

Unraveling Hierarchical Materials using Autonomous Research Systems

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Nature realizes extraordinary material properties through the hierarchical organization of polymers from the molecular to the macroscopic scale. Synthetically recapitulating this level of control has been a long-standing challenge as it requires mastery of each scale and an understanding of how to piece these levels together. In this talk, we describe our recent progress studying hierarchically structured polymers. Initially, we discuss our efforts to understand the nanomechanics of polymer films through an approach that combines finite element analysis and nanoindentation. We find that elastomeric thin films are stiffer than bulk samples in a manner that agrees with a newly proposed surface crosslinking model. While this level of understanding is important, there are too many distinct material classes, compositions, and processing conditions that can be chosen to tease out general truth using this conventional approach. Thus, new experimental paradigms are needed. To this end, we discuss the degree to which experimental research can be accelerated through the combination of automated experimental systems and machine learning to choose experiments. To explore the merits of such autonomous experimental systems, and study the mechanics of macroscopically structured polymers, we present a Bayesian experimental autonomous researcher that combines additive manufacturing, robotics, and mechanical characterization to rapidly print, test, and study mechanical structures. Using this platform, we study the elastic and plastic mechanics of polymer structures. In addition to developing an understanding of a family of mechanical structures, these experiments provide important lessons regarding how machine learning and automation can accelerate experimental research and mechanical design. Looking forward, we aim to combine this autonomous research framework with our recent efforts to use scanning probes to create and interrogate nanoscale libraries of polymers. Ultimately, understanding and leveraging the hierarchical arrangements of materials is a grand challenge. Autonomous research systems that span additive manufacturing, machine learning, and advanced characterization have the potential for transformatively advancing the pace of research to meet this challenge.

Dr. Keith A. Brown is an Assistant Professor of Mechanical Engineering, Materials Science & Engineering, and Physics and the Moorman-Simon Interdisciplinary Career Development Professor at Boston University. He earned a Ph.D. in Applied Physics at Harvard University under the guidance of Robert M. Westervelt and an S.B. in physics from MIT. Following his doctoral work, he was an International Institute for Nanotechnology postdoctoral fellow with Chad A. Mirkin at Northwestern University. The Brown group studies polymers and smart fluids to determine how useful properties emerge from hierarchical structure. A considerable focus is developing approaches that increase the throughput of materials research using scanning probe lithography, machine learning, additive manufacturing, and combinatorial chemistry. Keith has co-authored 64 peer-reviewed publications, five issued patents, and his work has been recognized through the reception of awards including the Materials Science and Engineering Innovation award from Boston University, the Omar Farha Award for Research Leadership from Northwestern University, as a “Future star of the AVS,” the AVS Nanometer-Scale Science and Technology Division Postdoctoral Award, and the National Defense Science and Engineering Graduate (NDSEG) Fellowship. Keith is currently serving on the *Nano Letters* Early Career Advisory Board and has organized symposia at the AVS International Symposium and at the MRS Fall Meeting.