[M/F] Oxidation assisted-strain localisation in Ni-based and Ti-based materials: numerical-experimental dialogue

<u>PhD offer :</u> ERC-SG_HT-S_4DefOx#6

<u>Context :</u>

Structural metallic/intermetallic materials operating at **high temperatures** (650°C-1200°C) in severe environments are commonly subjected to in-service **surface reactivity, *i.e.* oxidation, corrosion**. This issue is encountered in several industrial applications, especially when high temperatures, mechanical stresses, and highly corrosive atmospheres gather (power plants, aeronautic turbines, etc.)[1]. Environment-assisted degradation alters both the surface of the materials and their bulk properties due to a progressive selective consumption of elements involved in the surface degradation process and/or diffusion of oxidising elements (*e.g.* depleted sub-surface layer for Ni-based superalloys due to Al consumption to form Al_2O_3 [2, 3], brittle oxygen/nitrogen-enriched layer in Ti and TiAl alloys due to O and N solubility [4, 5], etc.). The material in a shallow region beneath the reactive surface subsequently presents a gradient of chemistry, microstructure and physical properties. **This gradient of microstructure and properties evolves with the time due to the oxide growth and diffusion processes.**

Each family of metallic/intermetallic materials reacts differently to the so-called "stress-corrosion", but also to the corrosive/oxidative-deformation. However, all the materials are potentially affected by these mechanisms due to the concomitant effects of surface reactivity, microstructure evolution and deformation. **Despite the negligible scale of the physical, chemical, metallurgical gradients (from 0.1 to 100 micrometres beneath the surface) in comparison with the dimensions of the structural components, the variability in mechanical behaviour within the gradient often drives premature damage and the progressive rupture of the component** [6]. Such material evolution and degradation could be included in the so-called "***stress-corrosion cracking***", investigated for decades for all the structural materials used at high temperature. **HOWEVER**, industrial and ecological motivations to use structural materials in ever-more extreme, severe, harsh conditions push them to their performance limits. **The synergy operating between inter- versus intragranular strain localisation and surface reactivity/diffusion processes promotes unexpected damage and high variability in lifespan of structural components exposed at "too high temperatures – too much (cyclic and/or steady) stresses"** [7]. A better understanding of the thermo-mechano-chemical elementary mechanisms responsible of early damage at the microscale is needed.

<u>Project motivations :</u>

To address this point, HT-S_4DefOx, a project funded by the European Research Council (ERC - Starting Grant), intends :

- To assess the mechanical behaviour within the time-evolving gradient of microstructure and properties, *i.e.* within the "sub-surface" material (micro- and mesoscale approach);
- To assess the variability in sub-grain mechanical behaviour of the metallic material at the metal/oxide interface (microscale approach). This interface, considered as the "extreme surface"; is on the front line for the thermo-mechano-chemical coupling;
- To model and simulate thermo-mechano-chemical coupling on time-evolving microstructures and properties of the "sub-surface" material with boundary conditions on the "extreme surface" adapted from Ref. [8].

References :

1. Young DJ (2016) High temperature oxidation and corrosion of metals, 2nd Ed. Elsevier Science
2. Bensch M, Preußner J, Hüttner R, et al (2010) Modelling and analysis of the oxidation influence on creep behaviour of thin-walled structures of the single-crystal nickel-base superalloy René N5 at 980 °C. Acta Mater 58:1607–1617. doi:10.1016/j.actamat.2009.11.004
3. Cassenti B, Staroselsky A (2009) The effect of thickness on the creep response of thin-wall single crystal components. Mater Sci Eng A 508:183–189. doi:10.1016/j.msea.2008.12.051
4. Finlay WL, Snyder JA (1950) Effects of three interstitial solutes (nitrogen, oxygen, and carbon) on the mechanical properties of high-purity, alpha titanium. JOM 2:277–286. doi:10.1007/BF03399001
5. Barkia B, Doquet V, Couzinié JP, et al (2015) In situ monitoring of the deformation mechanisms in titanium with different oxygen contents. Mater Sci Eng A 636:91–102. doi:10.1016/j.msea.2015.03.044
6. Pineau A, Antolovich SD (2009) High temperature fatigue of nickel-base superalloys - A review with special emphasis on deformation modes and oxidation. Eng Fail Anal 16:2668–2697. doi:10.1016/j.engfailanal.2009.01.010
7. Stinville JC, Echlin MP, Callahan PG, et al (2017) Measurement of strain localization resulting from monotonic and cyclic loading at 650 ∘C in nickel base superalloys. Exp Mech 57:1289–1309. doi:10.1007/s11340-017-0286-y
8. De Rancourt V, Ammar K, Appolaire B, Forest S (2016) Homogenization of viscoplastic constitutive laws within a phase field approach. J Mech Phys Solids 88:291–319. doi:10.1016/j.jmps.2015.12.026

Description of the PhD project :

The present PhD project will focus on the implementation of a thermo-mechano-chemical model and simulations of polycrystalline 2D then 3D aggregates. The modelled material will present a time-evolving gradient of chemical composition, microstructure, and subsequently mechanical properties due to the concomitant effect of localised deformation and surface reactivity. The reliable description and predictive simulations of the gradient of microstructure is necessary for a good prediction of the local mechanical properties. For the finite element framework, strain gradient crystal plasticity based on dislocation densities will be used, including anisotropic plasticity and size-dependence of plastic activity Ni-based and Ti-based materials subjected to oxidation.
Local mechanical properties will be assessed using advanced nanoindentation, microtensile and microcompression techniques in collaboration with another PhD student and postdoctoral fellows. The numerical simulation of the indentation test will aim to correlate the hardness and reduced modulus properties at the sub-grain level with both the contribution of the grain orientation and the local chemistry. Simulations on aggregates will be confronted to full field mechanical tests using high-resolution digital image correlation (HR-DIC) techniques from surface analyses.

In the present project, the PhD student will :

- Simulate nanoindentation test on anisotropic materials to identify elasto-plastic properties ;
- Compare these simulations with experimental data obtained on polycrystalline Ni-based and Ti-based materials, subjected or not to oxidation ;
- Develop a phase field-coupled finite element analyses on 2D aggregates ;
- Develop a phase field-coupled finite element analyses on 3D aggregates ;

- Simulate tensile tests on not oxidised 3D polycrystalline aggregates and compare the results with kinematics fields obtained using HR-DIC ;
- Simulate tensile tests on oxidised 3D polycrystalline aggregates and compare the results with kinematics fields obtained using HR-DIC;
- Discriminate the effect of strain localisation on "sub-surface" microstructure affected by stresses AND surface reactivity.

Expected skills and/or know-how :

The PhD student should have the following skills and/or know-how :
- Mechanical engineering (and more particularly at the microscale) ;
- Material sciences and/or computational solid mechanics ;
- Image analyses ;
- Scientific computing (Matlab and/or Python language and/or c++ etc.).

Administrative details :

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Salary : 2 135.00 € per month before taxes
PhD locations :

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AND

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