

## **Materials Data Sciences and Informatics: An Emerging New Discipline for Accelerated Design, Development, and Deployment of Advanced Materials**

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Georgia Institute of Technology  
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### Abstract

A majority of the materials employed in advanced technologies exhibit hierarchical internal structures with rich details at multiple length and/or structure scales (spanning from atomic to macroscale). Collectively, these features of the material internal structure constitute the central consideration in the development of new/improved materials. Although the core connections between the material's structure, its evolution through various manufacturing processes, and its macroscale properties (or performance characteristics) in service are widely acknowledged to exist, establishing this fundamental knowledge base has proven effort-intensive, slow, and very expensive for most material systems being explored for advanced technology applications. It is anticipated that the multi-functional performance characteristics of a material are likely to be controlled by a relatively small number of salient features in its hierarchical internal structure. However, cost-effective validated protocols do not yet exist for rapid identification of these salient features and establishment of the desired core knowledge needed for the accelerated design, manufacture and deployment of new materials in advanced technologies. The main impediment arises from lack of a broadly accepted framework for a rigorous quantification of the material's structure, and objective (automated) identification of the salient features that control the properties of interest. This presentation focuses on the development of data science algorithms and computationally efficient protocols capable of mining the essential linkages from large ensembles of materials datasets (both experimental and modeling), and building robust knowledge systems that can be readily accessed, searched, and shared by the broader community. The methods employed in this novel framework are based on digital representation of material's hierarchical internal structure, rigorous quantification of the material structure using n-point spatial correlations, objective (data-driven) dimensionality reduction of the material structure representation using data science approaches (e.g., principal component analyses), and formulation of reliable and robust process-structure-property linkages using various regression techniques. This new framework is illustrated through a number of case studies

### Bio

Surya Kalidindi is a Professor in the Woodruff School of Mechanical Engineering at Georgia Institute of Technology, Georgia, USA with joint appointments in the School of Materials Science and Engineering as well as the School of Computational Science and Engineering. Surya earned a Ph.D. in Mechanical Engineering from Massachusetts Institute of Technology in 1992, and joined the Department of Materials Science and Engineering at Drexel University as an Assistant Professor. After twenty years at Drexel University, Surya moved into his current position at Georgia Tech, where he also serves as the Lead MGI/ICME Strategist for Georgia Tech's Institute for Materials. Surya's research efforts have made seminal contributions to the fields of crystal plasticity, microstructure design, and materials informatics. Surya has been elected as a Fellow of ASM International, TMS, ASME, and Alpha Sigma Mu (Materials Honors Society). He has also been awarded the Alexander von Humboldt Research Award in 2013. In 2016, he and his group members have been awarded the top prize as well as one of the runner-up prizes in the national Materials Science and Engineering Data Challenge sponsored by the Air Force Research Lab in partnership with the National Institute of Standards and Technology and the U.S. National Science Foundation.