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SOME KEY ISSUES IN MULTISCALE MODELING OF MULTIFUNCTIONAL POLYMER NANOCOMPOSITES/COMPOSITES

Key issues in the development of a multiscale modeling strategy for multifunctional polymer composites and nanocomposites are addressed. Molecular dynamics (MD), computational micromechanics, and global finite element simulations are proposed, within an Integrated Computational Materials Engineering (ICME) framework, to determine composite material behavior from the molecular to global structural scales. Novel MD calculations were performed to investigate carbon nanofiber/matrix interphase formation and interfacial properties in thermosetting nanocomposites. Such properties are highly sensitive to the equilibrium redistribution of liquid resin monomers in the vicinity of the nanofiber surface prior to cure. An innovative crosslinking algorithm has been developed that accounts for key aspects of free radical polymerization. After crosslinking, MD nanofiber pullout simulations were performed to determine nanocomposite interphase properties and interfacial strengths for use in higher length scale models. Materials property data generated using MD simulations can feed directly into higher length scale micromechanical calculations. Modified versions of the Mori-Tanaka and self-consistent micromechanical models were developed to predict the effective elastic moduli and thermal/electrical conductivities of composites containing multiple distinct nanoheterogeneities (fibers, spheres, platelets, voids, etc.) each with an arbitrary number of coating layers. Predicted properties matched experimentally measured values for vapor-grown carbon nanofiber/polypropylene, exfoliated graphite flake/epoxy, glass micro-sphere/ polystyrene, cupric oxide sphere/epoxy, aluminum sphere/epoxy, and other composites. The homogenized properties for nanoreinforced materials may be readily implemented within a temporally concurrent, spatially sequential multiscale analysis framework using the NASA Micromechanics Analysis Code with the Generalized Method of Cells coupled with the ABAQUS finite element solver. This framework may be also used to account for the effect of statistical variations in material properties (e.g., continuous fiber strengths) on global structure failure. Progressive failure analyses can be performed that aim to establish structure-property relationships over a wide range of length scales, which account for the morphologies and geometries of real heterogeneous materials. Such analyses will facilitate development of a damage tolerance plan for multifunctional composites that accounts for loss of structural integrity as well as degradations in relevant aspects of multifunctionality associated with discrete source damage and in-service loadings.

Dr. Thomas E. Lacy Jr. received his Ph.D. in Mechanical Engineering from the Georgia Institute of Technology. He joined the J. Mike Walker '66 Department of Mechanical Engineering at Texas A&M as a Professor in 2018. He worked for nearly ten years as a practicing aerospace engineer. Dr. Lacy teaches graduate and undergraduate courses in solid mechanics and materials/structures. His research focuses on multifunctional composite materials for extreme environments, multiscale modeling, hypervelocity impacts, aerospace structures, computational solid mechanics, and durability and damage tolerance. Dr. Lacy has published 62 refereed journal articles, two book chapters, 59 conference proceedings, and over 25 technical reports in these areas and has been recognized for his contributions to both teaching and research. He received a 2009 SAE Ralph R. Teetor Educational Award and was selected to Who's Who Among America's Teachers and Who's Who in Engineering Education. Dr. Lacy has received a number of university-level awards for outstanding teaching, is a member of the Mississippi State University (MSU) Bagley College of Engineering (BCoE) Academy for Distinguished Teachers, received a 2012-2013 MSU Faculty Leadership Award, and won the 2017 MSU BCoE Outstanding Researcher Award. He has received over $3.5M dollars in external research as PI from the DoD, FAA, NSF, Boeing, and other sources. Dr. Lacy chaired 13 doctoral and 12 masters committees, and currently advises 11 graduate students. He served as a scientific advisor to Golf Digest magazine. Dr. Lacy is a fellow in the American Society of Mechanical Engineers and is an associate fellow in the American Institute of Aeronautics and Astronautics. Dr. Lacy is a member of the Sigma Gamma Tau National Aerospace Engineering Honor Society and is a founding university partner/ collaborator with the NASA Glenn Multiscale Analysis Center of Excellence. While at MSU, Dr. Lacy served as interim Head of the Department of Aerospace Engineering (2013-2016) and Chief Technology Officer in the Advanced Composites Institute (2018).

Interests: multifunctional composite materials for extreme environments, multiscale modeling, hypervelocity impacts, durability and damage tolerance