Current Opinion in Solid State and Materials Science 19 (2015) 212–226

Contents lists available at ScienceDirect

Current Opinion in Solid State and Materials Science

journal homepage: www.elsevier.com/locate/cossms

# Degradation science: Mesoscopic evolution and temporal analytics of photovoltaic energy materials

Roger H. French [a,b,c,d,*], Rudolf Podgornik [b,e], Timothy J. Peshek [a,b,d], Laura S. Bruckman [a,b], Yifan Xu [f,g], Nicholas R. Wheeler [a,c], Abdulkerim Gok [a,b], Yang Hu [a,b], Mohammad A. Hossain [a,h], Devin A. Gordon [a,b], Pei Zhao [a,i], Jiayang Sun [f,g,1], Guo-Qiang Zhang [i,j,1]

[a] Solar Durability and Lifetime Extension Center, Case Western Reserve University, Cleveland, OH 44106, United States
[b] Department of Materials Science and Engineering, Case Western Reserve University, Cleveland, OH 44106, United States
[c] Department of Macromolecular Science and Engineering, Case Western Reserve University, Cleveland, OH 44106, United States
[d] Department of Physics, Case Western Reserve University, Cleveland, OH 44106, United States
[e] Department of Physics, University of Massachusetts, Amherst, Massachusetts 01003, United States
[f] Department of Epidemiology and Biostatistics, Case Western Reserve University, Cleveland, OH 44106, United States
[g] Center for Statistical Research, Computing and Collaboration, Case Western Reserve University, Cleveland, OH 44106, United States
[h] Department of Mechanical and Aerospace Engineering, Case Western Reserve University, Cleveland, OH 44106, United States
[i] Department of Electrical Engineering and Computer Science, Case Western Reserve University, Cleveland, OH 44106, United States
[j] Center for Clinical Investigation, School of Medicine, Case Western Reserve University, Cleveland, OH 44106, United States

ARTICLE INFO

*Article history:*
Received 10 December 2014
Accepted 20 December 2014
Available online 20 January 2015

*Keywords:*
Photovoltaics
Degradation
Mesoscopic evolution
Real-world
Data science
Epidemiology
Reliability
Lifetime

ABSTRACT

Based on recent advances in nanoscience, data science and the availability of massive real-world datastreams, the mesoscopic evolution of mesoscopic energy materials can now be more fully studied. The temporal evolution is vastly complex in time and length scales and is fundamentally challenging to scientific understanding of degradation mechanisms and pathways responsible for energy materials evolution over lifetime. We propose a paradigm shift towards mesoscopic evolution modeling, based on physical and statistical models, that would integrate laboratory studies and real-world massive datastreams into a stress/mechanism/response framework with predictive capabilities. These epidemiological studies encompass the variability in properties that affect performance of material ensembles. Mesoscopic evolution modeling is shown to encompass the heterogeneity of these materials and systems, and enables the discrimination of the fast dynamics of their functional use and the slow and/or rare events of their degradation. We delineate paths forward for degradation science.



## 1. Introduction

Energy materials are essential in our modern world and are expected to have useful lifetimes that extend from 25 to greater than 50 years. The need for long lifetimes and large investments are barriers that new energy producing technologies must be surmounted if they are to provide a substantial proportion of global energy. These challenges were made evident by the Li-ion batteries in the Boeing 787 that were predicted to short circuit only once per 10 million flight hours [1–3]. Two adverse events grounded the whole fleet within four months of introduction, which was three orders of magnitude greater events than estimated. We know much about the synthesis, properties, and function of energy materials, but we do not yet know how to address the fundamental degradation science of energy materials under real-world conditions and time spans.

Since the first large testing of crystalline silicon photovoltaics (PV) module's reliability 40 years ago, we have seen widespread global adoption. The first 5 MW PV power plant, developed in the 1970s as part of the DOE Block Grant Program, was predicted to have a 20 year lifetime. The site power decreased 10× faster than the predicted rate and the failed plant was decommissioned after only 5 years [4]. Degradation-induced failures have been an ongoing characteristic of new and promising PV cells [5,6] and other energy materials even as producers continue to offer 25-year warranties.

The science of degradation of energy materials over time frames longer than >1 Gs (31.7 years) is a fundamental challenge of mesoscale science [7,8] and a transformational opportunity for energy

* Corresponding author at: White 536, 10900 Euclid Ave., Case Western Reserve University, Cleveland, OH 44106, United States. Tel.: +1 302 468 6667.
*E-mail address:* roger.french@case.edu (R.H. French).
[1] Equal contributing authors.

http://dx.doi.org/10.1016/j.cossms.2014.12.008
1359-0286/© 2015 The Authors. Published by Elsevier Ltd.

materials, for the following reasons. Realistic degradation studies face the same data and modeling challenges as in medicine, sociology or climate science, where "models and observational data together form an inseparable basis for scientific understanding and prediction" [9,10]. Degradation of energy materials distinguishes itself in that it evolves over long time-frames due to a multitude of distinct, complex, and interacting mechanisms that can lead to a variety of slow and/or rare events that eventually cause failure. There are severe knowledge gaps in identifying, modeling, and *reliably* predicting the mesoscopic evolution that produce degradation, and in *establishing an effective monitoring system* of the evolving process of degradation over the relevant timescales to prevent failures (especially catastrophic failures). It is essential to connect the mechanistic degradation pathways and their temporal evolution at the mesoscale so as to enable the identification of improved and longer-lived energy materials in real life. *Hence, the new degradation science examines degradation of a material or system, guided by real-world or realistic outcomes, whose fundamentals include modeling, monitoring, and prediction of a degradation process, as well as intervention, feature selection, and optimization aimed at improvement of materials and reduction of system failures*. A *new interdisciplinary approach to degradation science calls for the involvement of materials science, physics, chemistry, statistics, computer science, engineering, and energy industries in the investigation of real-world degradation of energy material over their lifetimes.* After reviewing current PV energy materials research approaches (Section 2) we shall illustrate how this should be done (Section 3), what has been done recently (Section 4), and what challenges and new directions lie ahead (Section 5).

### 1.1. Advances in nanoscience and data science

There have been transformative advances which provide the foundations for a new degradation science. First is the multitude of advances in nanoscience from the scientific community and, from the broader world, advances in computers, communication, and computation.

Since the National Nanotechnology Initiative in 2000 [11], there has been tremendous progress including detailed understanding of science at the nanometer scale and from the femto- to attosecond scale [12,13]. Fundamental advances in glasses [14], nanoscale materials [15–18], interactions [19], fabrication and assembly [20–24], and systems [25–28] have ensued. A detailed understanding of the basic nanoscience that underpins the beneficial function of energy materials provides the *first building block* of degradation science.

Within nanoscience, multi-scale modeling of materials [29] which connects microscopic/atomistic mechanisms with higher level, coarse grained, mesoscopic and even macroscopic models [30–34] helps us understand the fundamental origins of the *physical* properties of materials. This multi-scale modeling research has focused on spanning length scales underpinning the effective parameter passing approach, linking atomic scale behavior to experimentally determined macroscopic properties. The Materials Genome Initiative [35,36] is an example of accelerating materials discovery modeling at the micro- and mesoscopic levels to guide the experimental synthesis of new materials [37].

Still, multi-scale modeling has not elucidated the range from femto- to gigaseconds needed to provide fundamental guidance on the mesoscopic evolution of materials and their long term degradation in function and properties. For this challenge, we start with newly available data from large and diverse experiments. These varied datasets provide important information to fit appropriate *physical* and *statistical* models and identify the fundamental mechanisms of energy material degradation. These are then incorporated into a network model of their mesoscale evolution over lifetime. As nanoscience and multi-scale modeling advance, they will continue to provide mutual benefit by illuminating fundamentals and identifying critical contributors and effects.

The tremendous advances in computation and communications [38] and open access, code and data manipulation [39–45] over the past ten years are a *second building block* for the opportunities in degradation science. Distributed computing [46–48] improved Internet connectivity and mobility. The ubiquity of sensors make for unprecedented big data streams which can be utilized for experimental studies of energy materials in the laboratory and in real-world conditions [49]. Data science has grown beyond the purely computational advances which have been the focus of science (e.g., high performance computing). With increased data volumes and variety and the associated advances in informatics for petabyte scale analysis, it is now possible to study large populations of real (as opposed to idealized or simplified) energy materials under real-world conditions and over very long time frames. These epidemiological or population-based studies can complement our traditional small sample size, laboratory-based experiments, providing additional statistically sound information to bridge the 24 orders of magnitude in time required for femto- to gigasecond science.

### 1.2. Temporal evolution of mesoscopic energy materials

The Materials Genome Initiative and advances in nanoscience have allowed nascent energy materials to be developed; however, a predictive framework for those materials properties over time in real-world applications is lacking. For example, there is much research on new batteries and improved storage capacity for applications in electronics, transportation, and grid [50], yet degradation science must be applied to understand the contributing factors that limit the number of charge cycles and the basic mechanisms and pathways that lead to end-of-life failures [17].

Functional energy materials are complex materials with homo- and heterogeneous interfaces and substantial variances among samples in a population. By virtue of their energy function, they are non-equilibrium systems with cyclic operating conditions and stressors and thus have high spatio-temporal complexity. For energy applications spanning the time domain from femto- to gigaseconds, a new approach is needed that can distinguish the large dynamics of function from the slow/rare events of degradation and their differing temporal regimes. For example, damage initiation, accumulation, and growth will eventually lead to a transition such as a sudden precipitation or a possible bifurcation into a new regime. Similarly, environmental conditions, as encountered in permafrost or desert or given by daily or annual cycles of the seasons, can produce results quantitatively different from a well controlled laboratory-based study. To understand the degradation significance of each of the heterogeneous aspects of materials and devices across populations and characteristic time scales, all respective data needs to be accessible to scientific inquiry. The focus of this research is the development of mesoscopic-evolution network models which integrate *physical* and *statistical* models phenomena. These network models, exemplified in Fig. 1 for poly(methyl methacrylate) (PMMA) acrylic, link micro- and mesoscopic degradation in order to understand the stressor/mechanism-mode/responses of the PVs in real-world use over their lifetime.

## 2. Current PV energy materials research approaches

Three distinct communities (scientist, engineers, owners/operators) with distinct goals have worked in research and development of energy materials. Scientists typically pursue laboratory-based research topics related to materials performance. Engineers seek