

## IMAGE-BASED COMPUTATIONAL MODELING OF TITANIUM ALLOYS

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### ABSTRACT

The end-objective of this research is to identify critical microstructural features in metals such as grain morphology or crystallographic orientation mismatch between grains that may precipitate plastic flow, and therefore, cause degradation of mechanical performance at higher scales. The material focus is a titanium alloy— 21s. The three-dimensional (3D) microstructure in the mesoscale range was obtained using serial sectioning, optical microscopy, electron backscatter diffraction (EBSD) and computerized 3D reconstruction techniques. The reconstructed volumes provided information on morphology and crystallography for hundreds of beta-Ti grains; however, computational cost restricted modeling to a smaller number. This data was used as input into 3D finite element models to analyze the spatial evolution of state variables, such as stress, strain and crystallographic slip under simple loading conditions. Single crystal hypoelasticity and the assumption of only resolved shear stress causing crystal slip were used to represent microstructural material behavior. In the preliminary analysis of result data, some of the grain boundary interfaces where most plastic flow occurred were identified while work continues to establish definite structure-property relationships. Rendering of large reconstructions (hundreds of grains) into faithful but lean finite element meshes was recognized to be the critical issue in simulating accurate material behavior near grain boundaries, establishing definite structure-property relationships at mesoscale and reducing the computational cost.