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Hydrogen-enhanced interfacial damage in Ni-based single crystal superalloy

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ABSTRACT

The effect of hydrogen (H) on the interfacial damage in Ni-based single crystal superalloy is investigated by utilizing the molecular dynamics (MD) method. Accompanying the motion of misfit dislocation networks on the γ/γ′ interphase, more vacancies can form on the γ/γ′ interface with higher pre-charged H concentration. With the same H concentration, hydrogen-enhanced vacancies can more easily form at a low temperature than a high temperature. Meanwhile, hydrogen can facilitate the reaction and dissociation of interfacial dislocation segments, aggravating subsequent damage of the interfacial dislocation networks. These results shall enrich our understanding on the hydrogen embrittlement of the Ni-based single crystal superalloy.

Hydrogen, the smallest atom in nature, can enter the metallic lattice and diffuse rapidly until it is trapped by vacancy, dislocation, interface, crack or any other defects in metals [1,2]. The retention of hydrogen causes unforeseeable accidents by degrading the mechanical properties of metals [3,4] and their alloys [5–7], which is known as hydrogen embrittlement (HE) [2,8,9]. Ni-based single crystal superalloy, which has a unique two-phase microstructure with $L1_2$ ordered cuboidal γ′ precipitates embedded in the FCC γ matrix, is the preferred material for turbine blades on gas turbines and aero engines. When exposed to an aggressive environment, a turbine blade endures not only high pressure (HP)/high temperature (HT) but also the threat of HE due to the presence of hydrogen gas and its compounds. Besides, with the fast development and increasing utilization of hydrogen energy, HE of a Ni-based single crystal superalloy [10–12] is also becoming a severe challenge in the design and development of hydrogen-fueled engines in aerospace engineering. Under these circumstances, fundamental knowledge of the hydrogen effect on the Ni-based single crystal superalloy is critically important. Previous research has shown that hydrogen could boost dislocation accumulation in the γ matrix and cross-slip of super-dislocations, enhancing flow stress and work hardening [13]. In addition, the fatigue life of a hydrogen-charged Ni-based single crystal superalloy CMSX-2 is also significantly reduced compared with hydrogen-free CMSX-2 [14]. The fractographic analysis showed that the fracture surface of CMSX-2 transited from the octahedral {111} slip planes in uncharged samples to the {100} γ/γ′ interphases in hydrogen-charged samples [15]. First principles studies showed that the hydrogen can be segregated to the γ/γ′ interphase, causing severe embrittlement at the corresponding location [16,17]. Recent experiments also proved that hydrogen can significantly degrade interfacial integrity at elevated temperatures [18]. Presumably, hydrogen will also play an important role in the interphase failure of the Ni-based single crystal superalloy. As is known, to accommodate the misfit strain between γ/γ′ phases due to the lattice mismatch, dense misfit dislocations prefer to form on the γ/γ′ interphases [19–21] and tightly wrap the cuboidal γ′ precipitates. The destruction of interfacial dislocation networks can cut down the creep resistance [22–24] and accelerate the failure of the Ni-based single crystal superalloy. According to these results, hydrogen can be easily trapped by interfacial dislocation networks and can be segregated to γ/γ′interfaces after it enters the Ni-based single crystal superalloy [10,16,17]. How will these trapped or segregated hydrogen atoms damage the γ/γ′ interface in the Ni-based single crystal superalloy? This has always been one of the issues concerning hydrogen embrittlement failure in the Ni-based single crystal superalloy.

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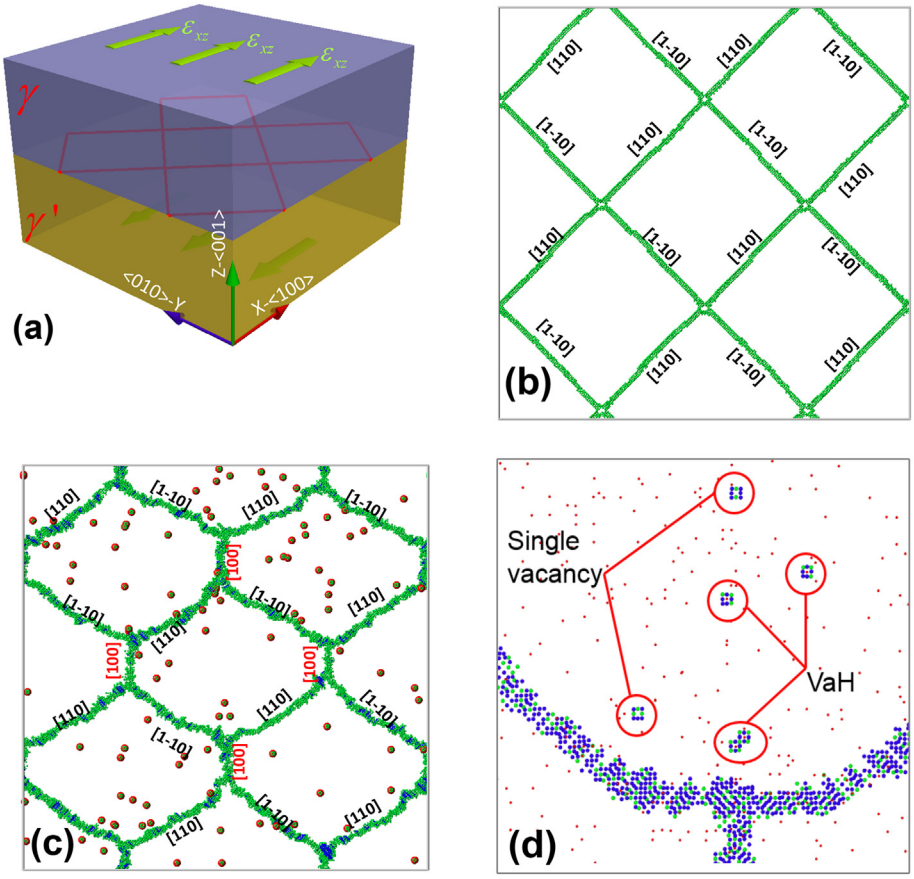

Fig. 1. (a) The illustration of the γ/γ′ bilayer model; (b, c) the configuration of interfacial dislocation networks at the shear stain of 25%, where T = 10 K and the H concentration is 0 and 5 at. % H, respectively; (d) atomic details of the single vacancies and Va-H complexes on the interface.

To uncover the mystery, the MD method, an effective approach to expose the deformation or failure mechanism at the nano-scale [25, 26], is adopted here. A bilayer model is constructed, as illustrated in Fig. 1(a). The orthogonal lattice directions in both γ and γ′ phases are aligned along [100], [010] and [001], respectively. Periodic boundary conditions are imposed along the x and y directions parallel to the interphase, while a free boundary condition is employed along the z direction. To include sufficient interfacial dislocations, a computational model with the dimensions of 53nm × 53nm × 20nm is considered. According to the selected embedded atom method (EAM) potential [27] which accurately describes theNi-Al-H system, the lattice constants of Ni and Ni_3Al are taken as $a_\gamma = 0.352$nm and $a_{\gamma'} = 0.3568$-nm.That can cause a lattice mismatch of about 1.35% on the γ/γ′ interphase [28] which is close to that of the fourth generation Ni-based single crystal superalloy. After carrying out energy minimization by utilizing the conjugate gradient (CG) algorithm, square-like interfacial dislocation networks form on the γ/γ′ interphase, as illustrated by the red lines in Fig. 1(a). To investigate the phenomenon that hydrogen prefers to be segregated to the γ/γ′ interface revealed by previous first principles studies [17], hydrogen atoms are randomly distributed within a 2 nm layer region in the vicinity of the γ/γ′ interphase, with three concentrations of 2, 5, and 7 at. % H considered, respectively. When energy minimization and heating process are imposed subsequently, hydrogen atoms are able to find their energy favorable Octahedral interstitial sites (O-site) in the γ phase and the O-sites surrounded by six Ni atoms in the γ′ phase. This is consistent with the result reported in literature [29]. Due to misfit dislocation networks on the γ/γ′ interface, some hydrogen atoms located near the interfacial dislocation segments are attracted to the tensile side of interfacial dislocation. Finally, shear strain ε_{xz} parallel to the γ/γ′ interphase is applied to the outermost layer of atoms in the ±Z directions, which drive the motion of the interfacial dislocation networks. The system temperature is maintained at 10 K, 300 K, or 600 K during the loading process, respectively, in order to investigate effects of hydrogen at different temperatures. The shear strain rate of $10^9 s^{-1}$ is adopted to reduce the computational burden. All simulations are performed using MD simulator LAMMPS [30]. The dislocation and vacancy details are identified by Atomviewer [31].

First, the results at low temperature are examined. Figs. 1(b) and 1(c) show the configurations of the interfacial dislocation networks at a strain of 25% with concentrations of 0 and 5 at. % H, respectively. For the H-free case, the interfacial dislocation segments glide consistently in the loading direction, neither the dislocation network's shape changes nor does any vacancy occur, as shown in Fig. 1(b) and Supplementary Movie 1. Nevertheless, as shown in Fig. 1(c), square-like dislocation networks gradually transform into hexagonal-like ones accompanying the movement of dislocation network segments in the H-charged case. This geometric structural change of the interfacial dislocation networks is sustained by the dislocation reaction of $a/2[110] + a/2[1\bar{1}0] = a[100]$, which has been observed in both numerical simulations [28] and experimental observation [19]. Meanwhile, an interesting phenomenon can be found. A large amount of vacancies (represented by large red spheres in Fig. 1(c)) form on the γ/γ′ interface accompanying the motion of the dislocation networks due to the presence of pre-charged H atoms (see also online Supplementary Movie 2). This indicates the pre-charged H facilitates not only the reaction of the interfacial dislocation network segments but also the nucleation of interfacial vacancies. A