

Letter to the Editor

Proliferation of Faulty Materials Data Analysis in the Literature

Matthew R. Linford¹, Vincent S. Smentkowski^{2*}, John T. Grant³, C. Richard Brundle⁴, Peter M.A. Sherwood⁵, Mark C. Biesinger⁶, Jeff Terry⁷, Kateryna Artyushkova⁸, Alberto Herrera-Gómez⁹, Sven Tougaard¹⁰, William Skinner¹¹, Jean-Jacques Pireaux¹², Christopher F. McConville¹³, Christopher D. Easton¹⁴, Thomas R. Gengenbach¹⁴, George H. Major¹, Paul Dietrich¹⁵, Andreas Thissen¹⁵, Mark Engelhard¹⁶, Cedric J. Powell¹⁷, Karen J. Gaskell¹⁸ and Donald R. Baer¹⁶

¹Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT 84602, USA; ²General Electric Research, Niskayuna, NY 12309, USA; ³Surface Analysis Consultant, Clearwater, FL 33767, USA; ⁴C.R. Brundle & Associates, Soquel, CA 95073, USA; ⁵University of Washington, Box 351700, Seattle, WA 98195, USA; ⁶Surface Science Western, University of Western Ontario, London, Ontario N6G 0J3, Canada; ⁷Department of Physics, Illinois Institute of Technology, Chicago, IL 60616, USA; ⁸Physical Electronics, Chanhassen, MN 55317, USA; ⁹CINVESTAV – Unidad Queretaro, Real de Juriquilla 76230, Mexico; ¹⁰Department of Physics, University of Southern Denmark, Odense 5230, Denmark; ¹¹Future Industries Institute, University of South Australia, Mawson Lakes, SA 5095, Australia; ¹²University of Namur, Namur Institute of Structured Matter, B-5000 Namur, Belgium; ¹³College of Science, RMIT University, Melbourne, VIC 3001, Australia; ¹⁴CSIRO Manufacturing, Ian Wark Laboratories, Clayton, VIC 3168, Australia; ¹⁵SPECS Surface Nano Analysis GmbH, 13355 Berlin, Germany; ¹⁶Pacific Northwest National Laboratory, Richland, WA 99354, USA; ¹⁷National Institute of Standards and Technology, Gaithersburg, MD 20899, USA and ¹⁸University of Maryland, College Park, MD 20742, USA

(Received 11 December 2019; revised 19 December 2019; accepted 19 December 2019)

As a group of subject-matter experts in X-ray photoelectron spectroscopy (XPS) and other material characterization techniques from different countries and institutions, we write this document to raise awareness of an epidemic of poor and incorrect materials data analysis in the literature. This issue is a growing problem with many causes and very undesirable consequences. It contributes to what has been called a “reproducibility crisis”, which is a recent concern of the U.S. National Academies of Science (Baker, 2016; Harris, 2017; NASE&M, 2019).

Over the past decade material analysis techniques have matured to the point that dedicated expert operators are often not considered to be necessary to collect and analyze data, especially when the samples are perceived as simple or routine. The tools in this growing arsenal, including XPS, are now used in academia, industry, and government laboratories to provide both compositional information and a mechanistic understanding of a wide variety of materials. This situation, coupled with increased accessibility of the equipment, improved instrument reliability, and the promise of useful data, has resulted in significant growth in the number of researchers using these characterization tools and reporting material analysis data. Although many of the resulting papers are of high quality, especially in journals that focus on materials characterization, others are unsatisfactory. In an ongoing analysis of XPS data in journals that emphasize next generation materials, we find that about 30% of the analyses are completely incorrect (Linford and Major, 2019). Thus, for some applications, inappropriate data analysis has reached a critical stage, making it difficult for researchers lacking the relevant expertise to find and readily identify reliable examples of what

would be considered good-quality data analysis. The errors we are observing in the literature are not limited to journals that may be deemed to be of lower impact—they regularly appear in what are identified as upper-tier/high-impact-factor journals. It is not uncommon to similarly find that 20–30% of the analyses of data from other material characterization techniques are also incorrect (Chirico et al., 2013; Park et al., 2017). The consequences of this issue are significantly greater than merely having a few poorly executed figures in otherwise good papers. Results and conclusions in a study hinge on the data collected and analyzed. If the characterization of a material is incorrect, an entire work may be fundamentally flawed. In some areas, the proliferation of advanced analytical instruments appears to have exceeded the world’s supply of expertise necessary to collect, interpret, and review the results obtained from them.

Some sub-disciplines in science only require a single analytical/measurement tool or just a few tools for a complete analysis of their systems. In contrast, materials analysis generally requires multiple advanced-characterization techniques to obtain an appropriate understanding of a new thin film or material (Baer & Gilmore, 2018). These techniques typically require an understanding of the physics and chemistry behind them, can be performed in multiple modes, and often require detailed first-principles and/or established empirical/semi-empirical modeling for their data reduction. Furthermore, each technique is supported by an extensive literature written by experts. Because of the need for information from these methods, the burden placed on materials researchers is heavy. In addition to a requirement to develop novel materials, they must characterize them at a high level with multiple analytical tools. Of course, not every materials problem requires advanced data analysis. Many important quality-control and device-failure problems have been solved by a basic application of one or more pieces of modern

*Author for correspondence: Vincent S. Smentkowski, E-mail: smentkow@ge.com
Cite this article: Linford MR et al (2020) Proliferation of Faulty Materials Data Analysis in the Literature. *Microsc Microanal* 26, 1–2. doi:10.1017/S1431927619015332