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Solute hydrogen effects on plastic deformation mechanisms of α-Fe with twist grain boundary

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ABSTRACT

The deformation mechanisms in the α-Fe twist bi-crystals (TBCs) containing differently angled twist grain boundaries (TGBs) are investigated carefully using the molecular dynamics modeling, with especial concerns on how solute hydrogen affects them. The results show that there are three main deformations in the TBCs, i.e. the dislocation glide-dominated mechanism, the twining-dominated mechanism, the dislocation glide and twining co-dominated mechanism, depending upon both the twist angle and the loading direction. In the dislocation glide-dominated TBCs, solute hydrogen increases the dislocation nucleation strength, dislocation mobility and dislocation density, further increases the vacancies concentration due to frequent interactions of solute hydrogen atoms with dislocations. In the dislocation glide and twining co-dominated TBCs, the solute hydrogen has weaker effect on the increase of dislocations density and the decrease of twins fraction with increasing tensile strain. However, in the twining-dominated TBCs, solute hydrogen assists the deformation twinning but doesn't increase significantly the vacancies concentration. So, it seems that twinning deformation is beneficial to resist hydrogen embrittlement (HE). These knowledge is helpful for us to understand the HE mechanism and develop new hydrogen-resistant high-strength materials.

Introduction

Hydrogen embrittlement (HE), which is an old topic since 19th century [1], exists extensively in various traditional and rising industrial fields, including aerospace engineering, oil and gas transportation, offshore platform, nuclear energy and so on. As the smallest atom in nature, hydrogen atom can easily enter the materials and then trapped by various defects (i.e. vacancy, dislocation, interface, void/crack etc.), forming various H-defect complexes. The retention of the hydrogen can heavily deteriorate the mechanical properties of advanced high strength materials, especially the ductility and toughness, which usually causes unexpected catastrophe in some important engineering structures. With the fast development and utilization of the hydrogen energy and nuclear energy, HE becomes increasingly important and a new intractable challenge for material scientists and engineers [2–6].

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Over the past more than 100 years, many scientists devoted themselves to find out the physical mechanisms causing HE. As a result of their efforts, several mechanisms were proposed to capture and explain the HE, including adsorption-induced dislocation emission mechanism (AIDE) [7], hydrogen-enhanced localized plasticity mechanism (HELP) [8], hydrogen-enhanced decohesion mechanism (HEDE) [9], hydride formation and cleavage [10,11], hydrogen-enhanced strain-induced vacancy stabilization mechanism (HEVM) [12,13] and so on. Although these mechanisms can be used to explain HE, there are still some disputes and even debates [14,15]. Strictly speaking, none of these mechanisms can explain convincingly all hydrogen embrittlement phenomena observed in different experiments. One possible reason is that the physical mechanisms causing HE are very complicated and elusive, which are affected by material chemical composition, internal microstructure and external load. In some situations, HE may be dominated by several mechanisms above mentioned at the same time. However, fundamentally speaking, the complexity of HE mechanism is mainly derived from those intricate interactions between hydrogen and various defects in materials [16]. So, an effective way to reveal the complicated HE mechanism is study those interactions of solute hydrogen with various defects.

As we know, there are various defects in materials, including the vacancy (point defect), dislocation (linear defect), interface/grain boundary (planar defect) and void/crack (volume defect). Among all interactions between hydrogen and various defects, one of the most important concerns is how the solute hydrogen influences the behaviors of dislocation which is the main carrier of plasticity. By means of the *in-situ* TEM technology, it was observed that hydrogen could enhance the dislocation sources operation [17] as well as the dislocation motion [18], which was considered a strong evidence of the HELP mechanism. An explain for the HELP mechanism is that hydrogen reduces the shear modulus, dislocation line energy and stacking fault energy [19]. Just recently, Xie et al. [20] employed the environmental transmission electron microscope to observe the dislocation motion in the compressed micro-pillars, they found that in hydrogen atmosphere some mobile dislocations loses their mobility, disagreeing with the HELP mechanism. They attributed the loss of dislocation mobility to the pinning effects of superabundant hydrogenated vacancies on the dislocations, supporting the HEVM [12] to some extent. Besides these, other experiments showed that hydrogen could affect the evolution of dislocations in a variety of ways. For instance, hydrogen was considered to play a role of temporary alloying addition and thus could increase the dislocation density in the cold-deformed Pd [21]; however, the positron lifetime spectroscopy analysis showed that hydrogen could enhance the generation of vacancies rather than dislocations in Fe [22]. Recently, in the shock-loaded Pd samples, it was found that hydrogen not only could cause a high density of dislocations but also small vacancy clusters by agglomeration of deformation-induced vacancies [23]. From these, it appears that there are still disagreement on whether hydrogen facilitates or inhibits the nucleation and movement of dislocations.

In addition to dislocation, twinning is another important carrier of plastic deformation. In recently developed TWIP steels which display excellent workability, deformation twinning is frequently observed due to lower stacking fault energy (SFE) [24,25]. As we know, hydrogen can lower the SFE of some materials [26,27] and thus contribute to the development of mechanical twinning and increase the work hardening of high strength materials. Although hydrogen is often considered to be a negative solute element that can heavily deteriorate mechanical properties of advanced high strength materials, it also can affect positively the tensile elongation and strength of materials in some situations. For example, in some hydrogen-charged single crystalline and polycrystalline austenite steels, hydrogen indeed promotes the development of twinning and a change in deformation mechanism from multiple slip to twinning. Due to a substantial activation of mechanical twinning in the hydrogen-charged samples, an increase in elongation to fracture is caused although a brittle component on the fracture surfaces still is observed [28–30]. Similar to this, in the equiatomic CoCrFeMnNi high-entropy alloy (HEA), hydrogen also can enhance its nano-twinning capacity, resulting in increase of the strength and ductility [31]. However, in the H-charged Inconel-725 Ni-base superalloy, twins at surface facilitate crack initiation but those in the interior resist crack propagation, playing dual role in HE [32]. Furthermore, owing to very high stress concentration at the deformation twin tip, deformation twins in the H-charged Fe–Mn–C TWIP steel can assist intergranular cracking and crack propagation and thus accelerate the HE [33]. These convincing experiments show that hydrogen also plays an important role in the twin deformation dominated plasticity, which can improve tensile elongation under certain optimal conditions by promoting deformation twinning but also can assist cracking and accelerate embrittlement.

By this token, hydrogen has negative and opposite effects on twinning and dislocation dominated plastic deformation and fracture in some pure metals or alloys, depending upon the microscopic structure and chemical composition of materials. A deeper understanding of hydrogen effect on the twinning and dislocation dominated plastic deformation is very necessary to exploit the hydrogen embrittlement mechanism. Motivated by this, the twist bi-crystals (TBCs), where dislocation glide or twinning dominates plastic deformation which closely depend upon the feature of initial twist grain boundary (TGB), are considered. Considering the MD simulation can capture the atom details and a large number of MD simulations have been successfully performed to shed light on HE mechanisms [10,34,35], it is employed here to reveal the hydrogen effect on the dislocation or twinning dominated plastic deformation mechanism in the TBCs. The paper is organized as follow: The details of the simulation setup are given in Section The details of simulation setup. The plastic deformation mechanisms and the solute hydrogen effects on them are presented in Section Main results. The hydrogen effects on the damage of TGBs are discussed in Section Discussion, followed by the main conclusions in Section Conclusions.

The details of simulation setup

The models of the bi-crystal with (001) TGB are constructed by rotating the grains 1 and 2 about the (001) crystallographic