Exceptional content with major impact potential

The second 2018 issue of the journal *Powder Diffraction* (PDJ) is filled with a very diverse and special set of papers. I believe you will find that this issue has exceptional content and is well worth reading each paper.

First, there are four invited papers from the 2017 Denver X-ray Conference Proceedings, Advances in X-ray Analysis (AXA). The first paper (Shigehiro Takajo *et al*.) uses neutron diffraction to study the spatial distribution of texture and strains within an additively manufactured and rapidly deformed 304 L stainless steel rod. Additive manufacturing has progressed since its inception and is now being used to manufacture parts for a diverse array of applications. The ability to spatially map out texture and strain should lead to valuable improvements in additively manufactured components. The second AXA paper (Bob He) provides a way to remove aberrations in powder data collected with flat two-dimensional (2D) detectors. The geometric corrections can be used as well to improve the merged data when the 2D detector is scanned. The third paper (Timothy Fawcett *et al*.) introduces a new capability for performing phase identification by using measured elemental composition (XRF for example) and comparing that with elemental composition information in the large, edited Powder Diffraction File™ (PDF®) database. The paper describes the Goodness-of-Fit tests used in conjunction with the chemical information in the PDF to identify the closest matching phase. Clearly, this approach will be enhanced in many ways in the next few years including the ability to be used in combination with powder diffraction search-match methods to more uniquely identify an unknown. It is applicable to all classes of materials, not just to minerals as were used to demonstrate in this paper the potential of the method. The fourth paper (Christopher Heirwegh *et al*.) describes an empirical derivation of the X-ray optic transmission profile for use in calibration of the Planetary Instrument for X-ray Lithochemistry (PIXL), a sub-millimeter focused X-ray fluorescence spectrometer selected for the Mars 2020 science mission. The goal is to develop an accurate calibration so that elemental composition of Martian specimens can be accurately measured.

An exceptional group of contributed Technical Articles, New Diffraction Data, and Data Reports in this issue may also have a major impact on the analysis of XRPD data and structure refinement. Particularly noteworthy are the set of three Technical Articles by Takashi Ida of Nagoya Institute of Technology on the usage of a deconvolution–convolution treatment on powder diffraction data collected on instruments equipped with Cu X-ray targets and Ni filters. In Ida's second paper he shows how the deconvolution–convolution treatment can also remove trace peaks arising from contaminant radiation arising from the target or incident beam path. In his third paper, the technique was used to remove the axial divergent aberration in data from instruments with Bragg–Brentano geometry. I feel this technique, once more widely tested and implemented on commercial instruments with X-ray tubes and Bragg–Brentano geometry, will become widely used and will provide significant improvements to the powder data collected on this class of widely used instruments.

A demonstration of the value of using combined XRF and XRD techniques is provided in the Technical Article by Fawcett *et al*. on studies of patinas on 3rd and 4th-century Roman coins. The power of using combined XRF and XRD characterizations is clearly demonstrated. Further, it is easy to see how the X-ray community can contribute to the knowledge about ancient metal production and minting of coins.

Another group of papers by Kaduk *et al*., report the structure solutions and refinements by the Rietveld method followed by optimization of the structures by density functional theory techniques. The large number of the contributions by Kaduk and colleagues that have been reported in *Powder Diffraction* over the last several years have applied advanced methods to solve and Rietveld refine the crystal structures of large-volume commercial pharmaceuticals and then optimize them using density functional theory techniques. It is likely that such advanced structure solution and optimization methods will someday become the norm in our field.

We look forward to your next contribution to *Powder Diffraction*.

Camden Hubbard
Editor-in-Chief

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