Journal of
Applied Crystallography
ISSN 0021-8898

Crystallography education and training for the 21st century

Katherine A. Kantardjieff,[a]* Anke R. Kaysser-Pyzalla[b] and Paola Spadon[c]

[a]Department of Chemistry, Center for Molecular Structure, California State Polytechnic University Pomona, 3801 West Temple Avenue, Pomona, CA 91768, USA, [b]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Wissenschaftliche Geschäftsführung, Glienicker Strasse 100, 14109 Berlin, Germany, and [c]Department of Chemical Sciences, Padua University, Via Marzolo 1, 35131 Padova, Italy

In reviewing crystallographic education and training pedagogy and progress, this issue of the journal considers current and ongoing developments, the potential of Web 3.0, and the challenges we face in the next decade.

Thirty-two years ago, a letter to the editor from the United States National Committee for Crystallography (USNCCr) Subcommittee on Interdisciplinary Activities appeared in *Journal of Applied Crystallography*, in which the USNCCr examined the current status of formal education in crystallography (Cohen, 1978). Five years ago, the USNCCr Education Subcommittee, together with the American Crystallographic Association Continuing Education Committee, re-examined the current status of the crystallography curriculum and produced a policy document on education and training in crystallography for the 21st century (Kantardjieff, 2006). Both efforts noted that methodological advances in the years preceding had provided opportunities for individuals with diverse backgrounds and preparation to use crystallography to answer structural problems in their hypothesis-driven research, and had greatly enhanced the need for many scientists and engineers, even if they were not directly in the field, to understand the results of diffraction analysis.

Crystallography remains a rich and interdisciplinary science. The role of crystallography across the sciences has been eloquently described for a broad scientific readership in two special volumes of *Acta Crystallographica Section A: Foundations of Crystallography* (Schenk, 1998, 2008), highlighting that the knowledge gained from analysis of crystallographic structures is a key underpinning of modern science and technology. Crystallography has gained importance for researchers in disciplines where it has not previously appeared and does not appear now in many curricula, such as engineering and solar energy technology. Technical advances, however, now enable users with little or no training, or deeper understanding, to often but not always produce quality results. Our readers will be familiar with recent high-profile and embarrassing retractions in the peer-reviewed literature, many the result of pathological science or inadequate review (Dauter & Baker, 2010; Harrison *et al.*, 2010).

Our objectives in publishing the articles in this special volume dedicated to education and training in crystallography are to provide an international forum for communicating the concerns in the crystallographic community about attracting, educating and training the next generation of scientists and professional crystallographers, as well as to share proven pedagogies, superior curriculum materials and innovations in teaching crystallography that utilize cyber-based tools and technology. Articles by E. Boldyreva, Z. Dauter and M. Jaskolski, M. Nespolo and B. Souvignier, and V. B. Pett provide materials and methods for teaching fundamentals. The use of databases and software tools to teach practical and skilful applications of crystallographic information is described in articles by G. M. Battle *et al.*, S. Dutta *et al.* and R. M. Hanson. Asserting that crystallography and molecular structure awareness should begin in elementary and secondary education as core components for implementing the established science standards, articles by K. A. Kantardjieff *et al.* and J. R. Luft *et al.* suggest ways to incorporate crystallographic science principles into the secondary curriculum and to engage both high school and beginning university students in projects utilizing crystallographic methods. In light of recent high-profile retractions due to methodological mistakes, as well as oversights in data analysis and peer review, B. Rupp discusses the importance of incorporating scientific reasoning and critical validation of data and structure models into the crystallography curriculum.

While crystallographic science forms the basis for a number of techniques utilized by researchers, in the past 15 years, crystallography as a science has largely migrated from a research specialty to a technique employed by a broad user community. With increasing use of neutron and synchrotron radiation sources, for example, a large and still growing user community aims to access crystallographic data to determine structure–property relationships of many substances, materials and even technical devices. Formal courses have all but disappeared from university course offerings, particularly in the United States, and in many European universities, former departments of crystallography have been dedicated to other allegedly more modern research fields. Moreover, the topic is rarely covered in undergraduate textbooks in biology, chemistry, geology or physics. These realities have led to growth of and dependence on independently funded workshops and summer schools in crystallography, as well as in related scientific areas (*e.g.* materials science) containing relevant aspects of crystallography. Such workshops are aimed largely at post-baccalaureate audiences. A notable example is the well known and highly regarded Cold Spring Harbor X-ray Methods in Structural Biology course. Held annually since 1988, this course provides both theoretical and hands-on sessions over an intensive, 16-day period, during which students carry out complete structure analyses from crystallization screens through structure refinement and presentation. Leaders in the field who developed the techniques and software give lectures and facilitate practical laboratory sessions. This 'total immersion' approach has been productive, training nearly 400 students so far, with many now heading their own research laboratories. An article by R. Sweet and A. Soares describes the RapiData practical course at the NSLS.

The crystallographic community has also come to rely increasingly on non-traditional curricular resources for instruction, such as web pages and, more recently, online courses. B. H. Toby provides observations on the use of such online materials for instruction in powder diffraction. As noted in the final article by K. A. Kantardjieff, the dynamic content and connectivity of Web 2.0 has facilitated practice and collaboration where the static pages of Web 1.0 could not provide practical experience. We have now entered the Web 3.0 decade, where the connectivity of Web 2.0 coupled with integration and mobility of information in Web 3.0 can provide practical experience through live, remote-enabling and realistic virtual environments. The new pedagogy made possible by Web 3.0 can facilitate deeper understanding among those who use and consume crystallographic information in related fields, and enable those teaching crystallography to transmit the fascination and excitement of the field necessary to attract a future generation of professional crystallographers.

Given past scientific achievements enabled by crystallographic science, including 25 Nobel Prizes, and the opportunities for new insights at the interface with other disciplines, it is an exciting time for crystallographic science but a challenging time for crystallographic education and training. We hope that this volume will provide ideas and useful materials that our readers can adapt and adopt in teaching crystallography, and that the insights presented herein will drive and stimulate discussion. The editorial office is extremely grateful for the contributions to this volume by the crystallographic community. We welcome your comments, and we hope to continue to serve as an international forum for informative and lively discussions on crystallography education and training for the 21st century.

References

Cohen, J. B. (1978). *J. Appl. Cryst.* **11**, 672–673.
Dauter, Z. & Baker, E. N. (2010). *Acta Cryst.* D**66**, 1.
Harrison, W. T. A., Simpson, J. & Weil, M. (2010). *Acta Cryst.* E**66**, e1–e2.
Kantardjieff, K. A. (2006). In Program Abstracts, American Crystallographic Association National Meeting, Honolulu, HI, USA.
Schenk, H. (1998). Guest Editor. *Acta Cryst.* A**54**, part 6, number 1.
Schenk, H. (2008). Guest Editor. *Acta Cryst.* A**64**, part 1.