Proceedings of the 7th International Conference on Mechanics and Materials in Design,
Albufeira/Portugal 11-15 June 2017. Editors J.F. Silva Gomes and S.A. Meguid.
Publ. INEGI/FEUP (2017)

PAPER REF: 6417

MODELING DUAL-PHASE STRUCTURES: A DREAM.3D-ABAQUS COUPLING

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ABSTRACT

A 3D finite element model was developed to simulate the influence of secondary phases (precipitates or aggregates) on the inelastic stress-strain distribution of nickel-based alloys and concrete structures. In both situations, the digital microstructure code DREAM.3D [1] was coupled to ABAQUS® finite element code through a MatLab® program.

Keywords: heterogeneous materials, digital structures, constitutive behaviour, cement paste, aggregates, inclusions, nickel-base alloys.

RESULTS AND CONCLUSIONS

Representative Volume Elements (RVEs) of similar edge size but different inclusion (aggregate) size, morphology and distribution generated with DREAM.3D were tested with ABAQUS to investigate the relation between micro (and/or meso) and macro deformation and stress variables. Virtual specimens subjected to continuous monotonic strain loading conditions, were constrained with 3D boundary conditions. In the case of dual-phase polycrystalline nickel-based alloys, the difference in crystallographic orientation, which evolves in the process of straining, and the incompatibility of deformation between neighbouring 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 through the strain hardening model documented in Bonifaz and Richards [2]. In the case of concrete structures consisting of aggregates and hydrated cement paste, individual experimental curves in compression and tension documented in Bonifaz, et.al [3] were considered in the nonlinear analysis.

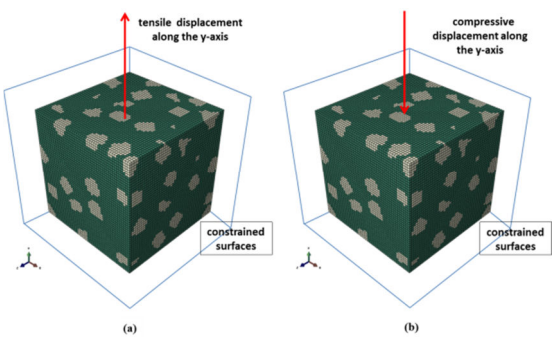

Fig. 1 - A dual-phase RVE constrained with 3D boundary conditions and subjected to continuous monotonic strain loading applied on the top face along the y-axis a) Tension b) Compression.

The effects of the phase type, inclusion size, morphology and distribution upon the composite (nickel alloy) local response are clearly observed in Fig. 2. The resistance to flow is higher in structures composed of finer and homogeneous spherical and/or cylindrical precipitates because the mises stresses and effective plastic strains are better distributed. Results demonstrate a strong dependence of flow stress and plastic strain on phase type, inclusion (or aggregate) size, shape and distribution as shown in Fig. 3. The effect of plastic deformation gradients imposed by the microstructure is clearly observed.

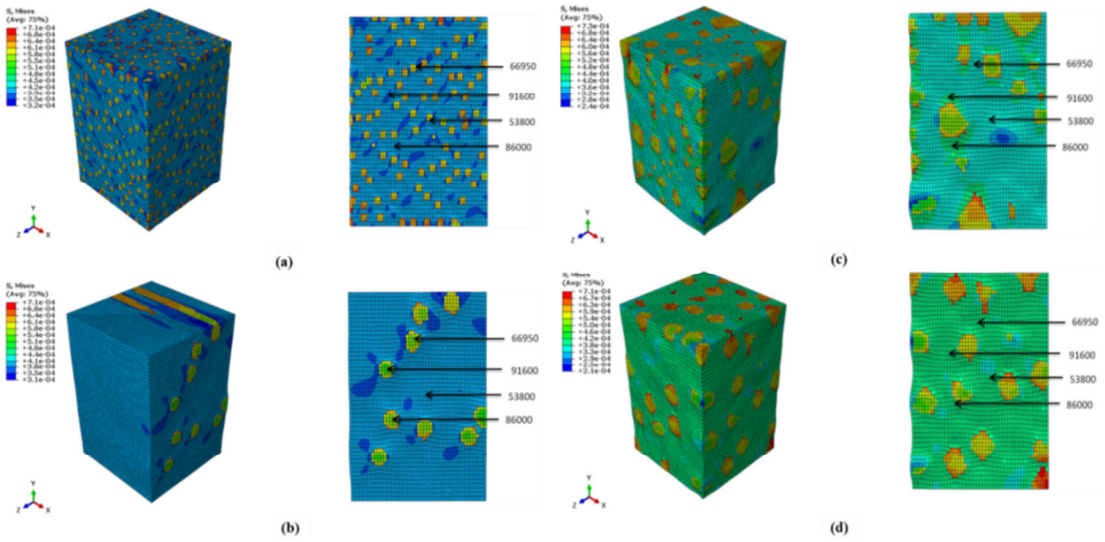

Fig. 2 - von Misses stress contours for a 50 micron RVE dual-phase nickel-based alloy under displacement loading along the y-axis a) Mesh 1 b) Mesh 2 c) Mesh 3 d) Mesh 4. The elements considered in the analysis are also shown on the right. Stress units in $\frac{N}{\mu m^2}$. Element size = 1 μm.

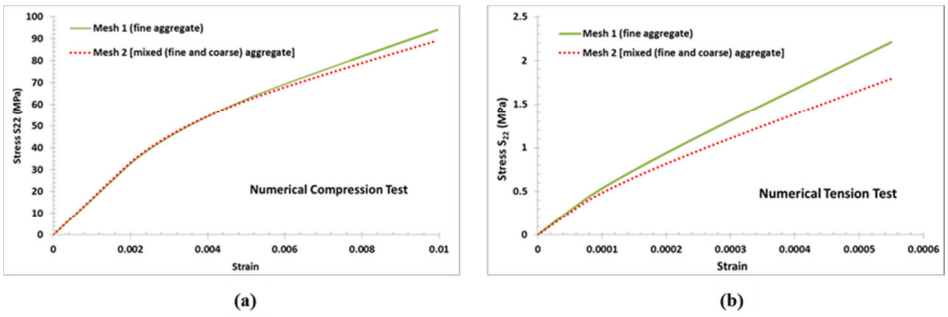

Fig. 3 - Stress-strain curves for the two analized concrete RVEs a) Compression test b) tension test.

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