Virtual Models for Processing and Testing

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As computational models are being developed with improved fidelity for use as virtual experiments, opportunities arise for reducing the number of costly tests needed and for extending the design space to include material configurations and process conditions that are too complex to determine by purely empirical methods. In this talk, we highlight case studies where high-fidelity models for such virtual testing have been employed. For instance, we are developing a platform to predict the optimal process parameters for cold spray additive manufacturing. The validated and integrated multi-physics, multiscale computational model consists of a multiphase supersonic gas flow model and a multiscale micromechanics model to simulate bonding at the mesoscale for particle impact and subsequent coating formation at the continuum scale based on the Eulerian framework and continuum scale finite elements based on micromechanics and homogenization theory. Atomistic models studying the metallurgical bonding mechanism and the localized material behaviour at the bonding interface are presented. In another example of virtual testing, we will present mechanistic arguments for the locus of cracks that initiate and propagate among fine-scale, stochastic, heterogeneous material without executing explicit fracture mechanics simulations. Specifically, the usefulness of graph theoretic methods for analyzing micro-cracking in continuous fiber composites loaded transversely to the fiber direction is explored.