Quantum Beam Science

Editorial

Quantum Beam Science—Applications to Probe or Influence Matter and Materials

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Received: 22 February 2017; Accepted: 22 February 2017; Published: 28 February 2017

1. Introduction

The concept of quantum beams unifies a multitude of different kinds of radiation that can be considered as both waves and particles, according to the quantum mechanical model. Examples include light, in the form of X-rays and synchrotron radiation, as well as neutrons, electrons, positrons, muons, protons, ions, and photons. While the past century saw the discovery of these types of radiation and particles along with the investigations of their physical properties and their fundamental interaction with matter, the current century focuses extensively on their applications to characterize and understand materials in their broadest context, under all imaginable conditions. X-rays diffract to deliver crystal structures, while muons probe for the local magnetism in such crystals. Similarly, neutrons diffract and probe for magnetism, while both γ-rays and positrons allow to measure the electronic density of states; or again X-ray, neutron or electron diffraction probes for crystal defects in addition to ion beam channeling. Because of their penetration, X-rays, neutrons and muons can be used for imaging, such as radiography and tomography. At the same time, the types of quantum beams are different in which information can be obtained when investigating a particular material. Take the difference in cross-sections between neutrons and X-rays, respectively emphasizing the light or the heavy elements in a compound or alloy. While neutrons diffract from nuclei and, as elementary magnets via their spins, they allow determination of crystal and magnetic structure via crystallographic methods. Muons, on the other hand, can be embedded as interstitials into crystals, locally probing the site and its surrounding electromagnetic potential landscape. There is much interest in the dynamics of matter—how electricity and heat are transported through a crystal, related to inelastic scattering of quantum beams. Again, neutrons win overall for the investigation of phonons, while visual light scattering in the form of Raman spectroscopy is much easier to conduct and delivers complementary information.

2. Facilities and Sources

Quantum-beam sources vary by many orders of magnitude in both beam parameters and physical size, ranging from the table-top to multi-billion-dollar large user facilities. The best example is X-rays. Any laboratory can afford an X-ray tube source, and a little more sophisticated, a rotating anode or even a modern liquid–metal–jet microfocus anode. The next step is particle-accelerator based synchrotron radiation, producing very soft X-rays with storage rings of only a 10 m circumference, climbing to 100 m ranging for very common 3 GeV machines and up to several 1000 m sized flagship synchrotrons that produce high energy X-rays. Such large facilities can host up to 50 beamlines in parallel and generate dedicated radiation from the infrared through ultraviolet to X-ray and gamma rays [1]. To top the brightness obtainable at synchrotrons, X-ray free-electron-lasers recently became operational at the Linac Coherent Light Source (LCLS) in the USA [2] and the SPring-8 Angstrom Compact Free Electron

Laser (SACLA) in Japan [3]. A European X-ray Free-Electron Laser (X-FEL) is being commissioned in Germany [4]. In those facilities, synchrotron-like insertion devices of typically a few meters in length are expanded to lengths of several hundred meters and X-ray light is emitted coherently [5]. All these sources and facilities cover differences in brilliance of over 25 orders of magnitude—some of the largest ranges of magnitude found in modern technology!

As large on a technological infrastructure and user-base scale are the neutron facilities. In the early laboratory-based days, neutron irradiating radioactive sources were used, until nuclear-reactor sources came along in the 1940s. Dedicated neutron facilities such as the Institut Laue Langevin (ILL), hosting over 40 instruments, became the state-of-the-art multi-user facilities where high-flux, compact cores are used, and beams are guided away from the reactor to dedicated instruments [6]. More recently, spallation sources have been developed, of which flagships are the Spallation Neutron Source (SNS) in the USA [7] and J-PARC in Japan [8], to be soon followed by the European Spallation Source (ESS) project in Sweden [9]. In such sources, highly accelerated proton beams are sent to a target evaporating neutrons from its nuclei, called spallation. Beams can be pulsed in time to allow energy-dispersive neutron detection by time-of-flight analysis, maximizing use of the created neutrons.

Because low-energy muons can be produced by a similar proton beam, such facilities are often located with spallation neutron sources. Furthermore, neutrons and muons cover an overlapping community for solid-state matter research, for whom the logistics of such a symbiosis is highly beneficial. Examples are the ISIS facility in the UK [10], J-PARC in Japan [11] and the Paul Scherrer Institute (PSI) in Switzerland [12], while the muon source at TRIUMF in Canada is based on a proton cyclotron [13].

Positrons are either produced by radioactive β^+ decay or by pair production from a high-energy γ photon, above 1.022 MeV. The latter is achieved at the reactor FRM-II in Munich, Germany by exploiting the neutron capture reaction ^{113}Cd (n,γ) ^{114}Cd yielding primary γ photons with an energy of 9.041 MeV [14]. Inverse Compton scattering of laser photons at accelerated electrons can reach these energies, meaning future positron sources will be based at neutron and accelerator facilities. The community is relatively small, however ambition is high to erect facilities with stronger beams.

The use of proton and ion-beam facilities is most diverse, as ions span in character from one single proton to heavy nuclei. Many ion beams are applied in conventional laboratories, such as focused ion beam milling for making nanoscopic specimens. Of high interest is the interaction of ions with matter, such as radiation damage, channeling, treating of tumors and ions as a characterization method (such as mass spectrometry). Stronger and high-energy ion beams are often used in creating exotic particles, as in nuclear physics at the borderline of stability, and for particles containing higher quark flavors. One of the largest projects is the international Facility for Antiproton and Ion Research (FAIR) being constructed in Germany [15], aiming at fundamental science studied along with applied research on bio- and hard materials.

Last but not least, lasers play a very important role in daily life and it will be out of scope to discuss all their applications here. Of interest in the context of *Quantum Beam Science* is the interaction of laser photons with other quantum beams, or with materials under extreme and exotic conditions, and in pump-probe arrangements. An example is above-mentioned inverse Compton scattering, nowadays developed and exploited at the Lawrence Livermore National Laboratory in the USA [16]. The Extreme Light Infrastructure (ELI) is a flagship project in Europe to produce laser driven quantum beams. Terawatt to petawatt lasers create plasmas and particle acceleration in the range 10 MeV up to 100 MeV, enough particle energy to create all kind of quantum beams including directly produced electrons, protons and ions, and secondary beams of X-rays, γ-rays, neutrons and positrons [17]. Such sources will pioneer not only capabilities in nuclear physics, but also the characterization of solid state materials and their properties. For example, high-flux, high energy γ photons not only allow for high-energy X-ray diffraction, but also to perform nuclear spectroscopy in solid state materials, related to novel imaging techniques.

3. Applications to Condensed Matter Physics and Materials

Much broader than the range of quantum-beam sources is their application to condensed matter and materials, including functional materials, structural materials, soft matter and medical treatment, i.e., the human body. It is out of the scope of this editorial to appraise the full capabilities of quantum beam applications. As a single example, I work with penetrating radiation of both neutrons and high energy synchrotron X-rays [18]. Neutrons typically show attenuation lengths in the many centimeter range while high-energy X-rays >100 keV penetrate up to a centimeter, say in steel and medium-heavy metals and compounds. This gives the opportunity to study bulk properties of crystalline and non-crystalline materials. When studying metals [19] interests range from engineering over characterization to fundamental science. Strain scanning for the characterization of residual stress is undertaken by both neutron and X-ray diffraction [20] and allow not only for the investigations of stresses but also to determine load partitioning between phases and crystal orientations [21,22]. Generally, neutron beams are larger and penetrate further, while high-energy synchrotron X-rays are of high brilliance and focused. They enable, respectively, fine statistical averaging, as needed for texture analysis and quantitative phase analysis in even coarse-grained material [23], versus single and multiple-grain studies scanned locally in a poly-crystalline matrix [24]. The complementarity in scattering contrast is exemplified by titanium aluminides, where the Ti scattering length for neutrons is negative while Al is positive, emphasizing large structure factors for superstructure reflections that describe atomic order. This is in contrast to X-rays, for which both scattering lengths are positive, rendering them sensitive to the overall structural packing [25]. Concepts of various quantum beams may be similar, such as the dynamical theory of diffraction [26,27], which can be used to trace crystal defects with neutrons [28], high-energy X-rays [29], and electrons [30], but on very different scales.

The advantage of using complementary and different quantum beams is well demonstrated by the study of magnetism. Here, neutron scattering is the conventional probe, as the neutron itself is a spin $\frac{1}{2}$ elementary magnet which interacts with spins of atoms in a crystal structure and thus reveals their arrangements. The interaction of X-rays with magnetism is extremely weak [31,32], however tuning the X-ray energy to the absorption edge of the magnetic atom enhances its scatting by orders of magnitude [33], making the method advantageous in certain situations, such as contrast variation attained by tuning through the resonance and working with small specimens. Here a third quantum beam comes into play, muons—elementary charged and spin $\frac{1}{2}$ magnetic particles which easily implant in crystal interstitials to probe the local magnetic fields, by techniques known as muon spin rotation and relaxation [34].

Again, although just two examples have been given, the importance of quantum beam science in thousands of disciplines cannot be emphasized enough. Quantum beams include synchrotron radiation, neutron beams, electrons, lasers, muons, positrons and ions, while materials can be crystalline, amorphous, magnetic, metallic, ceramic, biologic, hard and soft matter, warm dense matter, functional, structural and so on. *Quantum Beam Science* covers a broad range of disciplines including, but not limited to, solid-state physics, chemistry, crystallography, materials science, biology, geology, earth and planetary materials, and engineering. Examples of investigations are phase transformations in alloy development, modulated structures in spintronic systems, crystalline order and disorder, stresses in engineering specimens, changes in amorphous structure, excitations in functional materials, the interior of stars, electrochemistry in ion battery systems, imaging in life sciences, and propagation of dislocations in crystals.

4. Welcome to *Quantum Beam* Science

With this editorial I would like to welcome authors, institutions and readers to the new journal *Quantum Beam Science*. It is envisaged to cover sources, techniques, optics, properties and instrumentation, from a scientific point of view and to expose their innumerable applications to an interdisciplinary audience. *Quantum Beam Science* is supported by a renowned founding Editorial Board, seeking growth, and Guest Editors for Special Issues. We have started with the call for the special issue *Facilities*, aiming to lay a basis and awaken interest in the journal. A dedicated special issue *Laser-Driven Quantum Beams* is now in progress, demonstrating a new generation of powerful sources, while other special issues concentrating on quantum beam applications will follow shortly. The goal of the Editorial Board and the MDPI editorial staff is to make *Quantum Beam Science* a high-level scientific journal with short turnaround time, welcoming authors, institutions, and readers to a bright future!

Conflicts of Interest: The author declares no conflict of interest.

References

1. Liss, K.-D.; Chen, K. Frontiers of synchrotron research in materials science. *MRS Bull.* **2016**, *41*, 435–441. [CrossRef]
2. Emma, P.; Akre, R.; Arthur, J.; Bionta, R.; Bostedt, C.; Bozek, J.; Brachmann, A.; Bucksbaum, P.; Coffee, R.; Decker, F.-J.; et al. First lasing and operation of an Ångström-wavelength free-electron laser. *Nat. Photonics* **2010**, *4*, 641–647. [CrossRef]
3. Yabashi, M.; Tanaka, H.; Ishikawa, T. Overview of the SACLA facility. *J. Synchrotron. Radiat.* **2015**, *22*, 477–484. [CrossRef] [PubMed]
4. Altarelli, M.; Brinkmann, R.; Chergui, M.; Decking, W.; Dobson, B.; Düsterer, S.; Grübel, G.; Graeff, W.; Graafsma, H.; Hajdu, J.; et al. The European x-ray free-electron laser. *Tech. Des. Rep. DESY* **2006**, *97*, 1–26.
5. Geloni, G.; Saldin, E.; Samoylova, L.; Schneidmiller, E.; Sinn, H.; Tschentscher, T.; Yurkov, M. Coherence properties of the European XFEL. *New J. Phys.* **2010**, *12*, 035021. [CrossRef]
6. Büttner, H.; Lelievre-Berna, E.; Pinet, F. *The Yellow Book. Guide to Neutron Research Facilities at the ILL*; Institute Laue-Langevin Grenoble: Grenoble, France, 1997.
7. Mason, T.E.; Abernathy, D.; Anderson, I.; Ankner, J.; Egami, T.; Ehlers, G.; Ekkebus, A.; Granroth, G.; Hagen, M.; Herwig, K.; et al. The Spallation Neutron Source in Oak Ridge: A powerful tool for materials research. *Phys. B Condens. Matter* **2006**, *385–386*, 955–960. [CrossRef]
8. Maekawa, F.; Harada, M.; Oikawa, K.; Teshigawara, M.; Kai, T.; Meigo, S.; Ooi, M.; Sakamoto, S.; Takada, H.; Futakawa, M.; et al. First neutron production utilizing J-PARC pulsed spallation neutron source JSNS and neutronic performance demonstrated. *Nucl. Instrum. Methods Phys. Res. Sect. A: Accel. Spectrom. Detect. Assoc. Equip.* **2010**, *620*, 159–165. [CrossRef]
9. Åberg, M.; Ahlfors, N.; Ainsworth, R.; Alba-Simionesco, C.; Alimov, S.; Aliouane, N.; Alling, B.; Andersson, K.G.; Andersen, N.H.; Hansen, B.R.; et al. *ESS Technical Design Report*; European Spallation Source: Lund, Sweden, 2013.
10. Hillier, A.D.; Adams, D.J.; Baker, P.J.; Bekasovs, A.; Coomer, F.C.; Cottrell, S.P.; Higgins, S.D.; Jago, S.J.S.; Jones, K.G.; Lord, J.S.; et al. Developments at the ISIS muon source and the concomitant benefit to the user community. *J. Phys. Conf. Ser.* **2014**, *551*, 012067. [CrossRef]
11. Miyake, Y.; Shimomura, K.; Kawamura, N.; Strasser, P.; Koda, A.; Fujimori, H.; Ikedo, Y.; Makimura, S.; Kobayashi, Y.; Nakamura, J.; et al. Current status of the J-PARC muon facility, MUSE. *J. Phys. Conf. Ser.* **2014**, *551*, 012061. [CrossRef]
12. Kiselev, D.; Baumann, P.; Blau, B.; Geissmann, K.; Laube, D.; Reiss, T.; Sobbia, R.; Strinning, A.; Talanov, V.; Wohlmuther, M. The meson target stations and the high power spallation neutron source SINQ at PSI. *J. Radioanal. Nucl. Chem.* **2015**, *305*, 769–775. [CrossRef]
13. Pearce, R.M. *Experimental Facilities at TRIUMF*; Physics Department, University of Victoria: Victoria, BC, Canada, 1975.
14. Hugenschmidt, C.; Kögel, G.; Repper, R.; Schreckenbach, K.; Sperr, P.; Straßer, B.; Triftshäuser, W. The neutron induced positron source at Munich—NEPOMUC. *Nucl. Instrum. Methods Phys. Res. Sect. B: Beam Interact. Mater. At.* **2004**, *221*, 160–164. [CrossRef]
15. Spiller, P.; Franchetti, G. The FAIR accelerator project at GSI. *Nucl. Instrum. Methods Phys. Res. Sect. A: Accel. Spectrom. Detect. Assoc. Equip.* **2006**, *561*, 305–309. [CrossRef]
16. Hwang, Y.; Anderson, G.; Barty, C.; Gibson, D.; Marsh, R.; Tajima, T. LLNL Laser-Compton X-ray Characterization. In Proceedings of the 7th International Particle Accelerator Conference (IPAC'16), Busan, Korea, 8–13 May 2016; pp. 1885–1888.

17. Zamfir, N.V. Nuclear Physics with 10 PW laser beams at Extreme Light Infrastructure—Nuclear Physics (ELI-NP). *Eur. Phys. J. Spec. Top.* **2014**, *223*, 1221–1227. [CrossRef]
18. Liss, K.-D.; Bartels, A.; Schreyer, A.; Clemens, H. High-energy X-rays: A tool for advanced bulk investigations in materials science and physics. *Textures Microstruct.* **2003**, *35*, 219–252. [CrossRef]
19. Liss, K.-D. Structural Evolution of Metals at High Temperature: Complementary Investigations with Neutron and Synchrotron Quantum Beams. In *Magnesium Technology 2017*; Solanki, K.N., Orlov, D., Singh, A., Neelameggham, N.R., Eds.; Springer: Berlin, Germany, 2017; pp. 633–638.
20. Pyzalla, A.R.; Reimers, W.; Liss, K.D. A Comparison of Neutron and High Energy Synchrotron Radiation as Tools for Texture and Stress Analysis. *Mater. Sci. Forum.* **2000**, *347–349*, 34–41. [CrossRef]
21. Jimenez-Melero, E.; Van Dijk, N.H.; Zhao, L.; Sietsma, J.; Wright, J.P.; Van der Zwaag, S. In situ synchrotron study on the interplay between martensite formation, texture evolution and load partitioning in low-alloyed TRIP steels. *Mater. Sci. Eng. A* **2011**, *528*, 6407–6416. [CrossRef]
22. Iwase, K.; Sato, H.; Harjo, S.; Kamiyama, T.; Ito, T.; Takata, S.; Aizawa, K.; Kiyanagi, Y. In situ lattice strain mapping during tensile loading using the neutron transmission and diffraction methods. *J. Appl. Crystallogr.* **2012**, *45*, 113–118. [CrossRef]
23. Yan, K.; Carr, D.G.; Kabra, S.; Reid, M.; Studer, A.; Harrison, R.P.; Dippenaar, R.J.; Liss, K.-D. In situ Characterization of Lattice Structure Evolution during Phase Transformation of Zr-2.5Nb. *Adv. Eng. Mater.* **2011**, *13*, 882–886. [CrossRef]
24. Liss, K.-D.; Schmoelzer, T.; Yan, K.; Reid, M.; Peel, M.; Dippenaar, R.J.; Clemens, H. In situ study of dynamic recrystallization and hot deformation behavior of a multiphase titanium aluminide alloy. *J. Appl. Phys.* **2009**, *106*, 113526. [CrossRef]
25. Watson, I.J.; Liss, K.-D.; Clemens, H.; Wallgram, W.; Schmoelzer, T.; Hansen, T.C.; Reid, M. In situ Characterization of a Nb and Mo Containing gamma-TiAl Based Alloy Using Neutron Diffraction and High-Temperature Microscopy. *Adv. Eng. Mater.* **2009**, *11*, 932–937. [CrossRef]
26. Rauch, H.; Petrascheck, D. *Grundlagen für ein Laue-Neutroneninterferometer Teil 1: Dynamische Beugung*; Atominstitut der Österreichischen Universitäten: Wien, Austria, 1976.
27. Authier, A. Dynamical theory of X-ray diffraction. In *International Tables for Crystallography*; International Union of Crystallography: Manchester, UK; Volume B, pp. 626–646.
28. Kabra, S.; Yan, K.; Carr, D.G.; Harrison, R.P.; Dippenaar, R.J.; Reid, M.; Liss, K.-D. Defect dynamics in polycrystalline zirconium alloy probed in situ by primary extinction of neutron diffraction. *J. Appl. Phys.* **2013**, *113*. [CrossRef]
29. Bergmann, C. Quantitative Analyse Diffuser Röntgenstreuung an Sauerstoffnanopräzipitaten in Siliziumeinkristallen. Doctoral Thesis, Friedrich-Alexander-Universität Erlangen Nürnberg, Erlangen, Germany, 24 September 2015.
30. Whelan, M.J. Dynamical Theory of Electron Diffraction. In *Diffraction and Imaging Techniques in Material Science; Volume I: Electron Microscopy*; Amelinckx, S., Gevers, R., Van Landuyt, J., Eds.; North Holland Publishing Company, Elsevier: Amsterdam, The Netherlands, 2012; pp. 43–106.
31. Brückel, T.; Lippert, M.; Köhler, T.; Schneider, J.R.; Prandl, W.; Rilling, V.; Schilling, M. The Non-Resonant Magnetic X-ray Scattering Cross Section of MnF2. 1. Medium X-ray Energies from 5 to 12 keV. *Acta Crystallogr. A* **1996**, *52*, 427–437. [CrossRef]
32. Strempfer, J.; Brückel, T.; Rütt, T.; Schneider, J.R.; Liss, K.D.; Tschentscher, T. The non-resonant magnetic X-ray scattering cross section of MnF_2. 2. High-energy X-ray diffraction at 80 keV. *Acta Crystallogr. Sect. A* **1996**, *52*, 438–449. [CrossRef]
33. Hannon, J.P.; Trammell, G.T.; Blume, M.; Gibbs, D. X-Ray Resonance Exchange Scattering. *Phys. Rev. Lett.* **1988**, *61*, 1245–1248. [CrossRef] [PubMed]
34. Yaouanc, A.; De Réotier, P.D. *Muon Spin Rotation, Relaxation, and Resonance: Applications to Condensed Matter*; Oxford University Press: Oxford, NY, USA, 2010.