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Initializing type-2 residual stresses in crystal plasticity finite element simulations utilizing high-energy diffraction microscopy data

Kartik Kapoor, Michael D. Sangid*

School of Aeronautics and Astronautics, Purdue University, West Lafayette, IN 47907-2045, USA

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ABSTRACT

Crystal plasticity finite element models have advanced in recent years by increasing their fidelity via incorporating physically based deformation mechanisms and more realistic microstructures. In order to better understand their effectiveness, researchers have looked at comparing their results with that of experiments at the grain level. In most of these efforts, the importance of incorporating initial residual stresses, representing the true grain morphologies, and imposing correct boundary conditions, which may have a significant effect on the results, is often overlooked. This work utilizes an available dataset of high-energy X-ray diffraction microscopy experiments conducted on a titanium alloy, Ti-7Al, providing complete grain averaged elastic strain tensors to investigate these three issues in crystal plasticity models. In this study, a method to initialize grain-level residual stresses is formulated and its effect on the correlation of results between simulations and experiments, is evaluated. The effect of grain morphology on the simulation results is evaluated by comparing results from simulations using exact 3D grain morphology with that of simulations using tessellated grain structures. In addition, the importance of applying physically realistic boundary conditions, obtained directly from experiments is also investigated. The findings of this work indicate that initial residual stresses and physically realistic boundary conditions play a key role in the results obtained from CPFE simulations and it is imperative that more importance is given to them. On the other hand, using exact grain morphology is not of much benefit while comparing data on the grain averaged scale as long as the microstructure contains information about the position of the grains, as is the case with tessellations, although grain morphology plays an important role in predicting intragranular strain localization.

1. Introduction

Crystal plasticity finite element (CPFE) models have existed for quite some time, with one of the first implementation of crystal plasticity into finite elements (FE) being carried out in the early 1990s by Beaudoin et al. [1] and Kalidindi et al. [2]. Since then, these models have undergone a large number of developments, especially in the past decade. A vast number of models have been developed and used for a wide variety of applications, which have been reviewed by Roters et al. [3]. Broadly speaking, the majority of these applications can be divided into two categories: processing models and models used to understand material behavior. In the case of processing models, most of the literature deals with texture evolution in a number of deformation processes, like in the case of [2,4–7]. On the other hand, there have been a number of CPFE modeling studies to understand material properties and their behavior [8–12]. One of the many notable contributions in this field has been to extend these models to understand fatigue and damage, including predicting fatigue crack initiation in a number of metals and their alloys [13–17]. These models can span from simple phenomenological to more complex ones, like those based on strain gradient approaches [18].

Even with the advancements in these models over the years, proper verification and validation is essential in order to trust the results obtained from them. One of the most reliable ways to validate these models is to compare their results to experiments at the length-scale relevant to the microstructure, i.e. at the meso-scale, and there exist studies in literature that have done so. A number of these studies focus on comparing surface strains, obtained from digital image correlation (DIC) to those extracted from CPFE simulations [13,19–21]. But in order to develop a better and complete understanding of how these models compare with experiments, it is helpful if 3D data, in the form of entire stress or strain tensors is utilized for these comparisons. In recent years, a few studies have utilized high-energy X-ray diffraction microscopy (HEDM) experiments [22–25], which are capable of providing entire tensorial quantities of elastic strains for comparison with simulations [26,27]. In addition, HEDM can provide complete initial residual stress tensors, which is not possible in the case of DIC.

* Corresponding author.
E-mail address: msangid@purdue.edu (M.D. Sangid).

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Researchers have improved the representation of the underlying physics of these models [28–30], found new means to identify the CPFE parameters [31–35], incorporated detailed information about the material [36], and used techniques to incorporate exact grain morphologies in CPFE simulations [26,37–39]' in order to get reliable results that match experiments. However, in most of these efforts, three critical pieces of information are often neglected: the effect of initial conditions like residual stresses, the nature of the boundary conditions (BCs) prescribed during the simulations and the representation of the physical microstructure used for the simulations. Most materials have a non-zero value of residual stress due to its processing, handling, and loading history. Even in materials that have been stress relieved or have undergone heat treatment, there will be some amount of residual stress present necessitating the need to initialize residual stresses. This is true especially in metals and alloys with a HCP crystal structure, as shown by Turner et al. [26], who find that grain level residual stress is not insignificant even in a sample of annealed Ti-7Al. This can be attributed to the fact that the thermal expansion coefficients of the HCP crystal are highly anisotropic [40], hence grain level residual stresses are induced due to thermal expansion and contraction during heat treatment.

Broadly speaking, residual stress may be classified into three categories based on the length scale in consideration as follows: Type-1, which is generally on the scale of components; type-2, on the grain averaged scale and type-3 at the sub-grain or intra-granular level [41,42]. This classification of residual stresses across different length scales is illustrated in Fig. 1.

A number of simulation studies focus on understanding residual stresses and a few even look at incorporating them into CPFE simulations. Turner and Tome [43] utilize an elasto-plastic self-consistent simulation procedure to estimate residual strains in Zircaloy-2 and compare it with neutron diffraction experiments. Musinski and McDowell [44] use an Eigen-strain approach (analogous to thermal deformation) to incorporate residual stresses induced as a result of shot peening. However due to the isotropic nature of these Eigen-strains, only type-1 residual stresses can be incorporated. McNelis et al. [45] introduce a method to estimate the macroscopic residual stress field in a component using high-energy X-ray diffraction experimental data. They utilize a FE framework with an optimization routine to fit the residual stress distribution in a workpiece by ensuring that the macroscopic traction BCs and equilibrium are satisfied, which are treated as constraints in their optimization routine. The objective in their optimization routine is to reduce the difference between the lattice strains obtained from simulations and X-ray diffraction experiments. This optimization technique offers a unique way to estimate the type-1 residual stress in a material, but the work does not analyze the effect of this initial residual stress on the stress state of the grains during loading. All aforementioned studies provide insights into incorporating residual stresses within simulations, however they do not establish a robust framework to incorporate type-2 residual stresses for a wide variety of conditions. An effort in this direction has recently been made by Pokharel and Lebensohn [46], who propose a method to initialize grain averaged residual stresses in their elasto-viscoplastic fast Fourier transform based crystal plasticity framework. They utilize an Eshelby approximation to get an Eigen-strain field which is then equilibrated using their CP simulations to obtain grain averaged residual stresses. The Eshelby approximation is then modified using a scaling matrix in order to impose residual stresses that match experiments (synthetic experiments in their case). This is a powerful formulation for incorporating residual stresses but cannot be implemented in a commercially available FE code. In more recent work, Chatterjee et al. [47] initialize pre-existing residual stresses in their crystal plasticity simulation of Ti-7Al loaded in tension superposed with bending. In this work, the microstructure is created from HEDM data. The authors incorporate residual stresses by initializing a geometrically necessary dislocation (GND) field in their phenomenological mesoscopic field dislocation mechanics model, which is derived based on the difference in the experimental and simulated bending stresses. They assess the effect of incorporating an initial GND field using two-dimensional manifold learning. Manifold learning is a method of non-linear data-reduction. Using manifold learning, large datasets (stress history of grains in this study) can be reduced to smaller (2D in this study) datasets, making them easy to visualize. This visualization is utilized to compare experiments with simulations. The authors observe that incorporating the initial GND field improves the manifold structure and point distribution (corresponding to the stress history of the grains), indicating improvement in the simulation results compared to the experiments. At this stage, one perceived approach is to simply incorporate residual stress by pre-straining individual grains within the simulation volume. However if this approach is utilized, due to the nature of the FE method, satisfying the equilibrium condition, the residual stresses will relax away. This further strengthens the need for a new formulation.

It is well known that BCs may have a significant impact on the results obtained from any type of FE simulation. Zhang et al. [38] mention that using an accurate 3D microstructure along with correct BCs, it is possible to estimate the stress tensor in the grains being simulated with some degree of confidence. However, in many studies, the BCs prescribed in a CPFE simulation are generic to describe a microstructure sub-element loaded in uni-axial (uniform) tension. Since most simulations involving comparison with experiments incorporate volumes that are a subset of the actual samples being experimentally tested, it is difficult to extract the exact BCs that will act on the simulation volume. There have been some efforts in this regard by Buljac et al. [48], who propose using digital volume correlation based on 3D synchrotron imaging to extract BCs to be supplied to their FE simulations. Nonetheless, without the assistance of experimental techniques, it

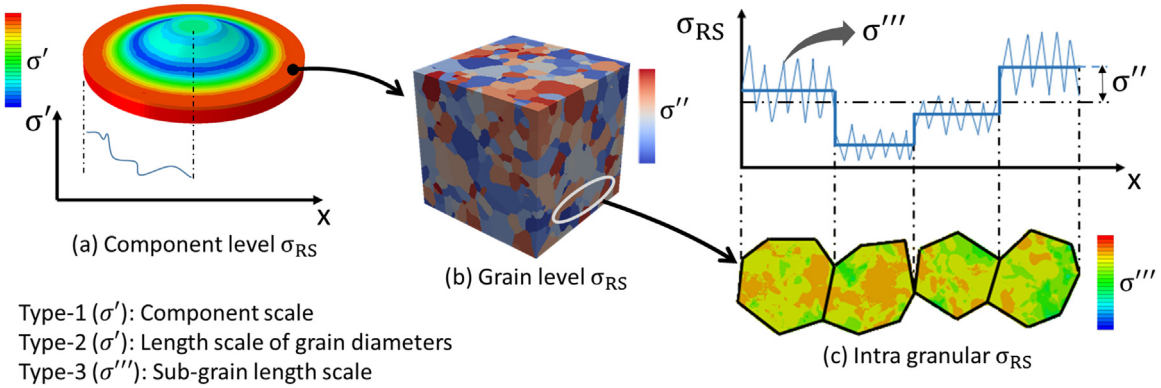

Fig. 1. Classification of residual stress based on length scale: (a) Variation of residual stresses on a turbine disc at the macroscopic scale; (b) grain by grain variation of residual stress at a point on the disc; (c) variation of residual stress within a set of individual grains (redrawn based on [42]).