Carnegie Mellon
Materials Science and Engineering Seminar Series

John Kieffer

Department of Materials Science and Engineering
University of Michigan

"Combining Experiments and Computation in Materials Research"

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10 A.M. Seminar in Baker Hall 136A

Over the past two decades computational science has evolved into a paradigm-changing research approach. In this time, computer speed has increased nearly a million fold, while the new algorithms and numerical methodologies that have been developed facilitate more accurate simulations and more efficient data exploration. This progress has had a profound impact on materials research, advancing computation to a tool for the design and discovery of novel materials that is on par with experimental characterization and measurement techniques. In this presentation I will give a brief historical overview and outlook with regards to the role of computation in science and engineering, and then present two examples from our own research illustrating the use of materials simulation. The first example pertains to the unveiling of the nature of anomalous thermo-mechanical properties of network glasses, i.e., the increase of the elastic modulus upon heating, its decrease upon compression, negative thermal expansion, etc. Using molecular dynamics (MD) simulations we generated glass structures in which the experimentally observed thermo-mechanical behaviors were reproduced and then analyzed the structure and dynamics of these configurations for the mechanisms that underlie these anomalous properties. We discovered that this behavior is universal to all major network glasses, and predicted the existence of previously unknown crystalline phases in common oxides. The second example, describes the investigation of the cure kinetics of cross-linked polymer systems. In this context we use concurrent Brillouin and Raman scattering to measure the complex mechanical modulus at the molecular level and monitor the structural evolution of the polymer network in situ as the reaction progresses. We use density functional theory (DFT) calculations to assign Raman peaks to the vibrational modes of the chemical species present. Using MD simulations we generate realistic structural models of the polymer networks by reproducing the underlying reaction and transport processes and predict their mechanical properties. By comparing experimental data and simulation results, we gain new insights into the complexity of the reactions that lead to the network formation and the relationship between the network topology and its mechanical properties.

John Kieffer is a Professor of Materials Science and Engineering. He received his M.S. in Metallurgy and his Ph.D. in Materials Science from Clausthal Technical University in Germany. He was a postdoctoral research associate at the Arizona State University in Solid State Science and at Purdue University in Physical Chemistry. After a brief industrial experience at Saint-Gobain Recherche in Paris, France, he became a faculty member at the University of Illinois in Materials Science and Engineering, where was for 12 years before coming to the University of Michigan in 2001. Kieffer's research interests include the (i) computational design of materials for energy applications, such as photovoltaics, fuel cells, and batteries, (ii) amorphous materials for optical and photonics applications, and (iii) thermal and mechanical properties of interfaces between dissimilar materials. He carries out both computational and experimental research. He is a Fellow of the American Ceramic Society and received the George W. Morey Award from the Glass and Optical Materials Division of the same society in 1999. As educator, Kieffer created several new courses, emphasizing the integration of computation and virtual experimentation with knowledge-based learning. He received the Amoco Award for Innovation in Undergraduate Instruction in 1992. Kieffer is active in stewardship of the materials science community by holding offices in professional societies. He served as Chair of the Amorphous Materials Special Interest Group of the American Crystallographic Association (1997-98); as Secretary (2000-03) and as Chair (2004-05) of the Glass and Optical Materials Division of the American Ceramic Society. He regularly organizes conference symposia at annual meetings of the Materials Research Society, the American Ceramic Society, and the American Crystallographic Association. He organized and directed the Annual Conference on Glass Problems at Illinois for 12 years.