Peter Moeck's Scholarly Agenda and a summary of his accomplishments at Portland State University

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Who I am and where I am coming from (metaphorically speaking)

I am, by education and career choices, a crystallographer and materials physicist. Materials physics may be considered as part of condensed-matter physics. While condensed-matter physics is mainly a fundamental science that explains the properties and behavior of macro-, meso-, and nano-scopic objects from their quantum mechanical foundations, materials physics has a more applied focus. Crystallography is generally considered to be *"part of the 'science of the structure of matter', the part associated with the atomic length scale"* [1]; see first footnote ([1]) for an alternative definition and suggestions for crystallography's place in a modern college science curriculum. Taken together, materials physics and crystallography are important parts of the scientific foundation of the double discipline Materials Science and Engineering.

Since my graduation with a Master of Science in crystallography in 1983, I have worked mainly on semiconductors in physics or materials science departments. Besides semiconductor crystal growth and processing, I mainly performed structural characterizations employing various modes of transmission electron microscopy, X-ray and electron diffraction, and X-ray topography at a synchrotron. Some of my best work was achieved by analyzing technologically relevant semiconductor growth or processing problems from a structural viewpoint by complementary methods and using my materials engineering background to elucidate the phenomenon/mechanism that caused the problems. This is what I like doing, want to continue doing, and have done well over the last 28 years in three different countries and at places as diverse as the University of Illinois at Chicago, the University of Oxford, Imperial College London, and the Humboldt University of Berlin.

Summary of prior and recent successes as researcher and educator / My place in the scientific enterprise

As a result of my scientific work, and because I have established highly productive collaborations, I have 73 scientific journal articles, 9 patents (including a pending patent application), 3 book chapters, 110 conference talks and seminars, and approximately 150 conference papers, posters, and abstracts to my credit. Two of our papers were selected for re-publication in the Virtual Journal of Nanoscale Science and Technology. Figures from one of our papers appeared on the cover of the June 2011 issue of an international materials science and engineering journal.

Since coming to Portland State University (September 16, 2002), I have published 47 peer-reviewed papers, three book chapters, 107 non-refereed papers, applied for three patents (2 granted, 1 patent application pending), presented 58 posters and 53 talks at scientific conferences, held 23 seminars at other institutions, and edited both a multi-author book as well as a special issue of the journal *Crystal Research and Technology* [2].

Within recent years, I was elected to memberships of the International Center for Diffraction Data [3] and the international advisory board of the Crystallography Open Database [4]. For several years I also served on the Technical Review Committee of the Nano Science and Technology Institute [5] as well as on the Editorial/Advisory Boards of the *Journal of Nano Education* [6] and the Internet-based publisher *Scientific Journals International* [7].

Since January 2011, I am a member of the Advisory/Editorial Review board of the above mentioned *Crystal Research and Technology* journal [8]. Having been invited to join such a board of an internationally highly regarded materials science and engineering journal (which had been founded in 1966 and is part of the Wiley journals portfolio) is so far the highest recognition of the significance of my scientific work.

Another significant recognition of my scientific achievements as well as of my engagements with the wider scientific community is the appointment to represent the Microscopy Society of America [9] at the US National Committee for Crystallography [10]. I also serve currently as a consultant in the Commission on Electron Crystallography [11] of the International Union of Crystallography [12].

Within the last few years, I received the "***Best Paper Award***" of the 2009 International Conference on Frontiers of Characterization & Metrology for Nanoelectronics, the (2008) "***Outstanding Project Award***" of the Northwest Academic Computing Consortium, and the "***Best Poster Award***" of the fall 2007 Meeting of the Materials Research Society. Note that all three of these competitive awards were in different scientific fields! (I will give brief introductions to these fields below.)

With this kind of background and track record, I am confident that my place within the scientific enterprise is right at the interface between materials physics and crystallography. It appears to me that the traditional boundaries between the scientific disciplines are disappearing with the emergence of nanoscience. In addition, new interdisciplinary developments typically start from niches at the interfaces between the traditional disciplines. My long-term goals are, therefore, to create, occupy, and expand my own scientific niches. I want to establish and expand my own scientific niches because I seek intellectual challenges and have, as documented by my patents, mastered such challenges with originality. Within my scientific niches, I strive to accomplish a seamless integration of my main activities as a faculty member: research, teaching, and community service.

These goals also fit seamlessly into the PhD program in Applied Physics of my department. Within our Applied Physics PhD program, there are strong components in Materials Physics and interdisciplinary Nano-Materials Science and Engineering. Further below, I will give examples of successfully created and occupied scientific niches. From these examples, a pattern will emerge about how I typically work and what kind of scientific problems I like to address.

At Portland State University, I have been teaching the two quarter undergraduate course "Introduction to Modern Physics" each year since the fall of 2002. Over the years, I also taught one quarter undergraduate/graduate courses on "Statistical Mechanics and Thermodynamics", "Introduction to Physical Metallurgy and Materials Science", and "Introduction to Nano-Materials Science and Engineering". The latter course is closest to my own research interests. I do like teaching in general and surely enjoyed teaching all of the courses mentioned above in the past!

The course "Introduction to Modern Physics" gives me the opportunity to "gently but persistently steer" the mindset of (300 level) undergraduates away from classical physics since the main topic of this course is quantum mechanics. This can be challenging at times for some of our students (who unfortunately lack proper preparation), but the reward of seeing the majority of the students grow intellectually is always great.

The four areas of my scholarly activities

Prior to coming to Portland State University (PSU), my publications covered three topical areas in materials physics and crystallography: (*i*) electron microscopy and diffraction, (*ii*) X-ray diffractometry and topography, (*iii*) compound (e.g. [Ga,In]Sb or GaN), element (e.g. Si or Sn), and other semiconductors growth, processing, and characterization by other methods (including scanning probe microscopy). As the recent entries in the attached lists of publications, patents, lectures, conference talks, posters, and seminars demonstrate, I am still active in each of these topical areas.

The division into topical areas is due to having worked in a variety of fields at different times and places. As a commonality of my work in these different topical areas, I have identified unsolved problems and found original solutions to them. This will be illustrated below using the examples of two of my recent innovations, i.e. ***structural fingerprinting in the transmission electron microscope*** *from either high resolution (lattice fringe) images or precession electron diffraction data* and ***crystallographic image processing for scanning probe microscopy***.

Since my coming to PSU, (in other words: since becoming an educator in addition to being a researcher), I have established activities in a 4th area: materials science and engineering education and Internet based outreach on crystallography. Taking on this new topical area of education and worldwide community service demonstrates my commitment to supporting PSU's reputation for excellence in education, community service, and sustainability. The community service aspect of my activities in this topical area, i.e. promoting open access crystallographic databases over the Internet, supports my long-term goals directly. It, therefore, establishes the desired connection between my education, research, and service efforts that a mature Scholarly Agenda is supposed to represent.

Integrating community service into my scholarly agenda

Initially as a community outreach project, I started the development of PSU's "Open Access Crystallography web space" [13] which associated open-access crystallographic databases in 2005. The work on developing the associated databases [14] was supported externally by one grant from the Research Corporation and three successive grants from the Northwest Academic Computing Consortium. A total of six physics undergraduate "summer students" from the Czech Republic and two graduate students (from physics and computer science) of Portland State University contributed to these developments.

I also teamed up with the international project "Crystallography Open Database" (COD [4]). At our websites at PSU [13], we provide three-dimensional interactive visualizations of crystal structures at the atomic level and of crystal morphologies in addition to selected COD datasets and our own datasets on technologically relevant inorganic nanomaterials. Our site is, therefore, both a free materials science education resource and a service to those parts of the condensed matter physics communities that work with inorganic crystalline materials. We also created two mirrors of the COD for the Americas [15].

Note that searches for "open access crystallography" on google.com consistently return our project ***first*** out of more than 300,000 search results. (Besides being smaller than the COD, we are actually ahead of it as far as popularity measured by means of google.com is concerned. It is probably the interfaced 3D interactive visualizations that make our site so popular.) From January 2008 onwards, we have counted the access to our crystallographic databases. As of today, there were more than 280,000 hits. In the summer of 2008, I also received the ***"Outstanding Project Award"*** of the NorthWest Academic Computing Consortium in recognition of our international community outreach efforts.

As a result of my research group's efforts since 2005, PSU now hosts mainly inorganic and educational subsets (with approximately 20,000 critically evaluated entries) of the COD's more than 155,000 entries, a dedicated "Crystal Morphology Database"[2], a dedicated "Nano-Crystallography Database", and the world's first open-access crystallography database in the "wikipedia format"[3]. The last of these databases was set up initially with a mineral subset (with approximately 9,000 entries) of the COD and is freely expandable and editable by the general public. Our Nano-Crystallography Database, on the other hand, is a research database with registered users and its purpose will be discussed in the context of the following section.

From community service to helping address the "nanocrystal problem"

Crystalline nanomaterials are arguably the future of materials physics because they possess size, morphology, and dimensionality dependent properties for the same (idealized) atomic structure. This means that within the nanometer size range, changes in morphology and dimensionality result in changes in a material's properties. Also (within the nanometer size range only), the properties of a material depend very strongly on the actual size of the crystals. (Colloquially, one may say *small* is *very different*.)

The deeper understanding of these properties that is required for device applications and optimized reproducible syntheses must be based on the (atomic) structure-size-morphology-dimensionality-property relationships of nanocrystalline materials. This is where the so called *"nanocrystal problem"* [16] arises. (While explaining this problem briefly may appear to be a slight digression, I consider it important for the illustration of how I typically work and what kinds of problems I am interested in solving.)

The nanocrystal problem has at least three compounding components, *(i)* many nanocrystals are *"crystallographically challenged"* [14], i.e. are far from the idealization of a periodic structure that is sufficiently large so that surface effects can be safely neglected, *(ii)* the standard X-ray diffraction based crystallographic techniques for both determining structures that are new to science and for recognizing structures that have already been determined (and possess, thus, an entry in a database) typically fail for nanocrystals [15], and *(iii)* there is no complete theoretical framework to describe nanocrystals. To me, this is a very interesting problem because its solution will lead to novel applications for decades to come.

Solutions to the nanocrystal problem are anticipated by both *(i)* coordinated efforts of researchers using complementary methods on materials from the same batch and *(ii)* the open sharing of the accumulated experimental data in a *"common computational global optimization framework"* [16]. I am working towards making PSU's Nano-Crystallography Database part of this framework.

Because I wanted to make experimental contributions to the solution of the nanocrystal problem as well, I have also been working on the development of novel crystallographic characterization methods using transmission electron microscopy. This work resulted from the realization that the industrially most important characterization technique for crystalline materials, i.e. powder X-ray diffraction, does not work for nanocrystals [17]. We started by developing structural fingerprinting from high resolution (lattice fringe) transmission electron microscope images in 2005 and won the ***"Best Poster Award"*** of the fall Meeting of the Materials Research Society in 2007 for these developments. Before publishing and presenting our core ideas at conferences, we applied for a patent on behalf of Portland State University [18]. The corresponding MS thesis work of one of my graduate students was supported by his spending of the summer of 2006 at the Technical University Chemnitz (in Germany).

In the fall of 2007, I was invited by the president the Brussels/Belgium based company NanoMEGAS to collaborate on the development of structural fingerprinting from precession electron diffraction data. This project constitutes a complementary branch of structural fingerprinting in the transmission electron microscope and is also covered by PSU's patent application [18]. (It is probably due to this patent application that this company selected us as partners of further developments of the scientific basis of their future products.) The Commission on Electron Crystallography of the International Union of Crystallography comments on their website [19] that "precession electron diffraction is rapidly maturing as a tool for structural fingerprinting". This is to a large extent the result of my research group's work at Portland State University.

The collaboration with the NanoMEGAS company has so far lead to the establishment of my laboratory as the first demonstration site for this company's precession electron diffraction systems (and associated electron crystallography[4] software) for the Americas. Income from this company to PSU is generated by my consulting and demonstration efforts to NanoMEGAS' potential customers, which are also our potential scientific collaborators. This income goes to a special account at Portland State University, from which I am allowed to support my own research projects.

Also, due to our special cooperative relationship, my laboratory was the first in the Americas where a novel (jointly developed) crystallographic analysis system was installed. On the basis of precession electron diffraction enhanced structural fingerprinting, this system allows for automated crystallite orientation and phase mapping in a transmission electron microscope. Figures from our first comprehensive paper on this subject [20] with three sets of international collaborators appeared in June of 2011 ***on the cover*** of an internationally highly regarded scientific journal [2]. Note also that two of our papers in the general field of addressing the nanocrystal problem were selected earlier for re-publication in the Virtual Journal of Nanoscale Science and Technology.

The corresponding projects for developing both branches of structural fingerprinting were funded for several consecutive years by the Office of Naval Research, the Army Research Laboratories, and the Oregon Nanoscience and Microtechnologies Institute. I was pursuing these projects both with external and PSU internal collaborators. As with most methodical developments, more specialized research is still ongoing on the basis of our earlier accomplishments.

Creating an entirely new research field by applying established techniques in a novel context

This section outlines another example of my successful creation and occupation of a scientific niche. (Although providing the scientific background briefly in an introductory manner may appear to be another slight digression, it is needed to clarify who I am and how I typically work.)

As a crystallographer, I am not only interested in Crystal Physics but also in the general field of Crystal Chemistry. I have, therefore, been following major developments in that particular field for more than a quarter of a century. I noticed, for example, that the "*supramolecular approach*" to nanofabrication [21] had received a Nobel Prize (in Chemistry) one year after the (Physics) Nobel Price for scanning probe microscopy [22].

While working on structural fingerprinting of nanocrystals on the basis of high resolution transmission electron microscope images (i.e. the above mentioned project that predates our collaboration with NanoMEGAS), I attended a seminar at the Technical University Chemnitz in the fall of 2007. During that seminar, I realized that further progress in the supramolecular manufacturing of "nanodevices" was hampered by the prevailing paradigm of scanning probe microscopy imaging.

As typical for all kinds of microscopical imaging, practitioners of scanning probe microscopy were mainly concerned with deviations from regular arrays of small to medium sized molecules with periodicities in two dimensions (2D). What that community did not assess optimally were the individual building blocks of the arrays themselves. For nanodevices that are manufactured by the supramolecular approach, it is, however, the atomic structure of the molecules and the resulting physical/chemical properties of the individual building blocks of the arrays that count most!

Determining the idealized atomic structure of the individual building blocks of 2D periodic arrays is not a typical microscopy problem by any stretch of the imagination. It can, however, be considered as simply solving a 2D crystallography problem by plane symmetry averaging over all selected experimental data, which happened to have been collected with a particular type of microscope. The same applies to determining application relevant physical properties of the array such as, e.g., the local 2D periodic density of electronic states (at the Fermi level) in case of scanning tunneling microscopy imaging. The plane symmetry averaging, or crystallographic image processing in other words, over all selected array building blocks leads to the average (idealized) building block at a significantly higher signal to noise ratio. One obtains, thus, a "much clearer" image of what really counts for fabricating nanodevices by the supramolecular approach. This is facilitated by the fact that all 2D periodic array building blocks are quantum mechanically identical when the arrays are self assembled.

Crystallographic image processing, on the other hand, originated with structural-molecular biologists in the context of high resolution transmission electron microscope imaging (and was part of another Nobel Prize in Chemistry [23]). I was familiar with the theory and practice of crystallographic image processing because I had just utilized this approach for the development of one branch of structural fingerprinting of nanocrystals as mentioned in the previous sections. It was, therefore, straightforward to generalize the core concepts of crystallographic image processing so that they became applicable to all kinds of scanning probe microscopes as well.

After securing a corresponding patent for Portland State [24], we processed scanning probe microscope images from our experimental collaborators at the Technical University Chemnitz, Humboldt University Berlin, the Pacific Northwest National Laboratory, PSU, and Washington State University. We, thus, created an entirely new research field and Portland State University possesses the fundamental patent in this field. The collaboration with Technical University Chemnitz was facilitated by having one of my graduate students spent the summer of 2008 there. In May of 2009, our scientific innovation was recognized by the wider nanometrology / scanning probe microscopy community when we won the ***"Best Paper Award"*** of the 2009 International Conference on Frontiers of Characterization & Metrology for Nanoelectronics.

Collaborative projects in the Pacific Northwest region

Within a large five year project[5] that was sponsored by the National Science Foundation, I was collaborating (as co-principal investigator, co-PI) on the development of ferromagnetic semiconductors with researchers from the University of Washington at Seattle, the University of California at Davis, the Pacific Northwest National Laboratory, as well as both the Lawrence Livermore and the Lawrence Berkeley National Laboratories. This project allowed me to send two of my graduate students and two of my undergraduate students over the summers of 2006 to 2009 to the Pacific Northwest National Laboratory, the University of California at Davis, and the National Center for Electron Microscopy at the Lawrence Berkeley National Laboratory.

Two smaller collaborative projects that involved researchers from the University of Oregon, Oregon State University, the Pacific Northwest National Laboratory, and my group were sponsored by both the Army Research Laboratory and the Oregon Nanoscience and Microtechnologies Institute. These projects involved me as co-PI and presented very interesting scientific challenges, i.e. atomic structure elucidation of incommensurate nanocrystalline materials (for prospective applications as thermoelectrics) by a combination of X-ray diffraction and electron crystallography[4].

Although I am interested in pursuing my own methodological developments, I also like to be part of larger interdisciplinary research teams. As such I feel confident to work on the structural characterization of any kind of crystalline material. I also had access (as principal investigator, PI) to sufficient research funds from the very first day onwards as a tenure-track assistant professor (i.e. since the fall of 2002). This required a sustained effort in writing research proposals. As a result of this effort, I have gained the professionalism to create and maintain successful research programs in the future.

From scientific project work to professional service

Analogously to the Pacific Northwest region and the Oregon Nanoscience and Microtechnologies Institute, the nanomaterials science and engineering community of the whole world is poised to benefit from further developments in electron crystallography[4]. For this reason, I organized the symposium "*Electron Crystallography for Materials Research*" at the 2009 spring Meeting of the Materials Research Society. I also served as the lead editor of the joint proceedings of two symposia of that meeting [25]. During my sabbatical at Humboldt University Berlin in 2010, I organized the International Three Day Workshop "*Facets of Electron Crystallography*" in conjunction with both the German Society for Crystallography and the Leibniz Institute for Crystal Growth [26]. Back at Portland State University in 2011, I helped organizing both a pre-conference (Sunday) workshop and the session "*Advances in Electron Crystallography for Materials Research*" at the annual joint meeting of the Microscopy Society of America and the Microbeam Analysis Society of America [27].

Establishing graduate materials physics and crystallography as well as interdisciplinary nano-materials science and -engineering undergraduate education at Portland State University

One of my aspirations since joining the Physics Department of Portland State University has been establishing graduate materials physics and (interdisciplinary) crystallography education at PSU. This aspiration is an outgrowth of my direct experiences at other universities at which I worked (and which have integrated materials physics and crystallography graduate education in their curricula)[6]. Because crystallography[1] is by itself interdisciplinary, it is a viable and valuable addition to the nanoscience[7] focus of interdisciplinary science and engineering programs at PSU, which are well aligned with the goals of the Oregon Nanoscience and Microtechnologies Institute.

Portland State University is fortunate because several of my colleagues in Physics, Chemistry, Electrical and Computer Engineering, as well as Mechanical and Materials Engineering are also interested in developing advanced courses in nanoscience and -engineering. Over the last four years, more than fifteen faculty members from these departments (including myself) volunteered their participation in PSU's interdisciplinary hands-on course "Fabrication and Characterization of Nanomaterials". (These faculty members are also members of the "Portland Nanoscience and Nanotechnology Academy" [28].)

In close collaboration with this interdisciplinary faculty group and in support of this hands-on course, I developed an interdisciplinary one quarter course that is concerned with materials science and engineering at the nanometer length scale. My "*Introduction to Nano-(Materials) Science and Engineering*" (PH 481/581) course, focuses not only on the scientific foundations that are concerned with the nanometer length scale, but also covers recent engineering breakthroughs that have already resulted in nanotechnology products[8]. Contributing to nanoscience and -engineering education and research from a materials physics perspective clearly benefits PSU and is at the core of the educational and service aspects of my scholarly agenda.

Note that a frequently quoted 2002 science policy document by the National Nanotechnology Initiative [29] spelled out the magnitude of the "*nanometer length scale*" challenge to undergraduate/graduate student education in the 21st century:
- "*about 2 million nanotechnology workers will be needed worldwide in 10 - 15 years*",
- by 2007 "*nanoscience and engineering education*" needs to be "*enabled in at least 25 % of research universities*". (Note that 40 to 45% of the *nanotech-workers* should be based in the USA [30].)

I am proud to have helped Portland State University meet the latter challenge and also look optimistically into the "*nanotech future*". This is because there should be 6 million "*nanotech-workers*" and a $3 trillion market for "*nanotech-enabled products*" in 2020 according to a recent study by the National Science Foundation [31]. A supporting charge by the US government to its college educators is to "*migrate education for the nanoscale from a supplement to traditional disciplines into its own specialties, e.g., nano-education organizations, degrees, and professional disciplines*" within the years 2010 to 2020 [32].

I am also happy to live in the state that created the Oregon Nanoscience and Microtechnologies Institute, which puts "*nanotechnology to work in microsystems*" [33] and has been a very reliable supporter of the above presented scholarly agenda. Note finally the growing "*nanotech footprint*" in both fields: Materials Science & –Engineering and Applied Physics [34]. On the basis of this worldwide study, one may state that the "*nanotech footprint*" by now covers more than half of all Materials Science & –engineering research and more than 40 % of all Applied Physics research.

[1] H. B. Bürgi, *Zeitschrift für Kristallographie, International journal for structural, physical, and chemical aspects of crystalline materials* **217** (2002) 288

[2] http://www.crystalresearch.com/crt/index_g.html (Where the cover of this special issue is displayed.)

[3] http://www.icdd.com

[4] http://www.crystallography.net; this open-access, Internet-based database is rapidly growing and currently contains more than 155,000 entries. At Portland State, we provide mirrors of this database at nanocrystallography.net and nanocrystallogrpaphy.org, (S. Gražulis, D. Chateigner, R. T. Downs, A. F. T. Yokochi, M. Quirós. L. Lutterotti, E. Manakova, J. Butkus, P. Moeck, A. Le Bail, Crystallography Open Database – an open access collection of crystal structures, *J. Appl. Cryst.* **42** (2009) 726-729, open access: http://journals.iucr.org/j/issues/2009/04/00/kk5039/kk5039.pdf

[5] http://www.nsti.org/Nanotech2008

[6] http://www.aspbs.com/jne.htm

[7] http://www.scientificjournals.org/index.htm

[8] http://www.crt-journal.org

[9] http://www.microscopy.org

[10] http://sites.nationalacademies.org/PGA/biso/IUCr/index.htm

[11] http://www.iucr.org/iucr/commissions/electron-crystallography

[12] http://www.iucr.org/iucr

[13] http://nanocrystallography.research.pdx.edu

[14] http://nanocrystallography.research.pdx.edu/CIF-searchable

[15] http://nanocrystallography.net, http://jcod.nanocrystallography.net, and http://nanocrystallography.org

[16] S. J. Billinge and M. G. Kanatzidis, Beyond crystallography: the study of disorder, nanocrystallinity and crystallographically challenged materials with pair distribution functions, *Chem. Commun*., April 7, 2004, 749-60

[17] N. Pinna, X-Ray diffraction from nanocrystals, *Progr. Colloid. Polym. Sci.* **130** (2005) 29-32

[18] P. Moeck, Database-supported nanocrystal structure identification by lattice-fringe fingerprinting with structure factor extraction, *US Patent* 2008/0275655 A1, issued November 6, 2008, priority date: May 3, 2007

[19] http://www.numis.northwestern.edu/IUCR_CED/

[20] P. Moeck, S. Rouvimov, E. F. Rauch, M. Véron, H. Kirmse, I. Häusler, W. Neumann, Y. Maniette, D. Bultreys, and S. Nicolopoulos, High-resolution automated crystal orientation and phase mapping of nanocrystals in a transmission electron microscope, *Cryst. Res. Technol.* **46** (2011) 589-706

[21] http://nobelprize.org/nobel_prizes/chemistry/laureates/1987/

[22] http://nobelprize.org/nobel_prizes/physics/laureates/1986/

[23] http://nobelprize.org/nobel_prizes/chemistry/laureates/1982/

[24] P. Moeck, Systems for assessing and enhancing the performance of scanning probe microscopes by quantifying and enforcing periodicities and symmetries in two dimensions, *US patent* 12/660,422, priority date: February 27, 2009

[25] P. Moeck, S. Hovmöller, S. Nicolopoulos, S. Rouvimov, V. Petkov, M. Gateshki, and P. Fraundorf (Eds.), *Electron Crystallography for Materials Research and Quantitative Characterization of Nanostructured Materials*, Material Research Society, Symposium Proceedings, Vol. **1184**, 2009

[26] http://nanocrystallography.research.pdx.edu/index.py/facets

[27] http://www.microscopy.org/mandm/2011

[28] http://www.pdx.edu/pnna (and old site http://www.pnna.groups.pdx.edu)

[29] M. C. Roco, The Vision and Action Plan of the National Nanotechnology Initiative, *Proc. Comp. Nanosc. Techn.*, vol. **2**, pp. 1-5, 2002

[30] M. C. Roco, Converging science and technology at the nanoscale: opportunities for education and training, *Nature Biotechnology* **21** (2003) 1247-1249

[31] Nanotechnology Research Directions for Societal Needs in 2020, Retrospective and Outlook, National Science Foundation, see also http://www.wtec.org/nano2/

[32] M. C. Roco, C. A. Mirkin, M. C. Hersam, Nanotechnology Research Directions for Societal Needs in 2020, Springer, Dordrecht, Heidelberg, London, New York, 2011, p. xl

[33] www.onami.us

[34] M. L. Grieneisen and M. Zhang. Nanoscience and Nanotechnology: Evolving Definitions and Growing Footprint on the Scientific Landscape, published online: 19 AUG 2011, DOI: 10.1002/smll.201100387, future 4 page paper in *small* (2011); see http://www.nanowerk.com/spotlight/spotid=22504.php for a brief discussion

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[1] Crystallography has also been defined recently as *"… the science of condensed matter with emphasis on the atomic or molecular structure and its relation to physical and chemical properties"*, P. Paufler, *Zeitschrift für Kristallographie, International journal for structural, physical, and chemical aspects of crystalline materials* **217** (2002) 357 (celebration issue of the 125th anniversary of the

continued existence of this journal). In the same issue, H. B. Bürgi, states that *"The structure and properties of crystals are such an important basis for physics, chemistry, materials sciences and even biology that they need to be integrated into the curriculum of every student in these fields. Whether such instruction is part of a program in physics, chemistry, biology or crystallography is of lesser importance, …"*

[2] Our Crystal Morphology Database has a strong educational component and is topical because there is a renewed interest in the knowledge of crystal morphology that is driven by the demonstration that not only the size of a nanocrystal matters with respect to its properties, but also its morphology. Catalytic properties of nanocrystals, for example, are controlled by crystal morphology, see e.g. N. Tian et al.: Synthesis of Tetrahexahedral Platinum Nanocrystals with High-Index Facets and High Electro-Oxidation Activity, *Science* **316** (2007) 732-735). Early mineralogists and crystallographers, on the other hand, developed a comprehensive and systematic crystal morphology description on the basis of the spatial arrangement of symmetry elements about 140 years ago. This framework can now be reused and expanded for nanocrystals, but needs to be popularized within the community of researchers and educators that deal with nanocrystals.

[3] We uploaded mineral data to our "Wiki Crystallography Database" because there are many people interested in mineralogy and many active mineral collectors worldwide. Inspired by the success of the wikipedia, we hope that some of these people will contribute at least some of their knowledge to the world's first website where everything about an inorganic crystal that is stable in the natural environment can be collected, searched, shared, and openly accessed.

[4] Solving and refining unknown crystal structures on the basis of either electron diffraction intensities, high-resolution phase-contrast (lattice fringe) transmission electron microscope images, or a combination of both is commonly referred to as either "structural electron crystallography" or simply "electron crystallography". The Commission on Electron Crystallography of the International Union of Crystallography defines *"Electron Crystallography is the branch of science that uses electron scattering and imaging to study the structure of matter"*, see http://www.numis.northwestern.edu/IUCR_CED/.

[5] $2,500,000 over 5 years shared between one PI and three co-PIs. My share was approximately $80,000 per annum for about three years. This covered salary and fringe benefits for one postdoctoral researcher (approximately $50.000) that worked under my co-supervision at both the Lawrence Livermore National Laboratory and the University of California at Davis. Approximately $30,000 was directly subcontracted to me at PSU each year.

[6] For example, the large Physics Department at the Humboldt University of Berlin, where I earned my Ph.D. more than 20 years ago and recently spent my sabbatical, had its own Crystallography/Materials Science Institute. The University of Illinois at Chicago, where I was a Research Assistant Professor, also had its own Solid State/Materials Physics cluster with several experimentalists and theorists in their Physics Department. The Condensed Matter Physics sub-department at the University of Oxford, where I was a Research Fellow, also had a large physical crystallography group.

[7] *"Because disciplines are barely distinguishable at the nanoscale, the current boom in nano education offers us a unique opportunity to rebuild science education, literally from the bottom up, doing away with the classical disciplinary barriers that are rapidly becoming obsolete in our global research communities."*; Robert P. H. Chang, Prof. of Materials Science, Northwestern University, General Secretary of the International Union of Materials Research Societies, Principal Editor of the *Journal of Materials Research*.

[8] Nanofabrication and nanocharacterization already being reality receive significantly more coverage than prospective nano-devices. The size-dependence of electronic, magnetic, optical, mechanical, thermal, and chemical materials properties is covered at an introductory level. Recent developments in structural-molecular biology and nano-bio-materials science and engineering are also discussed.