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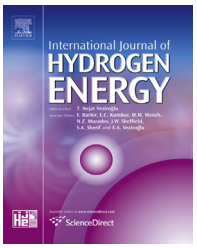

Influence of grain boundary misorientation on hydrogen embrittlement in bi-crystal nickel

Sathiskumar Jothi[*], *T.N. Croft*, *S.G.R. Brown*

College of Engineering, Swansea University, Singleton Park, Swansea SA2 8PP, UK

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A B S T R A C T

Computational techniques and tools have been developed to understand hydrogen embrittlement and hydrogen induced intergranular cracking based on grain boundary (GB) engineering with the help of computational materials engineering. This study can help to optimize GB misorientation configurations by identifying the cases that would improve the material properties increasing resistance to hydrogen embrittlement. In order to understand and optimize, it is important to understand the influence of misorientation angle on the atomic clustered hydrogen distribution under the impact of dilatational stress distributions. In this study, a number of bi-crystal models with tilt grain boundary (TGB) misorientation angles (θ) ranging between $0^\circ \leq \theta \leq 90^\circ$ were developed, with rotation performed about the [001] axis, using numerical microstructural finite element analysis. Subsequently, local stress and strain concentrations generated along the TGB (due to the difference in individual neighbouring crystals elastic anisotropy response as functions of misorientation angles) were evaluated when bi-crystals were subjected to overall uniform applied traction. Finally, the hydrogen distribution and segregations as a function of misorientation angles were studied. In real nickel, as opposed to the numerical model, geometrically necessary dislocations are generated due to GB misorientation. The generated dislocation motion along TGBs in response to dilatational mismatch varies depending on the misorientation angles. These generated dislocation motions affect the stress, strain and hydrogen distribution. Hydrogen segregates along these dislocations acting as traps and since the dislocation distribution varies depending on misorientation angles the hydrogen traps are also influenced by misorientation angles. From the results of numerical modelling it has been observed that the local stress, strain and hydrogen distributions are inhomogeneous, affected by the misorientation angles, orientations of neighbouring crystal and boundary conditions. In real material, as opposed to the numerical model, the clustered atomic hydrogens are segregated in traps near to the TGB due to the influence of dislocations developed under the effects of applied mechanical stress. The numerical model predicts maximum hydrogen concentrations are accumulated on the TGB with misorientation angles ranging between $15^\circ < \theta < 45^\circ$. This investigation reinforces the importance of GB engineering for designing and optimizing these materials to decrease hydrogen segregation arising from TGB misorientation angles.

* *Corresponding author.*
E-mail addresses: S.Jothi@swansea.ac.uk, jsathiskumar@gmail.com (S. Jothi).

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Introduction

Crystallographic interfaces and micro-textures such as GB misorientation are characterized by specific arrangements of their atoms. They play a prominent role in aerospace components which are typically made of high strength, high toughness, and corrosion resistant as well as high temperature metallic materials such as nickel, titanium and nickel-based super alloys. Nickel and nickel-based super alloys are made up of complex microstructures and have been used in aerospace applications for many years. Several catastrophic failures have occurred in nickel and nickel-based super alloys in aerospace components due to environmental cracking, hydrogen stress cracking and hydrogen embrittlement [1–4,53]. Hydrogen embrittlement is a costly problem in which structural degradation of the susceptible material leads to catastrophic failure. Atomic impurities in structural materials may occur any time during its life time, during fabrication in a manufacturing process or during operational use under service environmental conditions. It is not only a problem in the aerospace industries but also in many other sectors such as automotive, civil and construction, semiconductor, offshore, ship, oil and gas, nuclear power and renewable energy including wind energy, fuel cells and hydrogen energy. The susceptibility of structural materials to hydrogen embrittlement depends on many factors including hydrogen atom–microstructural interactions [1,3,11,12], microstructural intergranular engineering [6–8] and texture morphological behaviour [8–10]. By understanding and controlling some of these factors the susceptibility of materials can be reduced [12–16]. Even though there is a considerable amount of information available regarding the relationship between crystallographic micro-textures of materials such as TGB misorientation angles and hydrogen induced stress cracking [7,17,18,50], there has not been enough research done implementing this information into computational tools in order to understand material design and material design optimization based on GB engineering using finite element analysis (FEA). It is important to understand both the GB engineering and the relationship between misorientation angle and chemical and mechanical material degradation and properties at the design stage to develop new materials and to optimize existing materials to improve efficiency and increase the resistance of materials to hydrogen induced intergranular cracking, ideally implementing this approach into industrially applicable simulations.

The presence of GBs, interphase boundaries and the segregation of impurities are affected by GB misorientation significantly affects chemical, and mechanical properties as well as fracture processes such as crack nucleation and crack propagation in textured polycrystalline metallic materials [5–10]. It is already known that high densities of GBs (i.e. grain size), the type of GBs and GB misorientations with specific angles are important and could be optimized to increase properties such as strength, ductility and fracture toughness of textured polycrystalline metallic materials. On the other hand, GBs and GB misorientation can also be potential sites for segregation of impurities, cracks, fractures and their behaviour is responsible for GB embrittlement depending on the characteristics of the GBs misorientations within them [9–20]. It has been recently found that low angle grain boundaries and low Σ coincidence boundaries or coincidence site lattices (CSL) are immune to intergranular fractures that lead to intergranular cracking and intergranular embrittlement [9,10]. On the other hand high angle boundaries are preferential sites for fractures leading to crack nucleation and propagation [9,10,12,13]. Watanabe introduced the concept of 'grain boundary design and control' suggesting that GB misorientation and grain boundary character distribution (GBCD) are key microstructural parameters controlling the fracture toughness of polycrystalline metallic material [6–12]. Palumbo developed this concept as grain boundary engineering (GBE) and improved intergranular susceptibility by implementing GBE in nickel-based super alloys [21,11–16]. The GB misorientation and the distributions of GB misorientation angles are important parameters controlling the propensity of segregation of impurities and stress induced hydrogen fractures that can lead to catastrophic GB embrittlement failure of textured polycrystalline metallic materials. It is well known from the literature that texture and GB misorientation play important role in the impurities induced cracking [6–20]. Therefore, it would be of interest to implement GB misorientation in finite element modelling and develop a procedure to quantify the effect of GB misorientation and crystallographic texture on the stress induced mass diffusion of impurities in polycrystalline textured nickel developed for aerospace applications.

Most existing studies of the effect of environmental impurities (i.e. sulphur, hydrogen, oxygen, boron etc.) on embrittlement and cracking mechanisms in polycrystalline structural materials are based on global, macro mechanical properties. However microstructural inhomogeneity and micro-texture can result in micro-cracks and dislocation formation which may lead to macroscopic environmental failures of polycrystalline materials [1–4]. Since a polycrystalline material is an aggregate of crystal grains of various sizes and shapes, its macroscopic properties are affected by the properties of individual grains. Each individual crystal in polycrystalline nickel may exhibit elastic anisotropy due to its crystal symmetric characteristics. The elastic deformation of single crystals may exhibit anisotropy depending on the orientation of the crystal. The presence of microstructural inhomogeneity, morphological and crystallographic textures will certainly affect the correlation between experimental observation and prediction based on an assumed homogeneous deformation [22–26]. So with a better understanding of microstructurally local behaviour of high performance polycrystalline materials, the embrittlement problem may be reduced or perhaps solved by expanding the concept of microstructural local behaviour of polycrystalline engineering structural materials into design and analysis.

The local microstructural multi-physics stress induced hydrogen behaviours of the materials are strongly affected by the GB misorientation angles. The macroscopic environmental embrittlement cracking behaviour of materials is associated with local dislocation, stresses generated at the interface between crystals due to the GB misorientation angles and the accumulation, and segregation of hydrogen to

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