Atomic fundamental parameter determinations at PTB using well-known synchrotron radiation and calibrated instrumentation

Burkhard Beckhoff, Philipp Hönicke, Ina Holfelder, Yves Kayser, Michael Kolbe, Janin Lubeck, Matthias Müller, Beatrix Pollakowski-Herrmann, Rainer Unterumsberger, Jan Weser

Physikalisch-Technische Bundesanstalt (PTB), Abbestraße 2-12, 10587 Berlin, Germany

Author Email: Burkhard.Beckhoff@PTB.de

Progress in different x-ray metrology fields depends on reliable knowledge on x-ray fundamental parameters (FP). Since 2008 an international consortium of academic, industrial and metrology key players have organised an x-ray FP roadmap generation. Current research aims at improving the knowledge on FP data by means of experimental and theoretical methodologies by novel instrumentation, specimens and algorithms. The fundamental parameters approach to quantitative x-ray spectroscopy requires an extensive database from the field of atomic physics. These include (i) mass attenuation coefficients, (ii) (partial) fluorescence yields and Coster-Kronig factors, (iii) radiative transition rates, (iv) chemical effects and (v) (subshell) photo-ionisation cross-sections. The oft-heard and facile observation that such databases are well-established is incorrect since they are founded largely upon compilations of data measured in the 1960s and early 1970s. Inconsistencies and large discrepancies have been found in wide ranges of elements and x-ray energies in the available databases: the situation is particularly unsatisfactory in the soft x-ray range. In order to reveal more reliable FP data in line with the FP roadmap recommendations, PTB has been developing and using calibrated instrumentation, both energy- and wavelength-dispersive spectrometers, in conjunction with well-known synchrotron radiation of high spectral purity. Examples of recent PTB works on different FP determinations mostly of technologically relevant elements will be presented. In order to address this topic and to ensure validation, a broad experience in metrology, experimental physics, theoretical physics, and nanofabrication has to be combined in collaborations involving academic and industrial partners as well as NMIs. Improved FP data substantially contribute to traceable characterisations of modern nanomaterials as well as to reliable in-situ and operando metrology of both catalytic processes and energy storage systems such as batteries.

References

[1] M. Müller, B. Beckhoff, G. Ulm, and B. Kanngießer, Phys. Rev. A **74**, 012702 (2006)
[2] Ch. Zarkadas, A.G. Karydas, M. Müller, B. Beckhoff, Spectrochim. Acta B **61**, 189 (2006)
[3] M. Müller, B. Beckhoff, R. Fliegauf, and B. Kanngießer, Phys. Rev. A **79**, 032503 (2009)
[4] D. Sokaras, M. Müller, M. Kolbe, B. Beckhoff, Ch. Zarkadas, and A.G. Karydas, Phys. Rev. A **81**, 012703 (2010)
[5] D. Sokaras, A.G. Kochur, M. Müller, M. Kolbe, B. Beckhoff, M. Mantler, Ch. Zarkadas, M. Andrianis, A. Lagoyannis, and A.G. Karydas, Phys. Rev. A **83**, 052511 (2011)
[6] M. Kolbe, P. Hönicke, M. Müller, and B. Beckhoff, Phys. Rev. A **86**, 042512 (2012)
[7] P. Hönicke, M. Kolbe, M. Müller, M. Mantler, M. Krämer, and B. Beckhoff, Phys. Rev. Lett. **113,** 163001 (2014)
[8] M. Guerra, J.M. Sampaio, T.I. Madeira, F. Parente, P. Indelicato, J.P. Marques, J.P. Santos, J. Hoszowska, J.-Cl. Dousse, L. Loperetti, F. Zeeshan, M. Müller, R. Unterumsberger, B. Beckhoff, Phys. Rev. A **92**, 022507 (2015)
[9] Y. Ménesguen, M. Gerlach, B. Pollakowski, R. Unterumsberger, M. Haschke, B. Beckhoff and M.-C. Lépy, Metrologia **53**, 7 (2016)
[10] P. Hönicke, M. Kolbe, M. Krumrey, R. Unterumsberger, B. Beckhoff, Spectrochim. Acta B **124**, 94 (2016)
[11] P. Hönicke, I. Holfelder, M. Kolbe, J. Lubeck, B. Pollakowski-Herrmann, R. Unterumsberger, J. Weser and B. Beckhoff, Metrologia **54**, 481 (2017)
[12] Y. Ménesguen, M.-C. Lépy, P. Hönicke, M. Müller, R. Unterumsberger, B. Beckhoff, J. Hoszowska, J.-Cl. Dousse, W. Błachucki, Y. Ito, Metrologia **55**, 56 (2018)
[13] M. Guerra, J.M. Sampaio, F.Parente, P. Indelicato, P. Hönicke, M. Müller, B. Beckhoff, J. P. Marques, and J.P. Santos, *Theoretical and experimental determination of K- and L-shell x-ray relaxation parameters in Ni*, Phys. Rev. A (2018), in print
[14] Second roadmap on atomic Fundamental Parameters for X-ray methodologies, *International Initiative on X-ray Fundamental Parameters*, www.exsa.hu/news/wp-content/uploads/IIFP_Roadmap_V2.pdf , Dec. 2017