well studied, much less information is available for other Ln_2CuO_4 cuprates. However, one can expect that these compounds could be of interest since Ce-doped Nd_2 CuO_4 with T′-structure was found to exhibit promising properties for SOFC cathode application(Tu and Stimming, 2004).

High-temperature crystal structure of the layered cuprates Ln_2CuO_4, Ln = Pr, Nd and Sm with tetragonal T′-structure was refined using X-ray powder diffraction data. Substantial anisotropy of the thermal expansion behavior was observed in their crystal structures with thermal expansion coefficients (TEC) along *a*- and *c*- axes changing from TEC(*a*)/TEC(*c*) = 1.37 (Pr) to 0.89 (Nd) and 0.72 (Sm). Temperature dependence of the interatomic distances in Ln_2CuO_4 shows a significantly lower expansion rate of the chemical bond between Pr and oxygen atoms (O1) belonging to CuO_2-planes (TEC(Pr-O1) = 11.7 ppm K^{-1}) in comparison with other cuprates: TEC (Nd-O1) = 15.2 ppm K^{-1} and TEC (Sm-O1) = 15.1 ppm K^{-1}. High-temperature electrical conductivity of Pr_2CuO_4 is the highest one in the whole studied temperature range (298–1173 K). The trace diffusion coefficient (DT) of oxygen for Pr_2CuO_4 determined by isotopic exchange depth profile (IEDP) technique using secondary ion mass spectrometry (SIMS) varies in the range 7.2×10^{-13} cm^2 s^{-1} (973 K) and 3.8×10^{-10} cm^2 s^{-1} (1173 K) which are in between those observed for the manganese and cobalt-based perovskites.

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SYNTHESIS, CRYSTAL STRUCTURES, AND PROPERTIES OF NOVEL TERNARY COPPER PHOSPHIDES, $A_2CU_6P_5$ (A = SR, EU) AND $EUCU_4P_3$

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The recent discovery of superconductivity with T_c up to 55 K in layered iron pnictides (Kamihara *et al.* 2008) initiated intensive searches of both novel FeAs superconductors and novel element combinations which could give rise to other families of superconducting materials. Of the 3*d*-metal compounds, low-temperature superconducting properties have been found, apart from iron, for those of nickel (Clarke *et al.* 2008), and copper in a yet unique case of a $ThCr_2Si_2$-type compound $LiCu_2P_2$ (Jiantao *et al.* 2010). Layered multinary copper pnictides exhibit relatively rich structural chemistry approaching that of related Fe compounds. The copper oxypnictides are well studied and do not exhibit superconductivity; much less is, however, known about the ternaries beyond some structural data.

Three new ternary copper phosphides, $Sr_2Cu_6P_5$, $Eu_2Cu_6P_5$, and $EuCu_4P_3$, were synthesized from elements in evacuated silica capsules. $Eu_2Cu_6P_5$ and isostructural $Sr_2Cu_6P_5$ adopt the $Ca_2Cu_6P_5$-type structure (SG *I4/mmm*), while $EuCu_4P_3$ is isostructural to $BaMg_4Si_3$ (SG *P4/mmm*) and remains yet a lone representative of this structure among ternary Cu pnictides. $Eu_2Cu_6P_5$ is a ferromagnet with a T_c of 34 K, but these properties manifest themselves only in very weak external fields. $EuCu_4P_3$ exhibits a very complex magnetic behavior. Non-existence of isostructural compounds of alkaline earths and arsenic suggests that europium is partially trivalent in this compound.

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STRUCTURE, PHASE EQUILIBRIA, AND THERMOELECTRIC PROPERTIES OF THE Ca–M–Co–O (M = Sr, Zn, AND La) SYSTEMS

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Thermoelectric research is of increasing importance in the development of technologies for improving vehicular fuel economy and for mitigating green house gas emissions. There is a well-defined need for efficient energy conversion materials and environmentally friendly technologies over the next 20 years. For waste heat energy conversion applications, oxide materials that have high-temperature stability are potential candidates. In the Ca–M–Co–O (M = Sr, Zn, and La) systems, in addition to the well-known $Ca_3Co_4O_9$ phase (with misfit layered structure) that exhibits excellent thermoelectric property, other interesting phases include members of the homologous series, $A_{n+2}Co_nCo'O_{3n+3}$ (where A = Sr, Ca (Ca, Sr) or (Sr, Ca)), which consist of one-dimensional parallel $Co_2O_6^{6-}$ chains. While the members of the $A_{n+2}Co_nCo'O_{3n+3}$ series have reasonably high Seebeck coefficients and relatively low thermal conductivity, the electrical conductivity needs to be increased to achieve higher *ZT* (figure of merit) values. This paper discusses our phase equilibria/structural/property studies of selected cobaltites, including those in the SrO–CaO–CoO_x, CaO–ZnO–CoO_x, and CaO–La_2O_3–CoO_x systems.

CRYSTAL STRUCTURAL ANALYSIS OF MULTIPLE PHASES FORMED IN ZR2TIAL ALLOY SYSTEM BY THE MICRO X-RAY DIFFRACTION TECHNIQUE

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Zr_3Al is an intermetallic compound with a cubic structure, whereas the iso-electronic compound Ti_3Al is hexagonal. Crystallographic study of an alloy containing all three elements is important in advancing our knowledge of the phase behaviour across this pseudo-binary alloy system. A nominal composition of the Zr_2TiAl alloy was prepared by arc melting and subsequently vacuum annealed at 1050 °C for 30 days and 1000 °C for 20 days. Scanning electron microscopy (SEM) and energy-dispersive X-ray analysis (EDAX) showed the presence of three phases in the material. Among the three phases, the major phase was the stoichiometric Zr_2TiAl alloy. From the SEM micrograph, it was seen that the major phase grains varied in size from 10 to 50 μm. The polarized optical microscope image analysis showed that the 1050 °C, 30 days annealed specimen showed nearly 77% of Zr_2TiAl phase, whereas the 1000 °C and 20 days annealed specimen showed nearly 70%. Of the two minor phases present in the specimen, one is rich in Ti and the other in Al. To identify the peaks because of individual phases, micro-beam XRD was carried out, enabling the identification of all the three unambiguously. The stoichiometric phase Zr_2TiAl has $L2_1$ structure (space group *Fm*3*m*) with lattice parameter 6.8400. The theoretical XRD pattern generated using this lattice parameter and *Fm*3*m* space with atomic sites (0, 0, 0), (0, 0, 0.5) and (0.25, 0.25, 0.25) matches well with the micro-XRD pattern recorded on the grain. The Ti-rich phase has DO_{19} structure (space group $P6_3/mmc$) and the Al-rich phase has A_a structure (space group *I*4/*mmm*). A few other minor phase peaks are also present and with the help of micro XRD data the conventional XRD of the alloy is completely indexed.

THE PRESENCE OF POLYMERS IN THE POWDER DIFFRACTION FILE™ (PDF®)

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As technology progresses, the range of data suitable for incorporation into the Powder Diffraction File gradually grows. This advancement allows ICDD to better support the needs and interests of customers in various scientific fields. One recent update includes the incorporation of X-ray diffraction data of polymeric materials into the database. This has been an ongoing project for ICDD for the last 10 years; however, polymer chemistry and polymer research extend as far back as the early 1900s.[1] Although newly acquired polymer diffraction data can be easily included into the PDF, almost a century of data for natural, semi-synthetic, and synthetic compounds that were discovered before technological methods became available that could provide digital data, still remain. To bypass this limitation, ICDD began using digitizing software; allowing quality hard copy X-ray diffractograms to be converted to digital data. As a result, inclusion of more and more polymeric compounds in the PDF is possible. Consequently, the increased number of polymer compounds present has revealed a need for "polymer-based" quality marks, which has been addressed with the addition of quality marks "M" – minimal and "G" – good.

ENHANCEMENTS TO THE PDF-4/ORGANICS 2012

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One of the key features of the Powder Diffraction File's search/match option is the ability to search by common classes of materials. These subfiles are vital to the continuing growth of the database. The Editorial team introduced seven new organic subfiles in the PDF-4/Organics 2010 to add to the

[1] http://plastics.americanchemistry.com/Education-Resources/Hands-on-Plastics/Introduction-to-Plastics-Science-Teaching-Resources/History-of-Polymer-and-Plastics-for-Students.html#top

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previously popular subfiles such as pharmaceutical, forensic, and excipients. Since then, the Editorial team has enhanced the entries in the database. In the PDF-4/Organics 2012, we have integrated over 31 000 crystal structures to pre-existing entries, the majority of which are located in those specific subfiles. This integration allows the user to access features that are popular in PDF-4+ products such as 3D visualization and bond angle/distance calculations. This poster focuses on the analysis of the atomic coordinate subfile classifications in the PDF-4/Organics 2012.

THE STRUCTURE SOLUTION OF MOLECULAR CO-CRYSTALS AND SALTS FROM X-RAY POWDER DIFFRACTION DATA

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Molecular co-crystals are becoming increasingly important within the pharmaceutical industry as they represent a new source of solid-state materials which have the potential to provide optimal physical properties while retaining the chemical properties of the individual components. The ability to determine the crystal structures of these materials from powder diffraction data is vital, particularly when a stoichiometry or form is available only from synthesis by solvent-drop or dry grinding.

The development of direct space structure solution techniques has been a driving factor in the increasing number and complexity of crystal structures that can be determined by powder X-ray diffraction data. This poster will present some of our recent work on the development and application of the differential evolution structure solution technique which uses evolutionary principles to guide a highly efficient global optimization process. The structures presented are all multi-component molecular systems (molecular co-crystals and salts based on isonicotinamide, nicotinamide, and dicarboxylic acid synthons) prepared from both traditional solution and solid-based synthesis. The accuracy and reliability of the structural details obtained from both laboratory and synchrotron data will also be discussed.

ICDD.COM – RECENT IMPROVEMENTS FOR 2012

M. Kottenhahn
International Centre for Diffraction Data Newtown Square, Pennsylvania

The ICDD.COM website strives to meet the information and communication needs of ICDD members, customers, scholars, professionals, grant-in-aid participants, developers, and students.

This poster will highlight recent improvements to ICDD.COM including the translations area, knowledge center, product tutorials, social media outreach, bios of award honorees, Board of Directors' profiles, etc.

INTERNATIONAL CENTRE FOR DIFFRACTION DATA® (ICDD®) WELCOMES CAMBRIDGE UNIVERSITY PRESS AS THE NEW PUBLISHER FOR *POWDER DIFFRACTION*

Nicole M. Ernst Boris
International Centre for Diffraction Data Newtown Square, PA
(With special thanks to Carly Bray, Timothy Fawcett, Theresa Kahmer, and Monika Kottenhahn)

This poster highlights *Powder Diffraction* and its new publisher Cambridge University Press. Cambridge was chosen after several publishers were evaluated during a process that took several months. We are looking forward to a mutually beneficial relationship with Cambridge. ICDD has updated its website for the journal. The Publishing Agreement and Notes for Authors have also been updated. See the journal now on the Cambridge Journals Online (CJO) platform. Look for dynamic pages you can "flip" through like a book. In addition, content from 1986 through 2001 will soon be available for purchase or by subscription. We hope you will submit a manuscript to *Powder Diffraction* very soon using ScholarOne™, a manuscript and peer review submission system produced by Thomson Reuters. This user-friendly system has excellent help documentation. Should you have any questions, please contact me at boris@icdd.com

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