AJIT K ROY - AIR FORCE RESEARCH LABORATORY

BOTTOM-UP COMPOSITES MATERIALS

DESIGN FOR MULTIFUNCTIONALITY

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ABSTRACT

There are ample of evidence of materials hybridization at scale, even in nature, yields optimal respond to specific functions. In structural materials, hierarchical materials hybridization accounting for defects or porosity would offer optimal performance at reduced materials mass. Similar thought process goes for other performance functionalities, thermal, electrical, dielectric, etc. Materials hybridization, core to composites materials design, offers unprecedented design space for optimizing structural system and product performance. The atomic-scale materials hybridization, analogous to pointwise material optimization, is arguably the ultimate materials morphology optimization goal. Advent of multiscale (atomic to continuum) materials modeling, associated with evolving reliable materials characterization techniques, appears convincingly promising for atomic-scale hybrid materials design and development. Success in integrating the atomic scale materials performance attributes to higher domain (both in temporal and spatial scale) computational tools, such as density functional theory (DFT), Atomistic Molecular Dynamics (MD), tight-binding DFT, mesoscale Monte Carlo, Boltzmann Transport, Molecular Mechanics (MM), etc., shows early promise in this endeavor. In this presentation, examples of atomic scale hybrid material design unlocking specific performance goal, including concurrent multifunctional response, will be presented.

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BIO

Dr. Roy is a Computational Group Leader at the Materials and Manufacturing Directorate at AFRL. His research area is on materials innovations and development in structural, thermal, and electronic materials. His focus is in integrating multiscale computational methods to materials processing for accelerated materials development and technology transition. He pioneered carbon foam technology and nano-porous carbon as multifunctional materials for coatings, flexible electronics, and battery electrodes. His durable thermal interface concept transitioned to commercial product. He has over 28,000 Google citations of his published work, is a recipient of ASC Outstanding Research Award, Fellow of AFRL, AIAA, ASME, and ASC, and serves in journal editorial boards, and advisory panels. He received his Ph.D. in engineering mechanics from University of Minnesota in 1985.