# NUMERICAL MODELING OF Ti-6Al-4V MICROSTRUCTURE EVOLUTION FOR THERMOMECHANICAL PROCESS CONTROL

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## Abstract

Microstructure evolution modeling using finite element crystal plasticity (FECP), Monte-Carlo (MC), and phase field (PF) methods are being used to simulate microstructure evolution in Ti-6Al-4V under thermomechanical loading conditions. FECP is used to simulate deformation induced evolution of the microstructure and compute heterogeneous stored energy providing additional source of energy to MC and PF models. The MC grain growth model, calibrated using literature and experimental data, is used to simulate $\alpha$+$\beta$ grain growth. A multi-phase field, augmented with crystallographic symmetry and orientation relationship between $\alpha$-$\beta$, is employed to model simultaneous evolution and growth of all twelve $\alpha$-variants in 3D. The influence of transformation and coherency strain energy on $\alpha$-variant selection is studied by coupling the model with the Khachaturyan-Shatalov formalism for elastic strain calculation. This FECP/MC/PF suite will be able to simulate evolution of grains in the microstructure and within individual $\beta$-grains during typical thermomechanical processing conditions.

## 1. Introduction

Ti-6Al-4V is a dual-phase alloy, used mainly in aerospace and biomedical applications owing to its high specific strength, excellent high temperature properties, and corrosion resistance. In support of the Materials Genome Initiative, a collaborative effort combining simulation, experiments, and feedback control has been created to inform process design and control. An adaptive microscale simulator is being developed to examine the relationship between thermomechanical processing conditions and microstructure evolution. MC, FECP and microelasticity theory augmented PF simulation methods together with experimental observations will inform the process control algorithm. This approach allows for real-time control of microstructure using a scanning electron microscope with an in situ heating and tensile testing stage coupled with the use of feedforward and feedback control. Here, we present the modeling part of this effort.

## 2. Methodology

### 2.1. Overview

Fig. 1 shows the overall modeling approach. Microstructure images taken prior to the application of thermomechanical load are used to detect grain boundaries which are then used to create a model of the microstructure. FECP simulations are performed on the mesh generated from this model to simulate deformation induced evolution of the microstructure and compute heterogeneous stored energy, input to MC and PF models. A MC method, one of the most widely used methods to simulate grain growth in metals, is calibrated using literature data, to predict temperature driven grain structure evolution and to simulate BCC $\beta$-phase grain growth. Within an individual $\beta$ grain, the evolution is modelled using the phase-field model. The resulting predicted microstructures will be compared to directly observed microstructures to refine and determine the accuracy of the models.

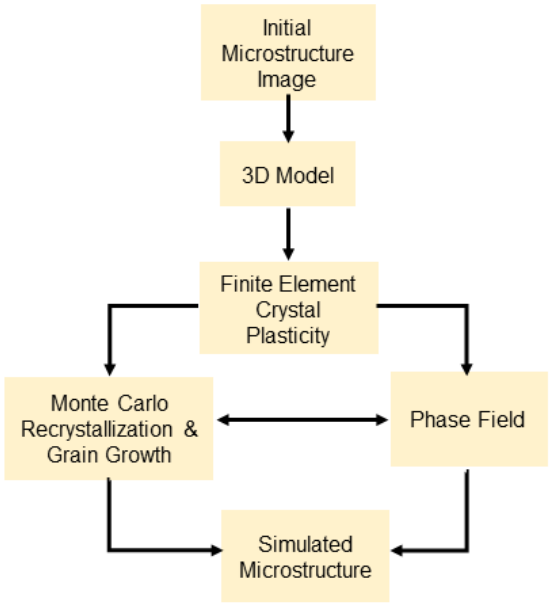



*Figure 1: Flow Chart explaining flow of information during the numerical simulation process.*

### 2.2. Finite Element Crystal Plasticity

A finite deformation crystal elastic-plastic constitutive model governs the mechanical behavior and its evolution implemented into a 3D parallel finite element framework following the work of Maniatty et al. [1]. The model starts with a multiplicative decomposition of the deformation gradient, into elastic and plastic parts. The elastic behavior is modeled assuming a linear, anisotropic relationship. The plastic deformation is associated with slip on the slip systems. The rate of shearing is related to the resolved shear stress on the slip systems through a power law, and the resistance to slip (hardening) evolves according to a Voce-Kocks model.

### 2.3. Monte Carlo Grain Growth

In this work, we use a MC method based on the Potts model, where a scaling relationship is established between the non-dimensional MC model and the physical dimensions of time, space and temperature, following earlier work by Tan et al. [2]. Based on this scaling relationship, the MC simulation is calibrated to the physical model, allowing for variations in the temperature field, in space and time, to be considered when modeling grain structure evolution.

### 2.4. Phase Field

A multi-phase field formalism is adopted to model the nucleation and growth of all unique

α-variants from a $\beta$ matrix. The multi-phase formalism is designed based on the model of Toth *et al*. [3]. The free energy functional for the model consists of three components. $F_{chem}$ contains the chemical free energy of the system, that includes the bulk free energies and the chemical interaction energies. $F_{int}$ contains the gradient energy penalty imposed on sharp interfaces. $F_{strain}$ contains the strain energy that arises as a result of the solid-state phase transformation from $\beta$ to α. The multiphase field model has been augmented with the microelasticity theory of Khachaturyan [4].

## 3. Preliminary Results

### 3.1. Finite Element Crystal Plasticity

The FECP approach is first tested on a simpler material system, pure Ni with a columnar grain structure (fig. 2), simulating 2% tensile strain.

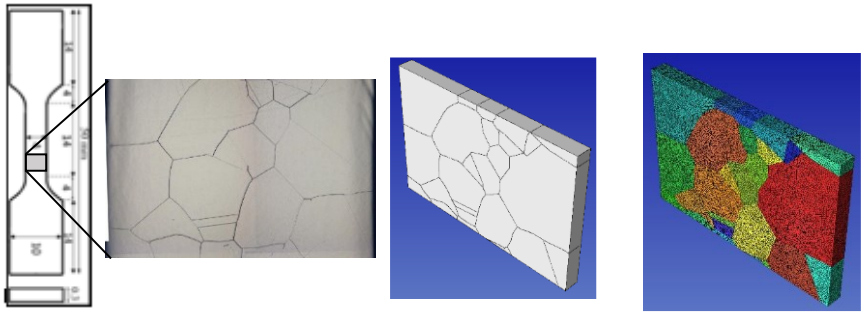


*Figure 2: Sample dimensions, microstructure (source: [5]), 3D model and mesh.*

Simulated macroscale tensile stress vs strain as well as local strains near the triple junctions will be compared with the experimental results produced by Li [5] to validate the accuracy of the CPFE model. A preliminary macroscale stress-strain calibration result is presented in fig. 3(a). Work is underway on simulating and comparing the microscale strains to measured local strains.

### 3.2 Monte Carlo Grain Growth

Ti-6Al-4V $\beta$-phase grain growth, in the early stages, follows closely the parabolic grain growth law for the average grain size $\overline{D}$ from initial average grain size $\overline{D}_0$

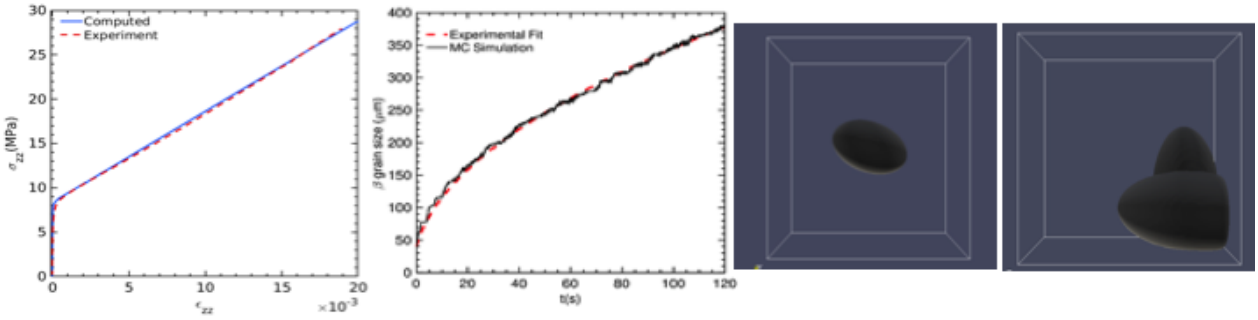
$$\overline{D}^2 - \overline{D}_0^2 = Kt\, exp(-Q/RT) = \lambda^2 C t_{mc}$$

where, the middle part of the equation relates the grain growth to physical time $t$ and temperature $T$, and the right side relates to the MC lattice spacing $\lambda$ and step $t_{mc}$. By equating the average grain size in the physical growth law to that in the MC growth equation, we can relate the MC step, $t_{mc}$, to the physical time $t$ and temperature $T$ [2]. Results at 1088°C [6] are shown in fig. 3(b).

### 3.3. Phase Field

Nucleation and growth of all 12 unique α-variants have been simulated by incorporating the crystallographic symmetry and the orientational relationship between the two phases. This relationship is reflected in each variant having a distinct eigenstrain associated with it. An example of isolated anisotropic growth of a variant within a α matrix is shown in fig.

3(c). Figure 3(d) shows the simultaneous growth of two variants with different eigenstrains, modeled with the multiphase formalism.




(a) (b) (c) (d)

*Figure 3: (a)Stress-Strain fit for dominant crystal orientation with Ni experimental data [5] and (b) Grain growth simulation fit to the experimental data [6] for Ti-6Al-4V at 1088°C. (c) Isolated growth of one $\alpha$-variant from the $\beta$ matrix. (d) Growth of two variants with different eigenstrains, multiphase formalism.*

## 4. Future Work

Work on defining a FECP formulation for Ti-6Al-4V, calibrating MC for $\alpha$+$\beta$ growth below $\beta$-transus, and developing a multi-phase PF formalism to model the influence of processing conditions on the strain-driven preferential variant selection of $\alpha$ variants or lack thereof are underway with the goal of developing an FECP/MC/PF suite.

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