COMPUTATIONAL MECHANICS IN ADVANCING THE INTEGRATED COMPUTATIONAL MATERIALS SCIENCE & ENGINEERING (ICMSE) INITIATIVE FOR METALS AND ALLOYS

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Focus Material: Metals, Composites,
Focus of the Presentation: Choose one.
(i) Physics-based multi-scale model development;

Abstract

The Integrated Computational Materials Science & Engineering or ICMSE initiative entails integration of information across length and time scales for materials phenomena. 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 and multi-scale spatial (scale-bridging) and temporal modeling methods for Titanium, Magnesium and Aluminum alloys and Nickel based-superalloys. Spatial scales will range from atomistic to component levels. Application domains will include both monotonic and cyclic loading and address properties such as time and location-dependent strength, ductility and fatigue life. The talk will begin with methods of 3D virtual image construction and development of statistically equivalent representative volume element 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. These 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 [1]. The method significantly enhances computational efficiency in comparison with conventional single time scale integration methods. Finally, stabilized element technology for analyzing this class of complex deformation problems will be discussed.

References

1. M. Anahid, M. Samal and **S. Ghosh,** "Dwell fatigue crack nucleation model based on using crystal plasticity finite element simulations of polycrystalline Titanium alloys ", *Journal of the Mechanics and Physics of Solids*, Vol. 59, pp. 2157-2176, August 2011.
