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John Ian Langford (1935–2013)

John Ian Langford was born in Chingford, Essex, UK, on 12 August 1935. It was at the Viriamu Jones Laboratory in the Department of Physics, University College, Cardiff, that he started his academic career in 1961. His contribution to powder diffraction has mainly been concerned with the development of high-resolution diffractometry with conventional and synchrotron X-ray sources, improving the accuracy of parameters derived from powder diffraction data, and developing procedures for studying the microstructural properties of materials. During his time at Cardiff, he collaborated with Professor A. J. C. Wilson in the development of a new method for analysing diffraction line profiles, based on their variance. This work was the subject of a thesis on *Variance and other measures of diffraction broadening*, for which he was awarded the degree of PhD by the University of Wales in September 1965.

In 1966, Ian moved to the Department of Physics, University of Birmingham, with Professor Wilson. A major contribution was his development of the variance method from a theoretical concept to a technique used in studies of structural defects from powder diffraction data. Later, an important contribution of Ian Langford to line-broadening theory and practice was his interpretation of direction-dependent line breadths in terms of the mean dimensions and shape of crystallites. This work initiated a close cooperation with D. Louër and his collaborators at the University of Rennes, where Ian was four times *Professeur Invité* from 1979. The theory was applied to high-symmetry materials, notably zinc oxide samples, and the results showed excellent agreement with theoretical predictions.

Figure 1
Ian Langford in his laboratory with the Picker diffractometer at Birmingham in about 1975 (picture taken by the Physics Department Photographer, David James).

While accurate methods for line-broadening analysis could only be applied to diffraction patterns with well resolved lines, the use of flexible analytical functions, *e.g.* the Voigt and pseudo-Voigt functions, opened the door to the fitting of a suitable model to the total diffraction pattern. A starting point for this work was the introduction of the Voigt function in powder diffraction, an idea proposed by several authors in the 1960s–1970s and described in detail by Ian Langford in 1978. This turned out to be a very convenient function which allows a straightforward separation of the instrumental and sample contributions and at the same time describes the form of the peaks adequately. A few years later E. J. Mittemeijer and colleagues at the Delft University of Technology approached Ian for cooperation on a specific project. This work, based on adopting the Voigt function for profile shape description, resulted in the now well known and manifold applied single-line method for size–strain analysis (de Keijser *et al.*, 1982). Later work on the correction for truncation of diffraction-line profiles also led to joint publications.

The availability of a suitable profile shape function led to pattern-decomposition methods. In 1985, in collaboration with E. J. Sonneveld and J. W. Visser from Delft University of Technology, an approach to the determination of microstructural properties of zinc oxide powders was reported. Moreover, the consideration of line broadening due to microstructural effects in the Rietveld method was developed in collaboration with E. J. Mittemeijer, Th. H. de Keijser and R. Delhez in Delft and D. Louër in Rennes. A chapter based on this work is included in the classic book on the Rietveld method (Young, 1993).

Extending the limits of applications of powder diffraction was a continued concern in Ian's work. The improved instrumentation and analytical techniques led him in the early 1990s to an association with the SERC Daresbury Laboratory synchrotron source. In the course of his research, Ian was involved in studies using synchrotron X-rays, and he contributed to the characterization of the breadth and shape of the instrumental line profile of the 9.1 high-resolution powder diffractometer at Daresbury, in collaboration with R. J. Cernik.

In the second half of the 1990s Ian became interested in the effect of a crystallite size distribution in line profile analysis. A fruitful collaboration was undertaken with P. Scardi, Trento University, who was working on a new pattern modelling approach, based on models of microstructural effects. The effect of crystallite size distribution was pointed out in the study of a nanocrystalline cerium oxide, with negligible microstrain, prepared at Rennes. The collaboration between Birmingham, Rennes and Trento resulted in a noteworthy article published in 2000 (Langford *et al.*, 2000).

Ian was involved in the activity of many organizations. In 1987, he was invited to serve in the newly created Commission on Powder Diffraction (CPD) and was elected Secretary, a post he held until 1990. He served as a Co-Editor of *Journal of Applied Crystallography*. He joined the British Crystallographic Association (BCA) in 1982. In 2001, Ian received the BCA Industrial Group Award for his work on line profile analysis. He was also a member of the International Centre for Diffraction Data (ICDD). Ian was a distinguished powder diffractionist with a thorough knowledge of most topics in powder diffraction. In relation with the dramatic increase in the use of powder diffraction in the late 1970s, he was invited to give a plenary lecture on this development at the 12th IUCr Congress in Ottawa in 1981 on the *Renaissance of powder diffraction: from ugly duckling to beautiful swan*. He contributed to several review articles (*e.g.* Langford & Louër, 1996).

Ian's interests and passions extended well beyond powder diffraction and science. For one, Ian was a good expert and author of Towpath Guides: *Staffordshire & Worcestershire Canal* and *Stourbridge Canal*. In later years, he had an interest in water mills in Shropshire. His study on *Granite millstones of Shropshire and adjoining counties* was recently published (Langford, 2011).

Ian was a patient and very friendly man. We will always remember our long discussions with him, which could take place even in the middle of the night, where controversial topics and conflicting scientific opinions were discussed in a way that was never aggressive and was characterized by mutual respect. We, and the powder diffraction community, by means of this interaction and cooperation, have learned a lot and are immensely grateful for that.

References

Keijser, Th. H. de, Langford, J. I., Mittemeijer, E. J. & Vogels, A. B. P. (1982). *J. Appl. Cryst.* **15**, 308–314.
Langford, I. (2011). *Wind Water Mills*, **30**, 2–31.
Langford, J. I. & Louër, D. (1996). *Rep. Prog. Phys.* **59**, 131–234.
Langford, J. I., Louër, D. & Scardi, P. (2000). *J. Appl. Cryst.* **33**, 964–974.
Young, R. A. (1993). Editor. *The Rietveld Method.* Oxford University Press.

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