X-RAY Spectrometry

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Editorial

The 12th International Conference on Proton Induced X-ray Emission (PIXE) and its Analytical Applications was held on the campus of the University of Surrey in Guildford, U.K. between 29th June and 2nd July 2010. The PIXE conferences have been held at approximately three year intervals since the mid 1970s and have reflected the development of the PIXE technique and its expanding range of applications.

This special issue of X-Ray Spectrometry contains papers based on conference contributions which have been selected to represent the latest developments in PIXE and its applications.

A major theme to emerge from the 2010 conference is the feeling that the understanding of the PIXE emission process and the quality of spectrum fitting and modelling software have now reached the point where the main factor determining the accuracy of elemental concentration determinations in homogenous samples is the accuracy of the physics database used in the model, especially the ionisation cross sections. Since there is little likelihood that the measurement of cross sections over the required range of Z and ion energy will ever be funded, improved theoretical calculations of these parameters will become increasingly important. This work is represented by the papers of Lapicki and Miranda and Taborda *et al*., which present new parametric expressions for ionisation cross sections. The paper by Mantero *et al*. presents the cross section parameterisation used for PIXE simulation in the Geant4 simulation package (http://www.geant4.org/geant4/), which will allow Geant4 to address PIXE related problems.

Another emerging strand of technique development concerns the use of X-ray detectors with high energy resolution which allow chemical information to be extracted from the fine structure of X-ray emission lines. The elegant paper by Reis *et al*. demonstrates the use of a novel calorimeter detector to reveal X-ray line fine structure which could provide information on the chemical or lattice environment of the emitting atoms. More conventionally, Tadić provides a numerical study of compact configurations of wavelength dispersive crystal spectrometer which are more compatible with a typical microPIXE target chamber than those normally used for WD-EDX and provide a much greater solid angle of acceptance. These miniature devices could permit the routine acquisition of WD-PIXE spectra in parallel with the more conventional ED spectra.

PIXE has long been perceived as ignoring the depth dimension, but the availability of fast computers coupled with novel software is opening the way to the goal of depth-resolved PIXE analysis, often in conjunction with complementary techniques such as RBS. Two papers in this volume (Reis, Dias *et al*.) explore this aspect of PIXE, which will allow the long penetration range of MeV protons to be fully exploited in exploring the depth distribution of trace elements.

Aerosol science has traditionally supplied a large proportion of the applications papers at PIXE conferences. Unusually, this conference saw significant drop in the number of aerosol papers, reflecting perhaps the shift in emphasis in climate change science away from inorganic elements and particulates. In their paper, Lucarelli *et al*. ask the question 'Is PIXE still a useful technique for the analysis of atmospheric aerosols?'. They conclude that it is; PIXE is unsurpassed for the rapid routine analysis of atmospheric particulates, especially in combination with other techniques. It is particularly useful in investigating local pollution events, as described by Maenhaut *et al*. or work-place exposure as shown by Matsuyama *et al*. and Szoboszlai *et al*.

The largest group of contributions to the conference concerned the analysis of biological and medical samples. PIXE is ideally suited for the study of trace metals in organic biological samples, and this can be exploited using a scanned proton microbeam to investigate how metals from the environment are transported and accumulated within the tissue of plants and insects. A review of this field is presented by Mesjasz-Przybyłowicz *et al*., while Gramigni *et al*. and Migula *et al*. describe investigations of metal metabolism in insects. The paper by Ohkura *et al*. takes a different approach to X-ray imaging of insects, using the X-ray emission produced by a proton microbeam as a quasi-monochromatic point source for projection micro-tomography of living insects.

The paper by Terakawa *et al*. is representative of the classical use of PIXE for determining bulk concentrations of metals in tissue (in this case the accumulation of platinum containing cancer drugs in tumours), but this is complemented by micro-PIXE measurements to confirm the microscopic distribution of the metal in the sample.

The use of PIXE in environmental science is represented in this issue by two papers. Thomyasirigul *et al*. use PIXE in a novel way to quantify small amounts of chromium accumulated on valence sensitive ion exchange medium to determine levels of Cr(III) and Cr(VI) in natural waters. This provides a much more precise measure of the environmental impact of Cr pollution, which is far more toxic in the Cr(VI) valence state. Šmit *et al*. use micro-PIXE to provide a detailed analysis and identification of a meteorite which fell in Slovenia in 2009.

The four remaining papers highlight the well-established use of PIXE in the study of ancient technologies. Beck *et al*. use the trace elements in the pigments used in Palaeolithic cave paintings to compare the pigment in the drawing with fragments of pigment raw materials found at the same site. Denker *et al*. exploit the 68 MeV external beam at the Helmholtz Centre in Berlin to analyse the metal alloy of a Roman bronze statue – beneath a thick protective varnish layer. Grime and Guttman-Bond have developed the use of external beam micro-PIXE to study ancient (Iron Age to mediaeval) agricultural manuring practices. Finally, Simon *et al*. use PIXE to develop trace element fingerprints for small scale glass factories in 17th and 18th century Germany and Poland in order to provenance fragments of glass bottles.

The conference took place during a period of uncharacteristically hot English summer weather; this enhanced the social programme which included a guided tour of the grounds of Guildford Castle and a day trip to the Portsmouth Historic Dockyard as well as the banquet in the Palladian surroundings of Clandon Park.

As outgoing chairman of the International Advisory Committee and as chairman of the Local Organising Committee I wish to express my gratitude to all those who contributed to the success of the 2010 PIXE conference: to the members of the IAC for their

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1 D.D. Cohen, 2 S. Thomyasirigul, 3 V. Havranek, 4 T. Calligaro, 5 Y. Miura, 6 J. Dias, 7 J. Miranda, 8 N. Dytlewski, 9 A. Mantero, 10 S. Matsuyama, 11 A. Markwitz, 12 F. Lucarelli, 13 C. Neelmeijer, 14 F. Olise, 15 B.N. Jones, 16 J. Mars, 17 J.C. Jeynes, 18 M.A. Reis, 19 C.A. Pineda, 20 N. Boyd, 21 J.L. Campbell, 22 S. Olabanji, 23 Z. Szokefalvi-Nagy, 24 P. Jobim, 25 D. Guseynov, 26 P. Comini, 27 T. Dupuis, 28 M. Christopher, 29 T. Saunders, 30 F. Eder, 31 S. Harada, 32 S. Calusi, 33 T. Tadic, 34 S. Fasinic, 35 J-O. Lill, 36 S. Kertez, 37 M. Roumie, 38 D. Jezerek, 39 K. Ishii, 40 G. Lapicki, 41 F. Folkmann, 42 N. Barapatre, 43 A. Denker, 44 W. Maenhaut, 45 W. Przybylowicz, 46 M.J. Merchant, 47 G.W. Grime, 48 R.P. Webb, 49 C. Jeynes, 50 M.J. Bailey, 51 K. Sera, 52 Z. Szoboszlai , 53 A. Terakawa, 54 H. Tamazaki, 55 C. dos Santos, 56 S. Bernardes, 58 D.G. de Kerckhove, 59 A. Taborda, 60 C. Chaves, 61 Z. Smit

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