UCI Samueli School of Engineering

Department of Materials Science and Engineering UCI

UNIVERSITY OF CALIFORNIA, IRVINE

DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING

SPECIAL SEMINAR

HOST: LORENZO VALDEVIT

DEFORMATION AND OXIDATION BEHAVIOR IN HIGH TEMPERATURE STRUCTURE ALLOYS

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Friday, September 20, 2024

11:00 AM - 12:00 PM

Engineering Tower, Conference Room 652

Abstract: Computational tools for materials discovery and design have in the past decade been extensively developed to study a wide range of properties. This talk will focus on two examples of such use cases. In the first example, we will show our recent results on the integration between thermodynamic calculations, first-principles modeling, machine learning, and experimental validation of mechanical properties and oxidation resistance in refractory complex, concentrated alloys (RCCAs). We will present a new machine learning for accelerated materials discovery (ML-AMD) framework that utilizes multi-fidelity and multi-cost experiments with physics-based modeling. New semi-high-throughput methods for characterizing hardness and oxidation resistance will be presented, and methods for implementing high-throughput simulations into the ML-AMD framework will be expounded. Promising alloys will be identified, and strategies for improving the oxidation resistance of RCCAs will be discussed. In the second example, we show how calculation of the generalized stacking fault energy (GSFE) surface can be used to predict deformation in a novel -Ni2(Cr,Mo,W)-strengthened superalloy, Haynes® 244®. Owing to its lower symmetry, the phase presents itself as 6 different orientation variants coherently embedded in the disordered FCC matrix and exhibits two close-packed planes and three unique deformation pathways. We show that the combination of these characteristics leads to the formation of microtwins at temperatures and strain rates ranging from 23 – 760 °C and 10-3 – 10-9 s-1, respectively. These results suggest that new structural alloys could be designed with unique precipitates that enable favorable deformation mechanisms for improved ductility and work hardening over a wide range of temperatures.

Bio: Prof. Michael Titus is a tenured Associate Professor and Technical Director of the Purdue Heat Treating Consortium at the School of Materials Engineering at Purdue University in West Lafayette, IN, USA. Prior to joining Purdue University in 2016, he earned his B.S. in Engineering Physics at The Ohio State University, 2010 and Ph.D. in Materials at the University of California Santa Barbara, 2015. From 2015 to 2016 he was an Alexander von Humboldt Postdoctoral Fellow at the Max Planck Institute for Iron Research in Dusseldorf, Germany. Prof. Titus Prof. Titus is the recipient of the NSF CAREER award (2018) and many professional society awards including the TMS SMD Young Leaders Professional Development Award (2017), TMS-JIM Young Leaders International Scholar (2020), and the ASM Bradley-Stoughton Award for Young Teachers (2021). He has co-authored over 35 peer-reviewed publications, has supervised 10 Ph.D. and Masters thesis students, and is currently advising 10 Ph.D. students. Prof. Titus' research has focused on elucidating fundamental deformation mechanisms in high temperature Ni-based superalloys, shape memory alloys, and refractory alloys using a combination of first-principles and thermodynamic theory and computational tools integrated with high-resolution experiments. Additionally, he has focused on improving the oxidation resistance of refractory alloys through machine learning-guided alloy design and discovery using a combination of multi-fidelity experiments and computational tools. Other research interests include improving performance of environmental barrier coatings through optimized heat treatments, recycling and rejuvenation of additive manufacturing metal alloy powder, and improving turbine engine components through coupled material-topology optimization.

Michael Titus Purdue Homepage -
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