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Finite Element Modeling of Dual-Phase Polycrystaline Nickel-Base Alloys

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RESUMEN

Un modelo 3D de elementos finitos fue desarrollado para simular la influencia de inclusiones en el comportamiento mecánico policristalino de aleaciones a base de Níquel de fase dual. Un modelo de endurecimiento por deformación basado en dislocaciones, construido en el llamado marco de Kocks-Mecking, se utiliza como la principal estrategia para el modelamiento constitutivo de las fases individuales. Un programa de MatLab fue desarrollado para acoplar el código de microestructura digital DREAM.3D con el código ABAQUS FE. Se observa una fuerte dependencia del esfuerzo de fluencia y la deformación plástica en el tipo de fase, el tamaño de la inclusión, la forma y la distribución en la respuesta local del agregado. El efecto de los gradientes de deformación plástica impuestos por la microestructura también es observado.

Palabras Clave: Microestructuras Digitales; Comportamiento Constitutivo; Elementos Finitos; Aleaciones a Base de Níquel; Dislocaciones

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. A MatLab program was developed to couple the digital microstructure code DREAM.3D with ABAQUS FE code. A strong dependence of flow stress and plastic strain on phase type, inclusion size, shape and distribution upon the aggregate local response is observed. The effect of plastic deformation gradients imposed by the microstructure is also noted.

Keywords: Digital microstructures; constitutive behaviour; finite elements; Nickel-base alloys; Dislocations

FINITE ELEMENT MODELLING OF DUAL-PHASE POLYCRYSTALLINE NICKEL-BASE ALLOYS

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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. A MatLab program was developed to couple the digital microstructure code DREAM.3D with ABAQUS FE code. A strong dependence of flow stress and plastic strain on phase type, inclusion size, shape and distribution upon the aggregate local response is observed. The effect of plastic deformation gradients imposed by the microstructure is also noted.

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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 ship-building 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; 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 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 fifteen years (Öztop, 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, 2013). On the other hand, due to the 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 phenomea (e.g. for a fixed inclusion v.f. in the range of few microns, the strength of MMCs increased with decreasing inclusion size) can be verified.

According 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, 2013). According to Meyers and Ashworth (1992), the difference in the elastic response between adjacent grains is responsable for the generation of stress incompatibility at the grain boundaries. These stress incompatibility, 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 affordabile 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 nonuniform 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 Representative Volume Element (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 Difraction, 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 size effects. For example, in polycrystalline MMCs microstructures with fine inclusions embedded within large grains, the local crystallography would be expected to decide the GND distribution. Single crystal plasticity based approaches are valuable in such scenarios, but they ignore the presence (influence) of pre-existing heterogeneously distributed initial dislocation density.

In its present state, dislocation density-related constitutive modeling is considered mature enough to be broadly used in finite element codes including viscoplasticity. In order to formulate the grain-size dependence of the total dislocation density, it is necessary to derive an equation to describe the accumulation of dislocations during deformation. The constitutive equation to describe the work hardening process in polycrystalline materials, however, has not been well established (Öztop, 2013; Rahaeifard et.al, 2014; Narutani and Takamura, 1991). In this work, the constitutive equations found in section 2 are used to describe the deformation behavior of polycrystals in uniaxial deformation. The constitutive model is constructed based on the so-called Kocks-Mecking model (Narutani and Takamura, 1991; Estrin and Mecking, 1984; Estrin, 1996; Kocks, 1976; Bonifaz and Richards, 2008). The 3D dislocation based strain hardening finite element model was developed to simulate the influence of inclusions on the polycrystalline mechanical behavior of Nickel-based alloys. Four affordable computational dual-phase Representative Volume Elements (RVEs) of similar edge size but different inclusion size, shape and distribution were tested to investigate the relation between micro and macro deformation and stress variables.The

mathematical modeling has been investigated with a view to generating numerical data to define an optimum parameter space for an ongoing experimental project in the processing of new metal alloys.

2. THE CONSTITUTIVE MODEL

The constitutive model used in the present FEA work is the dislocation based strain hardening model documented in Bonifaz and Richards, 2008.

$$\sigma = \sigma_0 + M\alpha Gb\sqrt{\rho^S + \rho^G} \tag{1}$$

$$\rho^S = \left[\frac{K_1}{K_2} \left(1 - e^{\frac{-MK_2\bar{\varepsilon}}{2}} \right) + \sqrt{\rho^0}\, e^{\frac{-MK_2\bar{\varepsilon}}{2}} \right]^2 \tag{2}$$

$$\rho^G \approx \frac{\bar{\varepsilon}}{4bd} \tag{3}$$

where $\bar{\varepsilon}$ represents the equivalent strain, ρ^S is the statistically stored dislocation density, ρ^G is the geometrically necessary dislocation density, ρ^0 is the initial dislocation density, G is the shear modulus, and the other parameters are defined in Table 1. According to Ashby (1970), the difference in crystallographic orientation between neighboring grains can be corrected by introducing the geometrically necessary dislocations (ρ^G), which are introduced to accommodate the incompatibility of deformation between grains. The presence of the GND densities introduces both a curvature as well as a strain into the crystal lattice. Formally, the relationship between the GND densities and the lattice distortion follows from a consideration of the compatibility of deformation in circumstances when multiple deformation mechanisms can be activated. The GND density (unit: 1/length^2), inherently contains a length scale, so GND densities are often invoked as state variables in strain gradient plasticity theories as a means of predicting the plasticity length scale effect (Öztop, 2013).

Table 1. Values of material parameters used in this study

Parameter	Matrix	Inclusion	Reference
Taylor factor, M	2.73	2.91	Thomson, 1977
Young´s Modulus, E	207 GPa	294 GPa	Reed, 2006
Critical Resolved Shear Stress, k_0	85.1 MPa	170 MPa	Bonifaz, 2014
Elastic limit, $\sigma_0 = \sqrt[2]{3}k_0$	147 MPa	295 MPa	Bonifaz, 2014
α constant	0.3	0.3	Ashby, 1970
K_1	9.47E5 1/cm	9.47E5 1/cm	Narutani and Takamura, 1991
K_2	6.12	6.12	Narutani and Takamura, 1991
Initial dislocation density, ρ^0	1.0E8 1/cm^2	1.0E8 1/cm^2	Kehoe and Kelly, 1970
Burguer´s vector, b	2.52E-8 cm	2.52E-8 cm	Sangal and Tangri, 1989
Average diameter, d	35 μm	16.8 μm	Bonifaz, 2014
Poisson´s coefficient, v	0.26	0.26	Reed, 2006

The mechanical behavior of each phase is assumed to be represented by the constitutive equations (Eqs. 1-3) with appropriate values obtained from Table 1. The constitutive material model is incorporated into ABAQUS code through the *PLASTIC option (isotropic hardening continuum plasticity). The single slip plasticity assumption was considered in all the aggregate. Fig. 1 shows a comparission of the calculated stress-strain curves of matrix phase and precipitate phase. The weak hardening at low and high strains observed in the matrix curve is due to the lower shear modulus *G*.

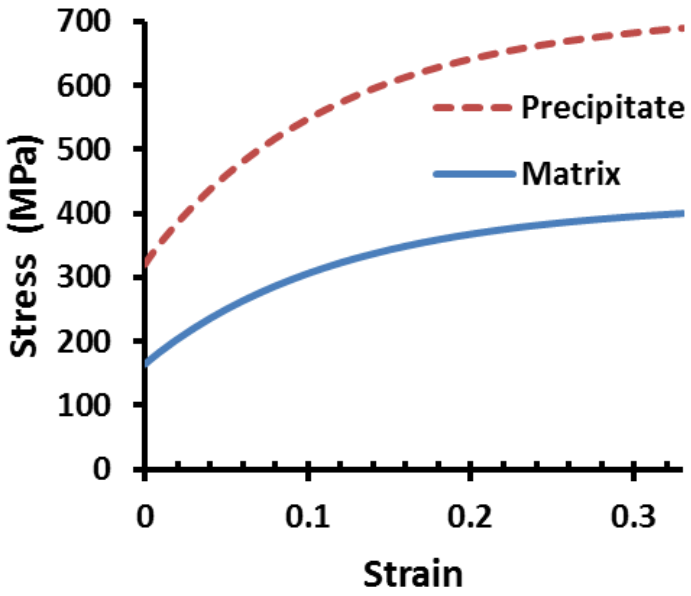

Figure 1: Stress-strain curves obtained with the dislocation based strain hardening constitutive model (Eqs. 1 to 3). Model parameters documented in Table 1.

3. THE FINITE ELEMENT MODEL

Three-dimensional grain-scale mechanical modeling of polycrystalline materials may provide valuable information for the design of enhanced materials. A cubic box with an edge size (l_o) is used to represent the polycrystalline aggregate. The four random polycrystalline aggregates (used in this work), generated with the software DREAM.3D, have a constant volume fraction ratio [70% (matrix phase) - 30 % (precipitate phase)]. Fig. 2 shows a dual-phase representative volume element constrained within 3-D boundary conditions. The individual contribution of the precipitates phase distributed in a random manner into the RVE models, are captured by the corresponding composite finite element mesh. The volume fraction ratio is kept constant in the four virtual specimens and corresponding simulations. To achieve the DREAM.3D and ABAQUS coupling, a MatLab® (Mathworks, 2015) program was developed. The program was constructed to identify the nodal information belonging to the cubic surfaces on which the load and boundary conditions were applied.

The macroscopic averaged stress σ (surface traction T_2 applied in the top surface) and strain ε in the traction direction are deduced from the resulting force on the face where the displacement is applied (for the stress) $\sigma = \frac{1}{A}\int_A \sigma_{22} dA$ and from the displacement itself (for the strain) $\varepsilon = \ln\left(1 + \frac{u_2}{l_0}\right)$. Here, u_2 is the applied displacement and l_0 is the cubic box edge size. Virtual specimens with different inclusion size, morphology and distribution were used in the finite element simulations. The single slip plasticity assumption was considered in all the dual-phase aggregate (matrix and inclusions). The boundary and load conditions in a dual-phase representative volume element are shown in Fig. 2.

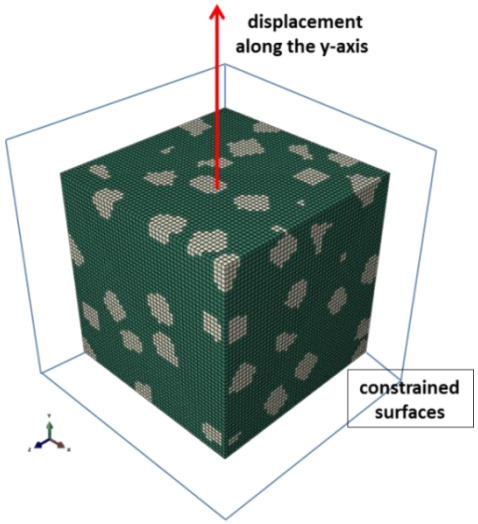

Figure 2: A dual-phase (matrix phase + inclusions phase) representative volume element constrained with 3D boundary conditions. Continuous monotonic strain loading applied on the top face along the y-axis.

The single oriented crystals (70 % matrix and 30 % inclusion grains) presented in Fig. 3, were uniformly meshed with ABAQUS® code, using 125000 low order 8 noded elements (C3D8). The matrix separated from inclusions and the inclusions separated from matrix are also shown in Fig. 3d.

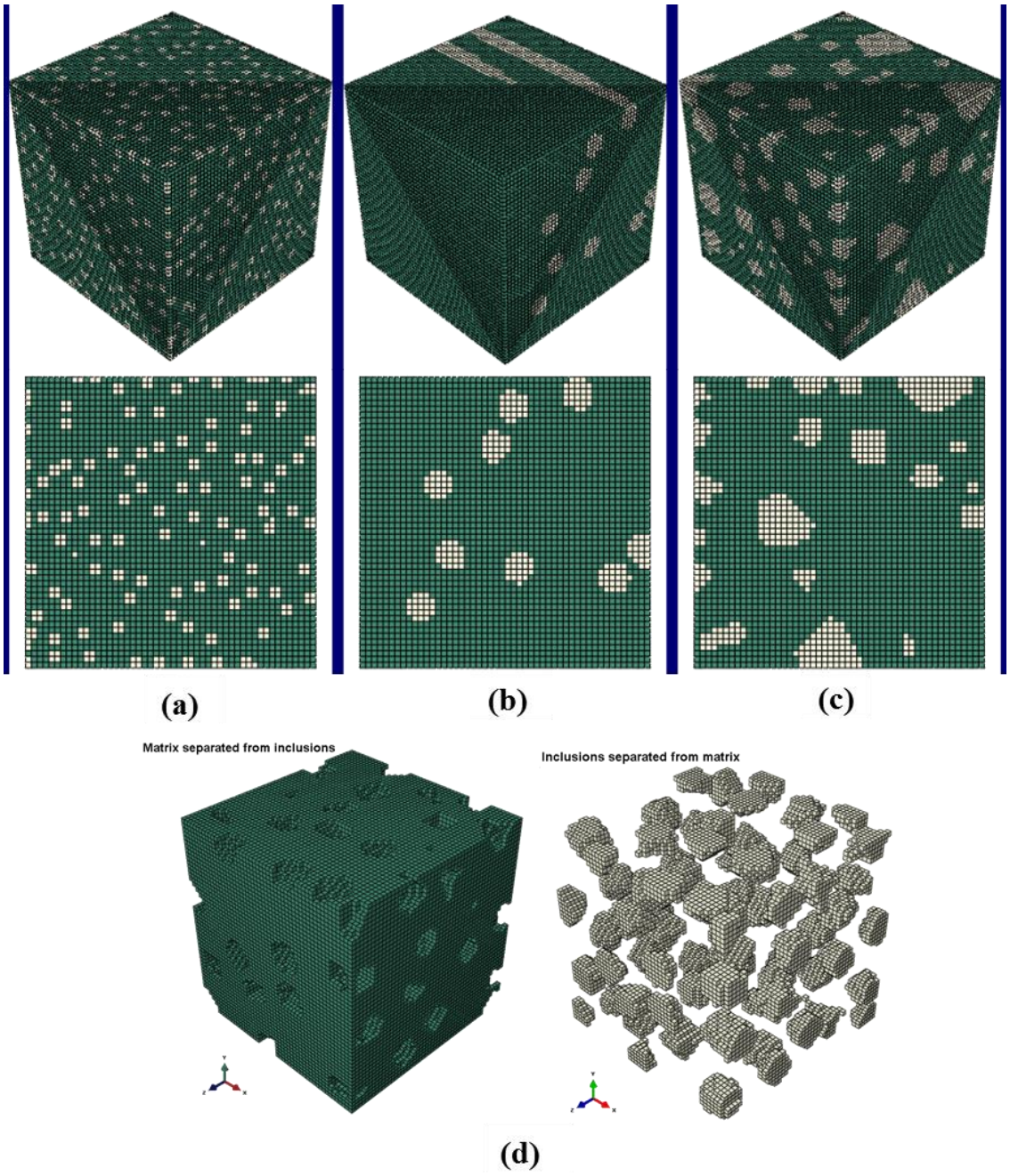

Figure 3: Four Representative Volume Elements (RVEs) for a dual-phase polycrystalline nickel-base alloy generated with the software DREAM.3D a) Mesh 1- fine spherical precipitate b) Mesh 2 – cylindrical precipitate c) Mesh 3- mixed spherical precipitate d) Mesh 4 – coarse spherical precipitate. Cubic box edge size (l_o = 50 μm). Element size = 1 μm.

4. RESULTS AND DISCUSSION

The difference in elastic (and plastic) response between adjacent inclusions and between matrix and inclusions are attributed to the generation of stress incompatibility at the inclusion boundaries.These stress incompatibilities, added to the resolved shear stress

due to the applied load, result in a total stress at the inclusion boundaries considerably higher than that experienced by the bulk of the inclusion or the matrix (See Mises stress contour values in Fig. 4). Results, shown in Figs. 4 to 6 demonstrate a strong dependency of flow stress and plastic strain on phase type, inclusion size, and inclusion distribution and morphology. It is noted that under the same load and boundary conditions, different points (four analyzed finite elements) located in the same matrix phase, present different mechanical behavior (see mixed spherical precipitate stress-strain curve profiles in Fig. 5). This phenomenon is attributed to the influence of the size, distribution and morphology of the inclusions. Of the same manner, for the four RVEs (mesh 1 to mesh 4), the difference in stress-strain behaviour and elastic limit observed in the same point (same element number) located either in the matrix phase or in the precipitate phase, also depends on inclusion size, shape and distribution (see Fig. 5a). The significance of the yield point variation is that once plastic deformation starts in a given area, the metal at this point is effectively softened and suffers a relatively large plastic deformation. This deformation then spreads into the material adjoining the region that already yielded because of the stress concentration at the boundary between the deformed and undeformed areas. In general, deformation starts at a position of stress concentration as discrete bands, as clearly observed in Figs. 4b and 6b. It is also confirmed that in RVEs composed with cylindrical inclusions (see Fig. 3b- mesh 2), the resistance to flow increases when the applied load is perpendicular to the inclusion longitudinal axis. Higher S22 stress values are reported for this condition in Figs. 5a, 5b, and 5d.

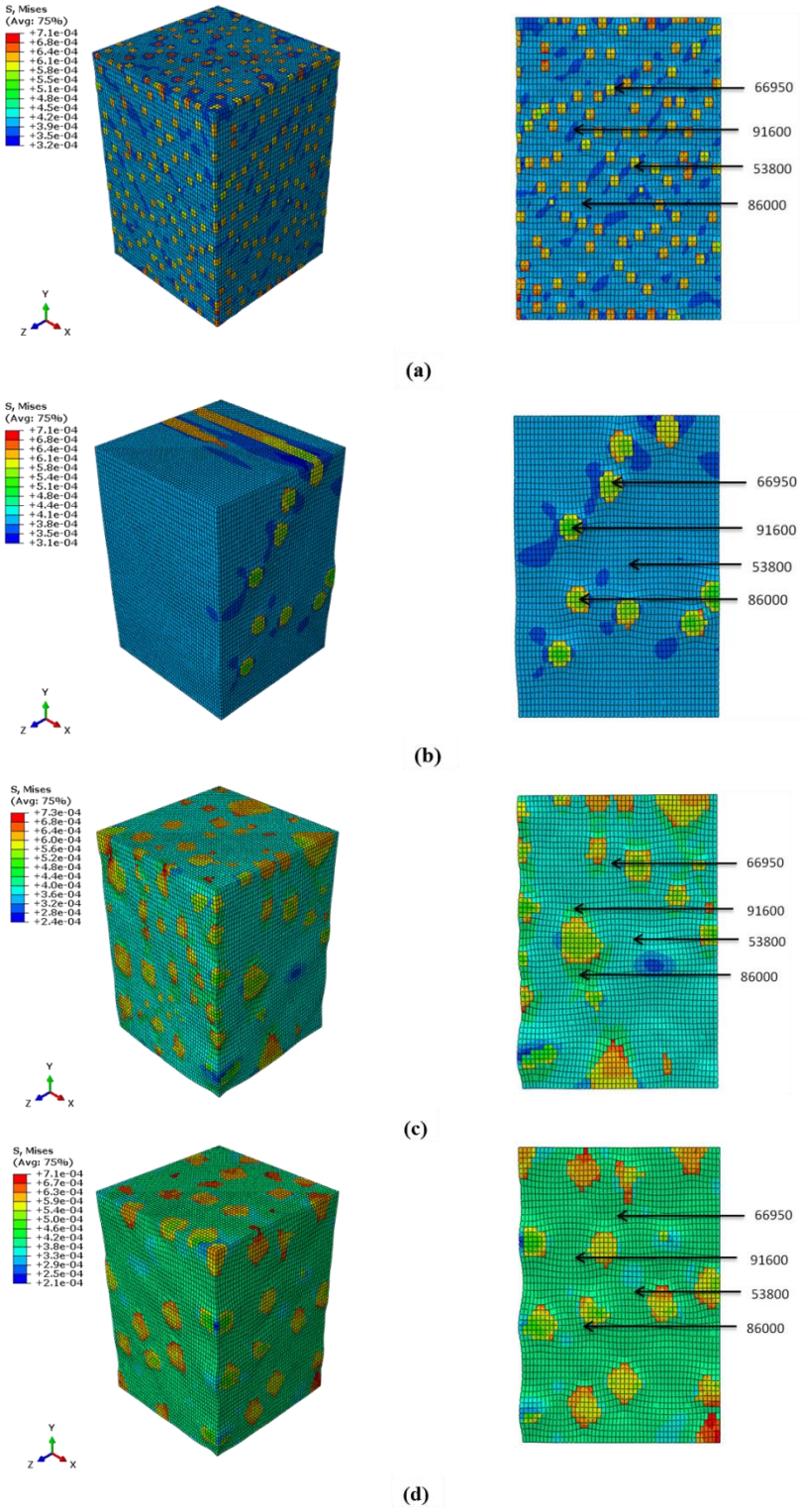

Figure 4: von Misses stress contours for the 50 micron Representative Volume Element (RVE) under displacement loading along the y-axis a) Mesh 1 b) Mesh 2 c) Mesh 3 d) Mesh 4. The elements considered in the analysis are also shown on the right. Stress units in $\frac{N}{\mu m^2}$. Element size = 1 μm.

Fig. 5 shows the stress-strain curves for the documented element number in the four representative digital microstructures stated in Figs. 3 and 4. Results reveal that the independent mechanical behavior of the analyzed element is affected for the phase type, inclusion size, distribution and morphology.

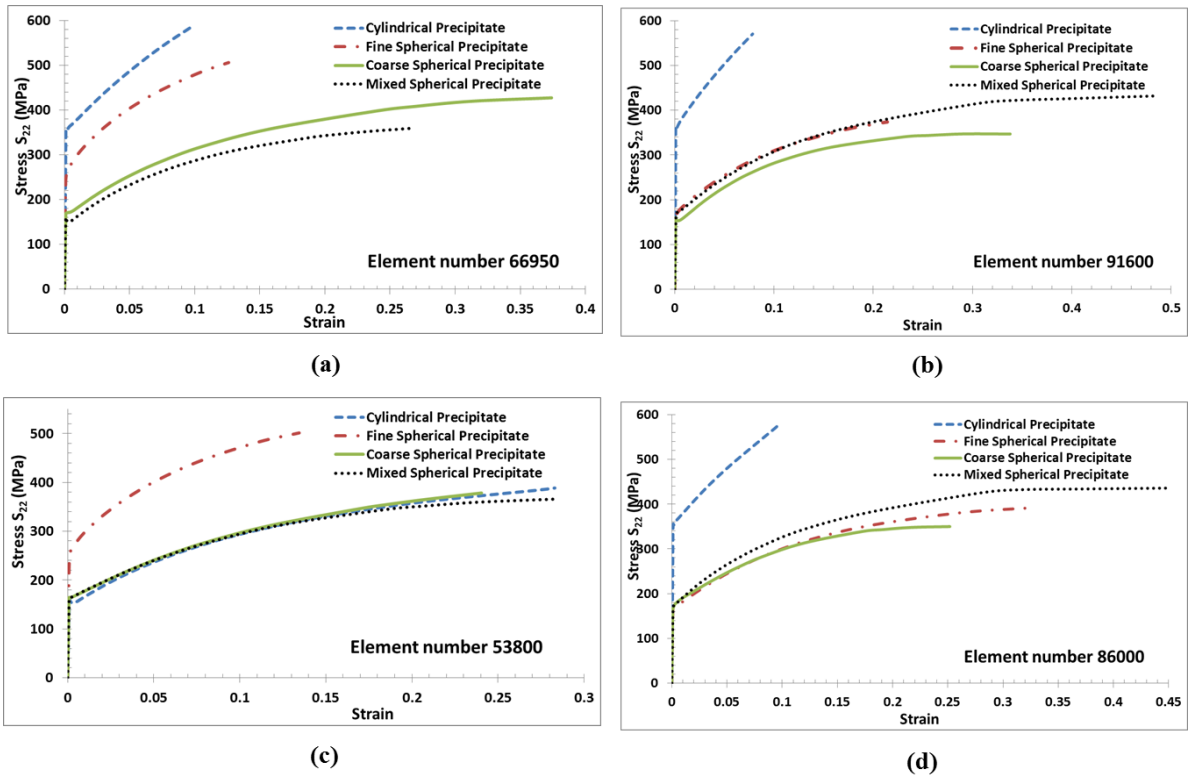

Figure 5: Element stress-strain curves obtained in the four RVEs subjected to displacement loading along the y-axis a) for element number 66950 b) for element number 91600 c) for element number 53800 d) for element number 86000. Element numbers documented in Fig. 4 are located in the righ surface of the cube.

Fig. 6 shows plastic effective strain (PEEQ) contours for the four 50 micron Representative Volume Elements (RVEs) after a 30 % displacement (15 microns) loading along the y-axis. Higher strain values are observed in meshes 3 and 4 when compared with meshes 1 and 2. Strain concentration areas appear as a result of the applied load, that is, the equivalent strain is not uniformily distributed through the aggregate. The effect of plastic deformation gradients imposed by the microstructure is clearly observed. The resistance to flow is higher in structures composed of finer and homogeneous spherical and cylindrical precipitates because the Mises stresses and effective plastic strains are better distributed.

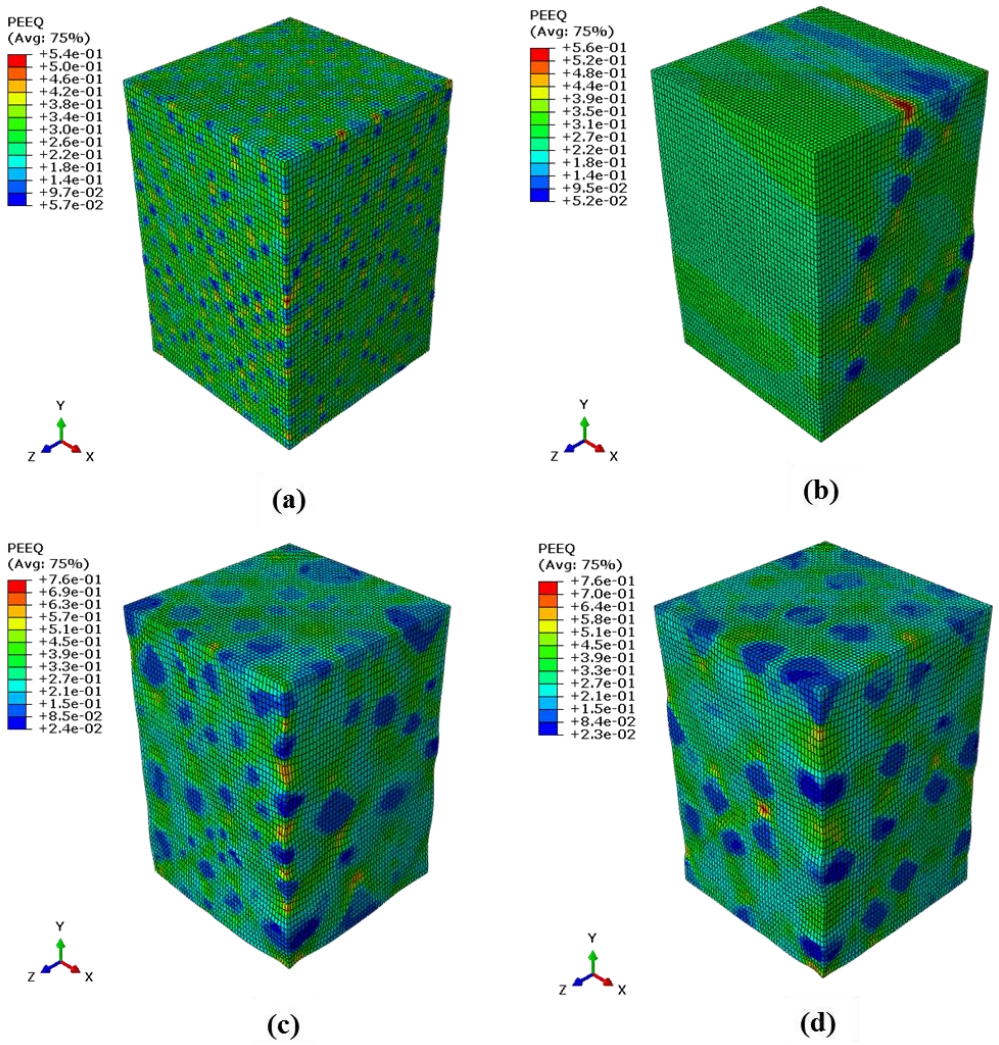

Figure 6: Plastic effective strain (PEEQ) contours for the 50 micron Representative Volume Element (RVE) under similar displacement loading along the y-axis a) Mesh 1 b) Mesh 2 c) Mesh 3 d) Mesh 4. Element size = 1 μm.

5. CONCLUSIONS

1. A 3D dislocation based strain hardening finite element model was developed to simulate the influence of inclusions in the polycrystalline mechanical behavior of Nickel-based alloys.
2. The effects of the phase type, inclusion (precipitate) size, shape and distribution upon the aggregate local response are clearly observed.
3. To couple the DREAM.3D digital microstructure code with ABAQUS finite element code, a MatLab program was developed. The program was constructed to identify the nodal information contained on the microstructure cube surfaces where the load and boundary conditions were applied.
4. Results demonstrate a strong dependency of flow stress and plastic strain on phase type, inclusion size, shape and distribution.

5. The effect of plastic deformation gradients imposed by the microstructure is clearly observed.
6. It is also confirmed that in RVEs composed with cylindrical inclusions, the resistance to flow increases when the applied load is perpendicular to the inclusion longitudinal axis.
7. For the same load and boundary conditions, different mechanical behavior is observed in a same element number when this is located in differents RVEs.
8. The resistance to flow is higher in structures composed of finer and homogeneous spherical and cylindrical precipitates because the Mises stresses and effective plastic strains are better distributed.
9. The difference in crystallographic orientation, 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 modulus.

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