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Linking Computational Multiscale Failure Analyses to Advanced Diffraction Measurements

Abstract

Despite significant advances in material lifetime studies, previous works on fracture and fatigue typically rely on *ex situ* microstructural characterizations and crack growth monitoring with replica techniques. An *in situ*, nondestructive, neutron and synchrotron X-ray diffraction, together with the multiscale simulations, will provide us a linkage between the stress analyses (top-down point of view) to the failure mechanisms on inter- and intra-granular scales (bottom-up point of view). Here we present two examples illustrating the computational studies in uncovering the deformation and failure mechanisms in advanced alloys. First, the general deformation characteristics near a fatigue crack tip include a plastic zone in front of the crack tip and a plastic wake left behind, where the cyclic loading and fatigue crack growth lead to a compressive strain. The magnitude and distribution of the compressive strain in this plastic wake depend on the stress multiaxiality, material properties, and crack growth increment in each loading cycle. We compare lattice strain measurements by the neutron diffraction technique and simulations by an irreversible and hysteretic cohesive-interface model, which is developed to simulate the fatigue crack nucleation and growth. Crystal plasticity simulations have been conducted to relate the macroscopic and lattice strains. Second, computational challenges in developing high temperature alloys are identified. Inter- and intra-granular strains and load partitioning mechanisms are studied for a creep-resistant, ferritic alloy with NiAl precipitates. A particular advantage is the capability of conducting high-temperature multiaxial tests at the Spallation Neutron Source (SNS) at ORNL.

Biosketch

Dr. Gao is an Associate Professor of the Department of Materials Science and Engineering, University of Tennessee, and a Joint Faculty in Materials Science and Technology Division, Oak Ridge National Laboratory. His research group focuses on modeling and simulation of plasticity at small length scales, thin-film growth, contact and friction, and constitutive behavior of amorphous alloys, among many others. Most of these projects are motivated from his colleagues' experiments at UT and ORNL. Dr. Gao holds a B.S. in Engineering Mechanics and a B.S. in Computer Science from Tsinghua University, Beijing, China, and a Ph.D. in Mechanical and Aerospace Engineering from Princeton University. Prior to joining UT/ORNL in August 2005, he worked as a post-doctoral research associate in solid mechanics group, Brown University, on surface plasticity and adhesion, microstructural evolution, and structural integrity. He is author or co-author of more than 50 research papers in mechanics of materials and has given more than 60 presentations (20 invited) at national/international conferences and academic institutions.