

A Theoretical Investigation on the Role of Microstructural Particularities on the Hydrogen Embrittlement of Nickel Alloys

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ABSTRACT

Precipitation hardened (PH) nickel alloys have been extensively used in diverse applications in the oil and gas industry due to its high strengths and outstanding corrosion resistance in several aggressive environments. Despite of their known high corrosion properties, hydrogen embrittlement is one common failure reported by the industry for this class of alloys.

PH nickel alloys exhibit complex microstructures, composed by diverse secondary phases. Numerous research activities to study the mechanisms behind hydrogen embrittlement have been carried out in the last years and are still a point of debate in the oil and gas community, mainly when it comes to the interaction of these microstructural features with the hydrogen uptake provided by the service environment. Several mechanisms have been proposed to explain the role of hydrogen in the microstructure of metallic materials. Hydrogen enhanced decohesion (HEDE) has been proposed as the mechanism behind the intergranular character of some of the fracture surfaces, being explained by the presence of grain boundary decoration. However, materials having a very limited amount of precipitates in the grain boundaries still can be susceptible to hydrogen embrittlement. When presenting a transgranular failure mode, the mechanism proposes that the cohesive strength between the metal atoms is reduced by the presence of hydrogen in the bulk. In spite of these observations, limited work is available in the literature in regards to microstructure features and a complete understanding of their roles on the hydrogen embrittlement.

This work is based on a cooperation with the Max Planck Institute for Iron Research in Düsseldorf, Germany. The interaction of hydrogen with microstructure elements primarily present in nickel-based alloys was fundamentally studied using ab-initio and atomistic models, showing that the strength and

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hardness levels are not primarily decisive for the susceptibility to hydrogen embrittlement, but rather the microstructure.

Key words: Precipitation Hardened Nickel Alloys, Hydrogen Embrittlement, ab-initio calculations, simulation and modeling, corrosion resistant alloys

INTRODUCTION

Precipitation hardened (PH) nickel alloys have been broadly used in various applications in the oil and gas industry thanks to its high strengths and outstanding corrosion resistance in several aggressive environments. Alloy 718 (UNS¹ N07718), Alloy 925 (UNS N09925), Alloy K-500 (UNS N05500), Alloy 725 (UNS N07725), and others are among the most used PH nickel alloys in the oil and gas industry. Despite of their known high corrosion properties, hydrogen embrittlement is one common failure reported by the industry for this class of alloys.¹⁻⁴

Most of the PH hardened nickel alloys, due to the fact of being alloyed with niobium, titanium and/or aluminum, are hardened through the precipitation of the intermetallic phases Gamma-Prime, a cubic face-centered $L1_2$ ordered $Ni_3(Al,Ti)$ phase, and Gamma-Double-prime, a cubic face-centered DO_{22} ordered Ni_3Nb phase. Additionally, these alloys may precipitate the non-avoidable carbonitrides, and the Delta and Eta phases, which can be detrimental to the alloy's mechanical and corrosion properties.

The precipitation of diverse secondary phases concedes to PH nickel alloys complex microstructures, which have been incentive for numerous research activities to study the mechanisms behind hydrogen embrittlement. The outcomes of these researches are commonly in debate within the oil and gas community, mostly in the matter of the interaction of microstructural features with the hydrogen uptake provided by the service environment.

Diverse mechanisms have been proposed to explain the numerous aspects observed. When the fracture surfaces present an intergranular character, the fracture is elucidated by the presence of grain boundary decoration. Hydrogen Enhanced Decohesion (HEDE) is the name given for this suggested mechanism. However, the current state of the art of manufacturing processes enables the production of materials having a very limited amount of precipitates in the grain boundaries. Even with grain boundaries with less precipitation or free of precipitation, PH alloys can still be susceptible to hydrogen embrittlement.⁵ In these cases, a transgranular mode of failure is usually detected. For these fractures, the mechanism proposes that the cohesive strength between the metal atoms is lowered by the presence of hydrogen in the bulk material. In spite of these observations, limited work is available in the literature in regards to microstructure features and a complete understanding of their roles on the hydrogen embrittlement.

The HEDE mechanism seems to be the most relevant for the present alloys, however it neglects the effects of hydrogen on the ductile processes.

AB-INITIO CALCULATIONS

Initial Considerations for system simplification

All of the phases present in the precipitation hardened nickel alloys obviously present a very complex chemistry. For example, in the Gamma-Prime phase, it is known that titanium may be present as a substitute element for aluminum in Alloy 718.⁶ Nevertheless, the inclusion of the full chemical complexity

¹ Unified Numbering System (UNS)

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of phases and matrix is not feasible on the simulations and therefore all of the participating phases were simplified to make the calculations possible. In Alloy 718, for example, the relevant precipitates are Gamma-Prime, Gamma-Double-Prime, Delta-Phase and the Niobium-Carbides. The Gamma-Prime was considered in the simulations to be composed only by nickel and aluminum (Ni_3Al). The Gamma-Double-Prime was considered to be composed by nickel and niobium only (Ni_3Nb), as well as the Delta-Phase. The carbide phase was considered to be formed by carbon and niobium, only. Taking that in consideration, example atomic cell arrangements of these phases are shown on **Figure 1**.

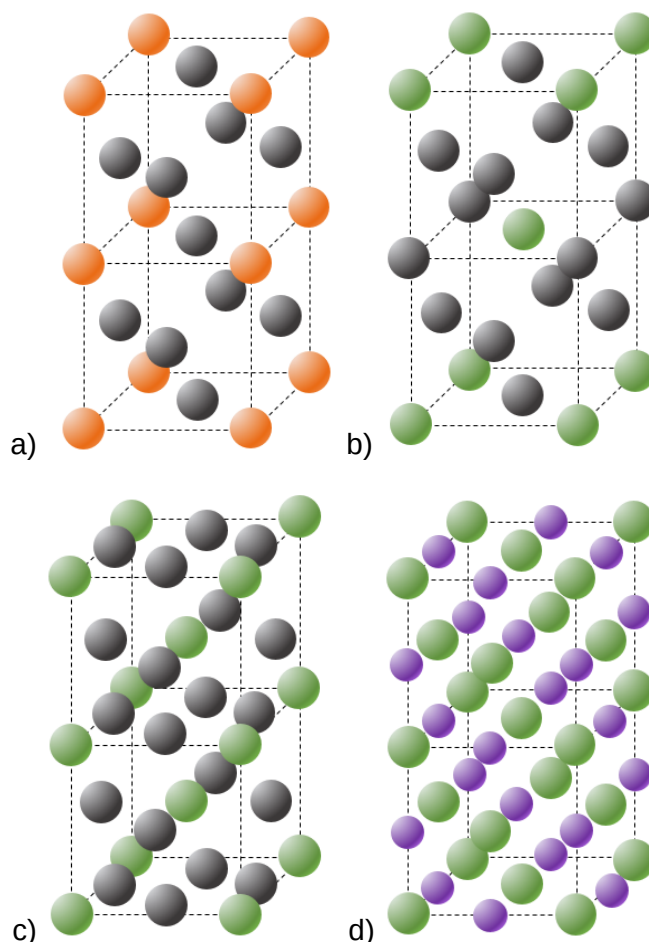


Figure 1: Atom cell arrangements of relevant phases precipitated on Alloy 718 a) Gamma-Prime, b) Gamma-Double-Prime, c) Delta-Phase and d) Niobium-Carbides. The grey spheres represent nickel atoms, the orange spheres represent aluminum atoms and the purple spheres represent carbon atoms.

It is believed that the present set of simulations, despite the simplifications assumed, provides genuine insight into features of the particular alloys.

Hydrogen Solution enthalpy on phase boundaries

The interaction of hydrogen with the microstructural features of PH nickel alloys has been investigated through the application of ab-initio calculation methods. First, the probability of incorporation of hydrogen into different positions at the relevant phase boundaries was established by taking in consideration the calculated solution enthalpies, which were calculated using ab-initio density functional theory (DFT).