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# Finite element modelling of dual-phase polycrystalline Nickel-base alloys

E.A. Bonifaz[a,b,*], J. Baus[a], A. Czekanski[b]

[a] Universidad San Francisco de Quito, Casilla Postal: 17-12-841, Circulo de Cumbayá, Quito-Ecuador
[b] Department of Mechanical Engineering, Lassonde School of Engineering, York University, Toronto, Canada

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ABSTRACT

A 3D finite element model was developed to simulate the influence of inclusions on the polycrystalline mechanical behavior of dual-phase Nickel-based alloys. A dislocation based strain hardening model, constructed in the so-called Kocks-Mecking framework, is used as the main strategy for the constitutive modeling of individual phases. To determine the influence of phase type, inclusion size, shape and distribution, on the inelastic stress-strain distribution, the digital microstructure code DREAM.3D was coupled to ABAQUS® code through a MatLab® program. Four dual-phase Representative Volume Elements (RVEs) of similar edge size but different inclusion size, morphology and distribution were tested to investigate the relation between micro and macro deformation and stress variables. The virtual specimens subjected to continuous monotonic strain loading conditions, were constrained with 3-D boundary conditions. A phenomenological approach is used to account for the effects of plastic strain gradients in hardening.The difference in crystallographic orientation, which evolves in the process of straining, and the incompatibility of deformation between neighboring grains were accounted for the evolution of geometrically necessary dislocation density, by the introduction of averaged Taylor factors, averaged Young´s modulus and single phase elastic limit. The effects of microstructural features upon the aggregate local response are clearly observed. Quantified results demonstrate a strong dependence of flow stress and plastic strain on phase type, inclusion size, shape and distribution. The results are in agreement with the expected output that the flow resistance is higher for structures composed of finer and homogeneously distributed inclusions.



## 1. Introduction

Polycrystalline materials (metals, alloys or ceramics) are commonly used in engineering applications ranging from delicate electronic components to very large structures in the nuclear and shipbuilding industries.Their microstructure is characterized by the topology, morphology, crystallographic orientation of the individual grains and their interfaces as well as microstructural defects within the bulk grains and at the inter-granular interfaces (Benedetti and Barbe, 2013). A given material´s microstructure can be thought of as being constructed using building blocks called “features” such as grains, inclusions, fibers, pores, corrosion pits, dislocations, individual atoms and many other possibilities. Although these features are very different in the “real world” material´s sense, they can digitally be simplified as groups of discrete mesh elements (Groeber and Jackson, 2014). The link between microstructure and material macroscopic properties, the *structure-property* relationship, is technologically interesting as it may provide valuable information for the design of enhanced materials (Hashin, 1983; Mura, 1987; Nemat-Nasser and Hori, 1999; Needleman, 2000; Watanabe and Tsurekawa, 1999; Dunne and Petrinic, 2005; Adams and Olson, 1998).

Groeber and Jackson (2014) state that under the Integrated Computational Materials Engineering (ICME) framework, engineering materials can be treated as series of models (empirical or physical) that link the processing history to a suite of properties (mechanical, thermal, optical, electromagnetic, etc). In the most general terms, processing models predict the internal structure of materials under some processing conditions, either directly or through a correlation with continuum state variables like thermal history and strain path. Similarly, property models predict a material´s performance under some operating conditions, given a description of its internal structure. Thus, it becomes obvious that the natural link between these models is the internal structure of the material that is output from one and input to the other. The internal

* Corresponding author.
*E-mail addresses:* ebonifaz@usfq.edu.ec (E.A. Bonifaz), juan.baus@estud.usfq.edu.ec (J. Baus), alex.czekanski@lassonde.yorku.ca (A. Czekanski).

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structure of nearly all materials is complex, multi-scale and not easily defined by a small number of parameters (Groeber and Jackson, 2014).

Several researchers demonstrated the existence of a length-scale effect in plasticity over the past 15 years (Öztop et al., 2013).Their experimental methods consisted either of bending, twisting or compressing small well-defined volumes of material, or by employing indentation on a material. As such the experiments characterized the global response of the specimens, but the experiments gave no direct information about the state of the material within the system (Öztop et al., 2013). On the other hand, due to the fact that classical continuum theory not only underestimates the stiffness and yielding load of micro-scale structures, but also is incapable of capturing the size-dependency observed in these structures, the non-classical continuum theories such as the strain gradient theory and the modified couple stress theory have been developed (Rahaeifard et al., 2014). Of this manner, by using an appropriate constitutive equation, observed length-scale phenomena can be verified.

According to Aghababaei and Joshi (2013), the strengthening and high hardening behavior of metal matrix composites (MMCs) occur due to the high triaxiality in the stress state within the matrix region at the inclusion-matrix interfaces. Nanocrystalline matrices (Barai and Weng, 2011; Legarth and Niordson, 2010; Farrokh and Khan, 2009; Khan et al., 2008; Lloyd, 1994) may be combined with fine-scaled inclusions that may strongly mediate the strengthening, ductility and failure of polycrystal MMCs. Likewise, in highly textured polycrystalline MMC architectures the overall crystallographic orientation would be expected to produce strong plastic anisotropy, which may also influence the geometrically necessary dislocations (GNDs) induced size effect. In other words, the MMC response becomes length-scale dependent- an effect that has been explained in terms of geometrically necessary dislocations. Common to all the aforementioned research approaches is the assumption of homogenized matrix plasticity in that they ignore the combined effects of crystallographic orientation, inclusion size and shape, which are important in discerning the local deformation fields that affect global composite response (Aghababaei and Joshi, 2013).

Under conditions in which the applied stress is homogeneous over large regions of the domain, approximately equal densities of dislocations of opposite signs accumulate within the crystal. Such an accumulation of dislocations is known as a statistically stored dislocation (SSD) density, which exerts no long-range influence with the material. However, when a significant gradient of stress exists within the domain, a net density of one sign of dislocations accumulates in certain regions of the crystal while a net density of dislocations of the opposite sign accumulates in neighboring regions. The net signed density of dislocations is known as the geometrically necessary dislocation (GND) density (Öztop et al., 2013). According to Meyers and Ashworth (1992), the difference in the elastic response between adjacent grains is responsible for the generation of stress incompatibility at the grain boundaries. These stress incompatibilities, added to the resolved shear stress due to the applied load, result in a total stress at the grain boundaries considerably higher than that experienced by the bulk of the grain. Hence, the grain boundary flows plastically prior to the bulk. The high dislocation density initiated from the grain boundaries can be classified as geometrically necessary. Their introduction will accommodate the two adjacent grains (crystals) and decrease the stress incompatibility, i.e., the plastic flow of the grain boundary region attenuates the stress concentration. As the applied stress increases, the ratio between interfacial and applied stress decreases. The stresses become homogeneous when the interfacial layer is completely covered.

Carvahlo et al. (2013) developed a user-friendly and time-efficient phenomenological model that incorporates details of the microstructure evolution at the grain scale with a limited number of material parameters. Particular attention had been focused on keeping a strong physical relevance in describing a wide set of interstitial free (IF) steels and dual phase (DP) steels and realistically reproducing the experimentally observed transients in the macroscopic behavior when strain-path changes occur. It was concluded that the proposed strategy allows avoiding the time-consuming mechanical characterization and identification procedures once a set of fixed physically-based constant parameters is identified. Component level phenomenological models, however, may not always be able to predict complex material behaviors, especially if damage initiation and evolution are of concern. It is today widely recognized that these aspects may be better understood if features of the material microstructure are considered and brought into the modeling framework (Benedetti and Barbe, 2013). Computational structural analysis of material's micro-structures requires the generation of reliable micro-morphologies and affordable computational meshes as well as the description of the mechanical behavior of the elementary constituents and their interactions (Benedetti and Barbe, 2013). The simulation of polycrystalline superalloys with a microstructural base is limited to few studies. Most of these analyses have been until recently restricted to two dimensional cases, due to the high computational requirements. In the last decade, however, the more affordable and increased computational capability has promoted the development of fully three-dimensional models (Benedetti and Barbe, 2013).

The problem of generating a suitable virtual microstructure, morphology and mesh, is particularly critical, especially when the analysis of a relevant number of grains in the three-dimensional case is of interest (Benedetti and Barbe, 2013). Analyses of this kind are of interest, for example, in predicting the strong dependency of flow stress and plastic strain on phase type and grain size. Polycrystalline aggregates are idealized as simple three-dimensional arrangements of grains called Representative Volume Elements (RVEs), where many elements per grain are used to represent non-uniform deformations within individual grains, seen as domains separated by boundaries of high misorientation. To investigate the link between micro and macro scale variables for the deformation and stress given a description of its internal structure through a conventional constitutive model, the RVE is subjected to continuous monotonic strain loading conditions and periodic boundary conditions.

Material microstructures are available in many different sizes and shapes and their features of interest have different dimensionalities. Data describing attributes of microstructure can be obtained using many different devices (Scanning Electron Microscopy, Transmission Electron Microscopy, Optical Microscopy, Electron Backscatter Diffraction, Energy Dispersive Spectroscopy, Wavelength Dispersive Spectroscopy, 3D Atom Probe, Atomic Force Microscopy, etc) (Groeber and Jackson, 2014). By abstracting the materials interpretation of the features and focusing only on how the feature is described digitally, DREAM.3D has been able to constitute a general, unified structure for digital data that assumes no prior knowledge of length-scale or material class (Groeber and Jackson, 2014).

As several experimental studies reported that the macroscopic behavior can be attributed to the evolution of the underlying microstructural details, such as dislocation structures, more physically based models are developed in order to take into account the consequence of the evolution of the dislocation structures on the macroscopic behavior and specifically when strain-path changes occur. One may envisage scenarios where crystallographic orientation effects are important in determining the inclusion-induced