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The Proliferation of Faulty Materials Data Analysis in the Literature

Matthew R. Linford,[1] Vincent S. Smentkowski,[2] John T. Grant,[3] C. Richard Brundle,[4] Peter M.A. Sherwood,[5] Mark C. Biesinger,[7] Jeff Terry,[8] Kateryna Artyushkova,[9] Alberto Herrera Gómez,[10] Sven Tougaard,[11] William Skinner,[12] Jean-Jacques Pireaux,[13] Christopher F. McConville,[14] Christopher D. Easton,[15] Thomas R. Gengenbach,[15] George H Major,[1] Paul Dietrich,[16] Andreas Thissen,[16] Mark Engelhard,[17] Cedric J. Powel,[18] Karen J. Gaskell,[19] Donald R. Baer[17]

[1]Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT 84602, USA

[2]General Electric Global Research, Niskayuna NY, USA

[3]Surface Analysis Consultant, Clearwater, FL 33767, USA

[4]C.R. Brundle & Associates, Soquel, CA 95073, USA

[5]University of Washington, Box 351700, Seattle, WA 98195, USA

[7]Surface Science Western, University of Western Ontario, London, Ontario N6G 0J3, Canada

[8]Department of Physics, Illinois Institute of Technology, Chicago, IL, USA

[9]Physical Electronics, Chanhassen, MN, USA

[10]CINVESTAV – Unidad Querétaro, Mexico

[11]Department of Physics, University of Southern Denmark, Odense, Denmark

[12]Future Industries Institute, University of South Australia, Mawson Lakes 5095, Australia

[13]University of Namur, Namur Institute of Structured Matter, Namur, Belgium

[14]College of Science, RMIT University, Melbourne, Victoria 3001, Australia

[15]CSIRO Manufacturing, Ian Wark Laboratories, Clayton, Victoria, Australia

[16]SPECS Surface Nano Analysis GmbH, Berlin, Germany

[17]Pacific Northwest National Laboratory, Richland WA, USA

[18]National Institute of Standards and Technology, Gaithersburg, MD 20899 USA

[19]University of Maryland. College Park, MD 20742 USA

As a group of subject-matter experts in X-ray photoelectron spectroscopy (XPS) and other materials 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.[1-3]

Over the past decade, materials-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 X-ray photoelectron spectroscopy (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, increased instrument reliability, and the promise of useful data has resulted in significant growth in the number of researchers using these characterization tools and reporting materials-analysis data. Although many of the resulting papers are of high quality, especially in journals that focus on materials characterization, in an ongoing analysis of XPS data in the recent literature, we are finding that more than 30% of the data or analyses are flawed and even completely incorrect in journals that emphasize next-generation materials.[4,5] For some specific 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. Based on other reports, it is not uncommon to similarly find that 20 – 30% of the analyses of data from other materials characterization techniques are also incorrect.[6,7] 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, 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.[8] In addition, each technique typically has multiple modes, they come out of an extensive literature written by experts, they require an understanding of the physics and chemistry behind them, and they often require detailed first principles and/or established empirical/semi-empirical modeling for their data reduction. 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.

This epidemic has a plethora of consequences. When too much of the literature is corrupted by poorly collected and poorly interpreted results, a resource that was designed to further the cause of research is compromised. Unfortunately, the literature does not have a generally accepted mechanism for identifying studies (or portions thereof) of questionable value, so these documents may influence the thinking, direction, and future research of other scientists and engineers. Anecdotally, we note that, as analysts, we are often asked to reproduce or follow an analysis approach from the literature that is fundamentally flawed. Incorrect precedent is sometimes cited in the literature, which perpetuates errors. Results from materials characterization influences business decisions, and graduate students and researchers who ought to be able to learn from the literature are misinformed.

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 characterization equipment. However, in mature industries and fields, advances are more often made through the development of a detailed, comprehensive understanding of materials. In these cases, a lack of proper data collection and analysis impedes progress.

In our view, the fact that many incorrect analyses are appearing in the literature is a systemic problem. Researchers are under intense pressure to publish, and without some change to the system they will most likely continue to do their work as they have in the past. Instrument manufacturers are, at least indirectly, if unintentionally, complicit; they have developed high quality and easy-to-operate systems that may mislead customers into believing that data collection and analysis from their instruments is a rather straightforward endeavor. This certainly may be the case for some routine samples, but not for all materials. Moderately to very complex materials such as nanoparticles, nanostructured and two- or three-dimensional materials, catalysts, anisotropic or graded materials, etc. require a more nuanced approach. Reviewers and editors of manuscripts are often experts in the synthesis and/or development of a particular type of material, and in this sense are appropriately chosen to evaluate certain classes of manuscripts. However, they often do not possess a detailed understanding of all the analytical methods that may have been used to characterize the new materials described in the documents they review. Thus, the structure, traditions, constraints, and pressures of the current scientific endeavor often lead to the publication of faulty or misleading data analysis.[8] A partial solution that some of us are applying to the review process is to only review portions of papers for which we have the needed expertise and to clearly inform the editors of the areas where we were not qualified to provide a needed evaluation. These are only preliminary suggestions. As this discussion and analysis of this problem progresses, our consensus of a solution has become

multifaceted, with emphasis on each level of stakeholder. A more detailed analysis of both the nature of the problem in XPS data, along with specific actions that can be taken to address the issues, is forthcoming.

Some of us are in the process of writing a series of guides, tutorials, and recommended protocol articles on XPS that are being published in the Journal of Vacuum Science and Technology.[9,10] We believe that these will be an aid to those who wish to acquaint themselves with the technique so that they can avoid some of the common pitfalls in its data analysis and reporting. Many of us have also been involved in developing documentary standards for XPS and other surface analysis methods that have been published by ASTM and the International Organization for Standardization (ISO). High quality surface analysis data have also been published in Surface Science Spectra.[11] The guides and papers we are developing will include lists of common errors made in XPS data analysis, recommendations to all the stakeholders in this issue, and a more detailed, quantitative analysis of the problem. Similar guidance and reference data, e.g., ASTM and ISO standards, have also been developed for other material-characterization techniques. We commend the efforts of other groups of experts that similarly teach appropriate data analysis of their methods and call upon the scientific community to pay greater heed to the more accurate work-up and publication of instrumental data.

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