Spatial and Temporal Multiscale Models for Advancing the Integrated Computational Materials Engineering (ICME) Initiative

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The Integrated Computational Materials Engineering or ICME initiative entails integration of information across length and time scales for relevant materials phenomena. Computational Mechanics plays an important role in this integration. This talk will present an integration of methods in Computational Mechanics and Computational Materials Science to address the deformation and failure characteristics of polycrystalline metals in various applications. Specifically it will address physics based modeling at different scales along with multi-scale spatial (scale-bridging) and temporal modeling methods. Materials considered will be Titanium, Magnesium and Aluminum alloys, as well as Nickel base-superalloys. Spatial scales will range from atomistic to component levels, depending on the application. Application domains will include cyclic loading and address properties such as time and location-dependent ductility and fatigue life.

The talk will begin with methods of 3D virtual image construction and development of statistically equivalent representative volume elements for materials at multiple scales. Subsequently it will discuss the development of novel system of experimentally validated physics-based crystal plasticity finite element or CPFE models to predict deformation and micro-twinning leading to crack nucleation. It will discuss stabilized element technology for analyzing heterogeneous deformation problems. The CPFE simulations will provide a platform for the implementation of physics-based crack evolution criterion that accounts for microstructural inhomogeneity. For crack evolution, a coupled molecular dynamics-continuum model for a crystalline material with an embedded crack will be discussed. A wavelet transformation based multi-time scaling (WATMUS) algorithm for accelerated crystal plasticity finite element simulations will be discussed as well. The method significantly enhances computational efficiency in comparison with conventional single time scale integration methods.