ISSN: 2692-5397
Modern Concepts in Material Science
DOI: 10.33552/MCMS.2020.03.000565
Iris Publishers

Opinion

The Reproducibility Crisis in Science from the Perspective of Thin Film Deposition: An Unexpected Approach

Carlos Morales[1]*, Leonardo Soriano[1] and Carlos Sánchez[2]

[1]*Department of Applied Physics and Nicolás Cabrera Institute, Autonomous University of Madrid, Spain*

[2]*Department of Materials Physics and Nicolás Cabrera Institute, Autonomous University of Madrid, Spain*

***Corresponding author:** Carlos Morales, Department of Applied Physics and Nicolás Cabrera Institute, Autonomous University of Madrid, Cantoblanco E-28049, Madrid, Spain, Email: Carlos.MoralesSanchez@b-tu.de.

Received Date: September 23, 2020

Published Date: October 12, 2020

Abstract

The publication of scientific results in all disciplines, and in particular in Material Science, has geometrically increased in the last decades. Although the quality of the published results seems to follow the same trend, the feeling that we could be facing a reproducibility crisis has become extended within the scientific community. We discuss this issue in relation to thin film deposition techniques such as atomic layer deposition, which should not present deviations on the reported results due to its self-limiting nature. In particular, we put the focus on the necessity of a multipolar approach that takes into account also the global environment in which researchers perform their work.

Keywords: Material science; Reproducibility crisis; Emotional and mental health

Abbreviations: ALD: Atomic Layer Deposition; CVD: Chemical Vapor Deposition

Introduction

The impressive technological development during the last hundred years has become the distinguishing mark of our contemporary era. If the ancient ages were identified by the name of the material that allowed a qualitative jump in terms of nature adaptation and territory control, i.e. stone, bronze and iron, very likely these are the days of silicon. The development of electronics, including its way through the micro and nano scales, has facilitated the greater and faster levels of information sharing and storage of the human history, changing the social uses, the relationships between different communities, our global perception of ourselves and, what particularly concerns us as scientists, the way of doing and sharing scientific results. Indeed, if until the beginning of the XX century the human knowledge was doubled every one hundred years, this time has been decreasing down to thirteen months in 2010. In that same year, the field of nanotechnology was doubling its knowledge every eighteen months [1].

This exponential improvement implies the domain of different bottom-up deposition techniques, most of them developed during the second half of the past century. In spite of the evident control of protocols and the successful results that translate into novel mass devices, there is also an extended feeling in the scientific community: we are within a reproducibility crisis that affects all disciplines, including Material Science [2]. Before moving forward, we would like to stress that this has nothing to do with a proliferation of fake results, but with difficulties on reproducing proper or external reliable results. The following lines will overview briefly the different deposition methods that may be used in thin film deposition. We will pause in atomic layer deposition (ALD), because its self-limiting reaction nature allows to compare and discuss the reproducibility among results from different groups. By extrapolating this reflection, we will discuss the current reproducibility crisis narrative.

Discussion

Thin film (from nanos to microns) deposition techniques can be divided in two large branches: physical and chemical processes [3]. Generally speaking, the first group covers those methods that imply a change on the physical state of the compound (liquid/solid-gas) before its deposition as thin film (gas-solid). The usual examples are sputtering or physical thermal evaporation (using different heating systems, such as e-beam or thermal Knudsen cells). On the other hand, chemical methods imply the formation of thin films by solid/gas or solid/liquid reactions, for instance, chemical vapor deposition (CVD) or ALD. Nevertheless, together with the variation of certain intrinsic parameters of the specific method, combinations of physical and chemical methods are very often used to grow oxides, to achieve film doping or some microstructure control. Reactive sputtering, which consists of standard sputtering under a reactive atmosphere, may well illustrate the former sentence. For example, from pure metallic targets, oxide films can be grown; by controlling the atmosphere composition intrinsic or extrinsic level of doping may be varied; and, finally, by changing pressure and temperature, the microstructure of the film also be tailored [4].

The limited length of the present contribution compels us to stop here the introduction of thin film deposition techniques. However, the aforementioned ALD technique constitutes an excellent example to continue our dissertation. The use of ALD has spread in the last decades due to its conformal growth on 3D structures and excellent control of thickness at the atomic scale, what makes it a very powerful technique in nano-devices production [5]. Although similar precursors to those of CVD are used, the difference between these two techniques is the self-limiting nature of ALD. The sample is alternatively exposed to the different precursors, limiting the reaction of each type with only those active sites available at the surface as a consequence of the previous reaction between the former precursor with the surface, what leads to a well-controlled growth of one layer per cycle (see Figure 1). Therefore, the advantage of ALD lies on the saturation of each one of the reactions that constitute a complete cycle. If saturation is reached, then extra time on the dosage of one precursor should not lead to changes on the deposition rate. Although secondary factors such as temperature or type of oxidant (in case of metal oxide growths) could lead to slight differences on the growth rate for a unique metalorganic precursor, the comparison of deposits under virtually exact conditions should lead to a very low dispersion of results. However, as very recently shown by H.H. Sønsteby et al. [6], there is a wide dispersion on reported growth rates for well-known materials such as Al_2O_3 (using Trimethylaluminu -TMA, $Al(CH_3)_3$- and water), TiO_2 (titanium tetraisopropoxide –TTIP, $Ti[OCH(CH_3)_2]_4$ - and water) or FeOx (ferrocene -$Fe(cp)_2$- and ozone). For example, Al_2O_3 growth rates between 1 and 3 Å/s are reported. This is a factor of three from the highest to the lowest value for a process that should be self-limiting, whatever the ALD reactor and for the same experimental conditions. Similar data dispersion apparently affects in different grades to the entire field of Material Science.

The perception of the reproducibility crisis that the previous example shows has gained attention in the last decade, as it demonstrates the evolution of records on the Web of Science database that mention this crisis on its title, abstract or keywords [7]. In particular, the survey published in Nature in 2016 by M. Baker drew the attention of the scientific community [2]. That work shows a survey to more than 1500 scientist where 52% of them recognized that there was a strong reproducibility crisis, followed by a 38% that, although recognizing the problem, lowered its depth. Only a 3% of surveyed people denied that such problem exists. Although chemists, physicists and engineers were the most confident regarding the work of their colleagues, more than 60% of them recognized problems in reproducing the results of other research groups. The lack of reproducibility within the same laboratory reached 50%. This value, slightly lower than the former could be explained by the diversity of laboratory equipment. Therefore, it seems clear that there exists a general perception of difficulties to reproduce previous published results and methods.

It is true that doing cutting-edge science may mean moving in the limits of reproducibility, in the sense that developing new lines of research means doing everything new. Therefore, despite describing correctly and in detail (not in all cases) the experimental method, same results may not be obtained because the focus of the description is not placed on important factors that remain hidden. Nevertheless, when scientists were asked in the quoted survey about the possible causes of this lack of reproducibility, more than 60% of them blame to pressure on publishing, selective reporting, low statistical power and non-enough replication of the original lab. In fact, the three last causes may be easily related to limited time and pressure to obtain and publish novel results. In short, the pressure to remain on the funding-publish-funding cycle seems to be the ultimate reason.

Moreover, the accumulative dynamic of such problems should have a high impact on science progress in the middle-long term. For example, the absence of an evident, visible gap between fundamental and more applied research, or the fact that retractions, errata or corrections in journals have not increased relatively to the amount

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of new publications [8], seems to indicate that this reproducibility crisis has not yet, if at some time should have, consequences. In fact, some authors as D. Fanelli consider that this crisis is not necessarily real, but a narrative put up by projecting personal experiences and idealizing scientific standards and models to all fields [7]. In particular, by metadata analysis from science databases such as Web of Science, this author argues that there are no evidences of an increase of the publications per author if the increase of co-authorship is taken into account, or that there is not a process of multiplication of published works by fractionating or simplifying results [9].

In our opinion, the statistical studies by D. Fanelli are of great interest and should be carefully studied. However, we consider that the wide dispersion of data regarding tests that should not depend on human bias, such as self-limiting ALD, reveals that there exists an important issue of reproducibility. Avoiding generalizations, at least on material science processing. In addition, the issue should be only tackled from an interdisciplinary view that should take into account the environment in which we are doing science. In this regard, we consider essential to relate the Baker's survey with the multiple studies regarding emotional and mental health of the scientific community, especially PhD students and young researches that carried out most of the laboratory work in many groups. For instance, the study by T.M. Evans [10] on twenty six countries indicates that PhD students are six times more prone to suffer from mental diseases than the rest of the general population, that is, a percentage of 39% versus 6%. When asked about symptoms associated with anxiety and/or depressive disorders, the 3600 participants from an equivalent survey performed in Belgium answered being under constant pressure (41%), feeling unhappy or depressed (30%), lacking confidence or simply useless (16%) [11]. Although it is true that policies on different countries and territories may imply differences on pressure suffered by the scientific community, similar studies have concluded similar trends in different countries. The perception (or narrative) of the reproducibility crisis and its causes cannot be explained without taking into account the whole picture. We believe that behind these two issues it may lie a deeper crisis related to the way by which science production is performed. As diagram of Figure 2 shows, this could especially be related to the accelerations of science times and the temporary and contingent positions of many researches, which contribute to increase the pressure to publish.

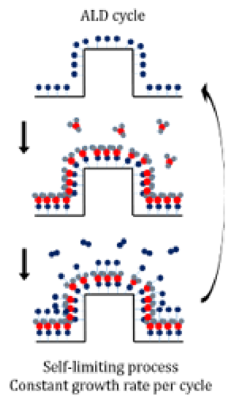

Figure 1: Schematic diagram of a single cycle of the ALD process. The self-limiting nature of surface reactions should impose a unique rate growth per cycle.

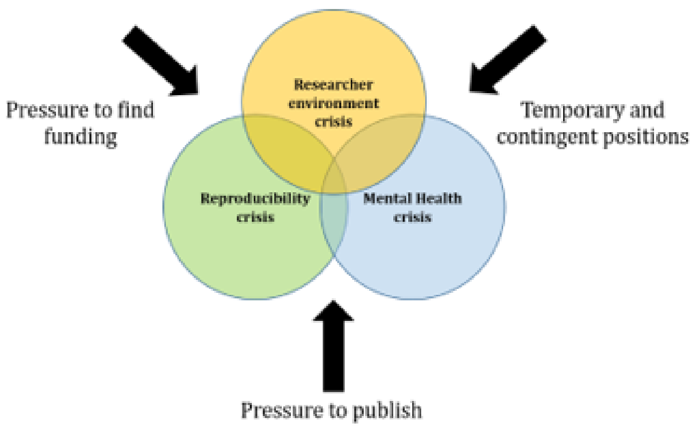

Figure 2: Diagram of complex interactions between different crisis in the scientific activity and possible main causes.

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Conclusion

Scientific knowledge, and in particular Material Science, are undoubtedly in a golden age. However, in the last years an increasing interest has appeared on the reproducibility crisis in all scientific disciplines. The pressure to publish has been pointed out as the ultimate possible cause. Moreover, the conclusions of different studies regarding metadata of published records show no evidence of such crisis but a narrative built up from personal experiences and erroneous generalizations. We believe that objective experimental techniques, such as the self-limiting ALD, shows the existence of such reproducibility crisis without the critical concurrence of any human bias. Besides, the study of the causes of the reproducibility crisis, that may not yet let to sever consequences, should be related to other facets of the scientists social and labor environment.

Acknowledgement

Members of MIRE Group acknowledge the financial support of the Spanish MICINN under project RTI2018-099794-B-I00.

Conflict of Interest

The authors declare no conflict of interest.

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