Atomistic Study on the Microscopic Mechanism of Grain Boundary Embrittlement Induced by Small Dense Helium Bubbles in Iron

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Abstract

The helium bubbles induced by 14 MeV neutron irradiation can cause intergranular fractures in reduced activation ferritic martensitic (RAFM) steel, which is a candidate structural material for fusion reactors. In order to elucidate the susceptibility of different grain boundaries (GBs) to helium-induced embrittlement, the tensile fracture processes of 10 types of GBs with and without helium bubbles in body-centered cubic (bcc) iron at the relevant service temperature of 600 K were investigated via molecular dynamics methods. The results indicate that in the absence of helium bubbles, the GBs studied here can be classified into two distinct categories: brittle GBs and ductile GBs. The atomic scale analysis shows that the plastic deformation of ductile GB at high temperatures originates from complex plastic deformation mechanisms, including the Bain/Burgers path phase transition and deformation twinning, in which the Bain path phase transition is the most dominant plastic deformation mechanism. However, the presence of helium bubbles severely inhibits the plastic deformation channels of the GBs, resulting in a significant decrease in elongation at fractures. For bubble-decorated GBs, the ultimate tensile strength increases with the increase of the misorientation angle. Interestingly, the coherent twin boundary $3\{112\}$ was found to maintain relatively high fracture strength and maximum failure strain under the influence of helium bubbles.

Full Text

Preamble

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Abstract

Helium bubbles induced by 14 MeV neutron irradiation can cause intergranular fractures in reduced activation ferritic martensitic (RAFM) steel, a candidate structural material for fusion reactors. To elucidate the susceptibility of different grain boundaries (GBs) to helium-induced embrittlement, we investigated the tensile fracture processes of ten types of GBs with and without helium bubbles in body-centered cubic (bcc) iron at the relevant service temperature of 600 K using molecular dynamics methods. Our results indicate that in the absence of helium bubbles, the studied GBs can be classified into two distinct categories: brittle GBs and ductile GBs. Atomic-scale analysis reveals that the plastic deformation of ductile GBs at high temperatures originates from complex mechanisms, including the Bain/Burgers path phase transition and deformation twinning, with the Bain path phase transition being the dominant mechanism. However, the presence of helium bubbles severely inhibits these plastic deformation channels, resulting in a significant decrease in elongation at fracture. For bubble-decorated GBs, the ultimate tensile strength increases with increasing misorientation angle. Interestingly, the coherent twin boundary $3\{112\}$ maintains relatively high fracture strength and maximum failure strain even under the influence of helium bubbles.

Keywords: Helium bubble; Grain boundary; Embrittlement; Reduced activation ferritic martensitic steel; Molecular dynamics; Bain path

1. Introduction

Reduced activation ferritic martensitic (RAFM) steel and its improved variants, such as oxide dispersion strengthened (ODS), thermomechanically treated (TMT), and castable nanostructured alloys (CNA) steels, are primary candidate structural materials for future fusion and advanced fission reactors due to

their excellent irradiation resistance, high-temperature performance, and high technological maturity [**?**]. However, in fusion reactor service environments, high-energy neutron irradiation introduces large quantities of helium atoms (up to 10–15 appm/dpa) into structural steel through (n, α) reactions [**?**]. Due to the extremely low solubility of helium in metallic alloys, helium atoms strongly tend to coalesce into nanometric bubbles. These bubbles preferentially nucleate and grow at intrinsic or irradiation-induced defects with substantial free volume, such as grain boundaries (GBs) and dislocations. While helium can contribute to safe material performance in some fission reactor applications, such as protecting fuel rod cladding integrity [**?**], it is detrimental to fusion reactor structural materials. A high density of helium bubbles at GBs can significantly weaken GB cohesive strength, reduce fracture stress, and exacerbate RAFM steel failure through intergranular fracture. Therefore, elucidating the underlying mechanism of helium-induced GB embrittlement and establishing the relationship between helium embrittlement susceptibility and GB structural characteristics is essential for exploring methods to improve RAFM steel resistance against helium-induced GB embrittlement.

Few experiments have investigated the mechanical response of individual GBs to helium. Miura et al. [**?**] studied the effect of helium on fracture properties of six different non-coincidence site lattice GBs in austenitic stainless steel using micro-tensile tests combined with electron backscatter diffraction (EBSD) and focused ion beam (FIB) techniques, finding that GB segregation capacity for helium impurities plays an important role in GB helium embrittlement. However, no such micro-tensile test results have been reported for RAFM steels.

Atomic-scale simulation methods provide a convenient approach for investigating the mechanical behavior of different GB types under helium bubble influence. Terentyev et al. [**?**] used uniaxial tensile simulations to study helium bubble effects on fracture processes of six different GBs with <110> tilt axis at 0 K in body-centered cubic (bcc) iron, demonstrating that helium bubbles substantially affect GB fracture stress and strain while intensively suppressing slip-related plastic deformation. Our previous work [**?**] investigated the effect of small helium-vacancy clusters on tensile deformation of two symmetric tilt grain boundaries (STGBs) with <110> and <100> tilt axes at 0 K and 300 K, revealing that helium-vacancy clusters significantly suppress GB sliding and that cluster size effects appear stronger than He/V ratio effects. However, whether the helium embrittlement mechanism changes for different GBs remains unclear.

Moreover, previous simulation studies created single helium bubbles by removing Fe atoms from spherical regions and filling them with helium atoms, without considering GB effects on helium segregation. In our recent work [**?**], we comprehensively investigated how GB characteristic parameters affect helium segregation, bubble nucleation, and growth processes in bcc iron under high-energy neutron irradiation conditions. Spatial distributions of helium bubbles in bubble-decorated bicrystal models were obtained through kinetic evolution at 600 K with a helium concentration of 2000 appm. In this paper, we performed

uniaxial tensile simulations of ten different clean GBs (four with <100> tilt axis and six with <110> tilt axis) and their corresponding bubble-decorated GBs at 600 K using molecular dynamics methods. Experimental characterization of ferritic steels has shown that several of these GBs appear at higher concentrations than random GBs [**?**, **?**]. By comparing and analyzing tensile processes of clean and bubble-decorated GBs, we studied the microscopic mechanism of helium-induced GB embrittlement at high temperatures and correlated fracture strength and strain of bubble-decorated GBs with GB misorientation angle to characterize helium embrittlement susceptibilities of different GBs.

2. Simulation Methods

We used the parallel molecular dynamics (MD) code LAMMPS [**?**, **?**] to simulate tensile processes of GBs in bcc iron with and without helium bubbles. The s-band Fe-He many-body potential [**?**], combined with the Fe-Fe potential of Ackland and Mendelev [**?**] and He-He potential of Aziz [**?**, **?**], was selected to describe interatomic interactions in the Fe-He system. Based on this potential set, calculated properties show good agreement with experimental and ab initio data demonstrated in previous works [**?**].

Based on coincidence site lattice (CSL) theory, we constructed ten types of STGBs that experimental studies have observed at higher concentrations than random GBs [**?**, **?**] using the bicrystal method. The GB is located at the interface between two perfect grains with different orientations. Detailed parameters for these GBs are listed in Table 1. To obtain equilibrium GB structures, we sampled over 10,000 structures using rigid body translations. The displacement shift complete lattice was used to characterize the translational vector, with the equilibrium structure identified as the optimized lowest-energy configuration. Table 2 compares GB energies calculated in this work with results from DFT calculations [**?**] and other MD calculations [**?**, **?**]. Most GB energy values from our work are consistent with other MD calculations but slightly lower than DFT results. Details of the bicrystal method for GB structure construction can be found in Refs. [**?**]. In the simulation box Cartesian coordinate system, the tilt axis aligns with the z-direction and the GB normal is parallel to the y-direction. Figure 1 shows side views of supercells for the ten different STGBs, with structural units comprising each GB marked in the figure.

Table 1. Detailed parameters of the studied STGBs. These include tilt axis (<110> and <100>), coincidence index ( ), GB plane index, misorientation angle ( ) in degrees, total number of iron atoms (NFe), initial supercell dimensions (Lx, Ly, and Lz) in nanometers, number density of GB helium bubbles (DHe) in m^{-3}, and average diameter of GB helium bubbles (Da) in nm.

Tilt Axis	GB Plane	(deg)	NFe	Lx (nm)	Ly (nm)	Lz (nm)	DHe (10^{26} m^{-3})	Da (10^{-1} nm)
<110>	{111}	109.47	300000	17.5	24.8	–	–	–
<110>	{112}	70.53	302400	17.3	25.2	–	–	–
<110>	{114}	38.94	286400	17.1	24.2	–	–	–
<110>	{221}	141.06	300160	17.0	25.5	–	–	–
<110>	{113}	50.48	297440	17.4	24.7	–	–	–
<110>	{332}	129.52	285120	17.0	24.1	–	–	–
<100>	{210}	53.13	299488	17.9	24.5	–	–	–
<100>	{310}	36.87	297920	17.2	25.3	–	–	–
<100>	{320}	67.38	296072	17.5	24.7	–	–	–
<100>	{510}	22.62	313152	17.5	26.1	–	–	–

Note: Some parameter values were not fully preserved in the original text.

Table 2. Comparison of GB energies (EGB, in J/m^2) calculated in this work with literature values.

STGB Type	EGB (J/m^2)	MD Calculations	DFT Calculations
3<110>{111}	1.308	1.308a, 1.295b	1.51e, 1.52f, 1.53g
3<110>{112}	0.260	0.260a, 0.262b	0.34f, 0.43g, 0.45h
5<100>{210}	1.113	1.113a	1.61g, 1.64h
5<100>{310}	1.008	1.008a, 1.19c	1.48e, 1.49f, 1.53g
9<110>{114}	1.286	1.286a,b, 1.40d	1.50e,h, 1.38g
9<110>{221}	1.168	1.172a, 1.167b	1.66h, 1.71i, 1.62j
11<110>{113}	1.113	1.113a, 1.03c	1.45h, 1.44j
11<110>{332}	1.019	1.02a, 1.00d	1.38g, 1.47h, 1.49i
13<100>{320}	1.108	1.108a	1.53h
13<100>{510}	1.005	1.005a	1.40h

aRef. [**?**]; bRef. [**?**]; cRef. [**?**]; dRef. [**?**]; eRef. [**?**]; fRef. [**?**]; gRef. [**?**]; hRef. [**?**]; iRef. [**?**]; jRef. [**?**].

The helium concentration in structural steels for a fusion power plant first wall can reach 1090 appm after 5 years [**?**] and 2000 appm after longer service times [**?**]. Therefore, we set the initial helium concentration in our simulations to 2000 appm to study GB mechanical properties at high He concentrations. Initially, all helium atoms were randomly distributed in the bicrystal model. A stable helium bubble distribution was obtained after 1.6 ns of MD evolution with the NPT ensemble at 600 K. This bicrystal model with helium bubble distribution was then used as the initial configuration for GB tensile simulations. Detailed procedures for building bubble-decorated GB initial models and quantitative helium bubble information can be found in our previous work [**?**]. Due to high

helium yields, spallation neutron irradiation is widely used to test fusion reactor candidate materials. The distribution of high-density, small-sized helium bubbles on GBs in our bubble-decorated bicrystal models (Fig. 2(b)) is consistent with bubble distributions observed on GBs in spallation neutron-irradiated RAFM steel specimens (Fig. 2(c, d)) reported in Refs. [**?**, **?**].

Uniaxial tensile simulations for GBs with and without helium bubbles were performed under identical conditions. The tensile strain rate was set to 10^8 s^{-1} after comparison tests with 10^7 s^{-1} and 10^9 s^{-1} showed that GB deformation mechanisms remain unchanged across different strain rates. At 10^8 s^{-1}, relatively accurate fracture strength and strain values can be obtained while significantly reducing computational costs. The uniaxial tensile load was applied perpendicular to the GB plane. Periodic boundary conditions were applied along the x and z directions. To avoid boundary atom interactions in the y-direction, iron atoms more than 120 nm from the GB plane were removed to create a vacuum layer, as shown in Fig. 2. Iron atoms located 115–120 nm from the GB plane were fixed to control tensile strain. Strain was applied by moving both fixed layers—one in the positive y-direction and the other in the negative y-direction—while remapping remaining atom coordinates. Each strain step increased strain by 0.01%, followed by 1.0 ps relaxation with the NVT ensemble. This process was repeated cyclically until bicrystal fracture occurred. After each strain step relaxation, strain and stress in the y-direction were recorded to analyze GB tensile deformation. Atomic configuration visualization and analysis were performed using dislocation extraction analysis (DXA) and common neighbor analysis (CNA) as implemented in OVITO [**?**].

Figure 2. Uniaxial tensile models of (a) clean GB and (b) bubble-decorated GB, using 3<110>{112} GB as an example. Red spheres in panel (b) represent helium atoms, while blue spheres in both figures represent iron atoms. Vacuum layers, fixed layers, and GB planes are indicated by black, red, and green rectangular boxes, respectively. Panels (c) and (d) [**?**] show high-density distributions of small-scale helium bubbles at GBs in RAFM steel irradiated by spallation neutrons.

3. Results

The studied GBs can be classified into two categories based on clean GB tensile behavior: (1) brittle GBs with no plastic deformation stage, including 3{111}, 9{114}, and 9{221} GBs (hereafter, tilt axis notation is omitted), and (2) ductile GBs with a plastic deformation stage. Ductile GBs exhibit complex plastic deformation mechanisms at high temperatures, which we classify into three categories: (1) Bain path phase transition with lath structure, occurring in 5{210}, 5{310}, 13{320}, and 13{510} GBs; (2) deformation twinning, which only occurs in the twin boundary 3{112}; and (3) holonomic Bain/Burgers path phase transition, occurring in 11{113} and 11{332} GBs. To comprehensively study plastic deformation behaviors of different clean GBs and elucidate helium bubble effects on tensile deformation, we investigated GB tensile processes in detail

by combining stress-strain curve analysis with atomic configuration analysis.

Figure 3 shows tensile deformation processes for 5{210}, 5{310}, 13{320}, and 13{510} GBs via the first mechanism: Bain path phase transition with lath structure. The results indicate that during uniaxial tensile simulations, all four clean GBs underwent a plastic deformation stage where stress first dropped rapidly then increased slowly. Using 5{310} GB as an example, Fig. 3(b–e) shows atomic configurations of the bicrystal at different deformation stages, with corresponding stress and strain values indicated by stars in Fig. 3(a). The initial GB configuration remained intact at high temperatures (Fig. 3(b)). During the elastic stage, stress increased linearly with strain without initial phase transition. When strain reached 7.28% and corresponding stress reached 9.77 GPa, the GB region in the upper grain began undergoing Bain path phase transition (bcc to fcc) (Fig. 3(c)). As tensile strain increased, the phase transition region expanded toward the fixed ends in both upper and lower grains, forming fcc lath grains in the transition region (Fig. 3(d)). With further strain increase, the phase transition region continued expanding, increasing lath grain size. Fig. 3(i) shows the largest phase transition region covering nearly entire grains. After strain reached 18.95%, cracks initiated at the GB plane. However, Fig. 3(a) shows that with helium bubbles present, none of the four GBs exhibited a plastic deformation stage. Elongation at fracture decreased sharply, and ultimate tensile strength also decreased. Fig. 3(f–i) shows atomic configurations of crack initiation in bubble-decorated 5{210}, 5{310}, 13{320}, and 13{510} GBs. No phase transition regions appeared in grains before bicrystal fracture. When applied stress surpassed a certain threshold, dislocation loops nucleated around helium bubbles in the bulk, gradually growing until reaching the fixed end of the bicrystal model and absorbing part of the strain energy. Additionally, helium bubbles at the GB reduced boundary bonding area, leading to decreased cohesive strength. In this case, fracture stress was lower than the critical stress for Bain path phase transition, meaning helium bubbles at the GB inhibited the Bain path phase transition channel, causing brittle rupture at the GB.

Figure 3. Stress-strain curves and atomic configurations of GBs with Bain path phase transition and lath structure. (a) Stress-strain curves of 5{210}, 5{310}, 13{320}, and 13{510} GBs with (dotted line) and without (solid line) helium bubbles. Panels (b–e) illustrate atomic configurations of clean 5{310} GB at different deformation stages. Blue, green, red, and white spheres represent iron atoms with bcc, fcc, hcp, and other structures, respectively. Panels (f–i) illustrate atomic configurations of crack initiation in bubble-decorated 5{210}, 5{310}, 13{320}, and 13{510} GBs, respectively. Parts of curves are horizontally translated for clarity. Blue spheres, red spheres, green lines, and pink lines represent iron atoms, helium atoms, ½<111> dislocations/dislocation loops, and <100> dislocations/dislocation loops, respectively. Black rectangles indicate crack initiation regions.

The tensile deformation process of 3{112} GB via the second mechanism—deformation twinning—is analyzed in Fig. 4. 3{112} GB is a unique twin

GB, and tensile loading along the <112> orientation activates its twin system {112}<111> [**?**, **?**]. Fig. 4(a) shows the stress-strain curve for clean 3{112} GB, exhibiting a fluctuating increase during plastic deformation. Atomic configurations of clean 3{112} GB during uniaxial tensile testing explain this phenomenon (Fig. 4(b–f)), with corresponding stress and strain values indicated by stars in Fig. 4(a). Unlike other GBs, the initial 3{112} GB configuration is a narrow region consisting of two atomic layers, reflecting its peculiarity as a twin GB (Fig. 4(b)). Stress increased linearly with strain during the elastic stage without phase transition. When tensile strain reached 8.13% and corresponding stress rose to 12.78 GPa, the GB plane began slipping along the (1-21)[111] slip system toward the fixed end, forming deformation twins perpendicular to the original GB plane (Fig. 4(c, d)). The structures of these deformation twins were entirely consistent with the original twin boundary. Thereafter, deformation twin shape and size were gradually optimized under applied stress (Fig. 4(e)). Fig. 4(h) shows that these deformation twin structures closely match those observed in RAFM [**?**, **?**] and austenitic steels [**?**] via TEM. However, the critical stress for deformation twinning differed significantly, mainly due to the high strain rate in MD simulations. During twinning, tensile stress rose in a fluctuating manner. With further strain increase, the high-stress state at the fixed end led to Bain path phase transition near the newly formed twin boundaries (Fig. 4(f)). Deformation twinning refined the newly formed grains, quickly hindering phase transition region expansion. Eventually, the bicrystal fractured at the interface between the deformation twin boundary and fixed end, consistent with experimental findings that deformation twins can act as micro-crack initiators (Fig. 4(i)) [**?**]. The stress-strain curve for bubble-decorated 3{112} GB is shown as a dashed line in Fig. 4(a). Compared with clean 3{112} GB, fracture strength and elongation of the bubble-decorated GB are much lower, with fracture stress below the critical stress for deformation twinning. Although deformation twinning was inhibited, the twin boundary retained some plasticity under helium bubble influence, deriving from relatively active dislocation evolution at the crack tip (Fig. 4(g)).

Figure 4. Stress-strain curves and atomic configurations of 3{112} GB with deformation twins. (a) Stress-strain curves of 3{112} GBs with (dotted line) and without (solid line) helium bubbles. Panels (b–f) illustrate atomic configurations of clean 3{112} GB at different deformation stages. Blue, green, red, and white spheres represent iron atoms with bcc, fcc, hcp, and other structures, respectively. Panel (g) illustrates crack initiation atomic configuration of helium bubble-decorated 3{112} GB. Blue spheres, red spheres, green lines, and pink lines represent iron atoms, helium atoms, ½<111> dislocations/dislocation loops, and <100> dislocations/dislocation loops, respectively. Panel (h) [**?**] shows deformation twin structure observed during tensile tests under TEM. Panel (i) [**?**] shows microcrack initiation caused by deformation twins.

Figure 5 shows tensile deformation processes for 11{113} and 11{332} GBs via the third mechanism: holonomic Bain/Burgers path phase transition. Fig. 5(a) shows that both clean GBs underwent plastic deformation with constant

stress during uniaxial tensile simulations. However, atomic-scale analysis revealed different phase transition mechanisms. Fig. 5(b–e) shows atomic configurations of 11{332} GB with Burgers path phase transition (bcc to hcp) at different stages, with corresponding stress and strain indicated by stars in Fig. 5(a). Fig. 5(g–j) shows atomic configurations of 11{113} GB with Bain path phase transition at different stages, with corresponding stress and strain also indicated by stars in Fig. 5(a). Initial configurations of 11{332} and 11{113} GBs differed, with some atoms at the 11{332} GB plane having configurations similar to hcp crystals, providing numerous nucleation sites for Burgers path phase transitions, while 11{113} GB lacked such structure. When strain increased to 7.64%/7.0%, Burgers/Bain path phase transitions began progressing steadily perpendicular to the original GB plane in 11{332} and 11{113} GBs, respectively (Fig. 5(c, h)). As strain increased, bcc-structure atoms on both sides of the GB continuously transformed into hcp or fcc structures while the bcc-hcp or bcc-fcc phase boundary moved toward the bicrystal fixed end. During this period, stress remained almost constant with increasing strain. Once strain reached 10.86%/13.00%, hcp/fcc region volume reached maximum values for 11{332} and 11{113} GBs, respectively (Fig. 5(d, i)). Typically, phase transition continues until the phase boundary reaches the fixed end at 0 K [**?**]. However, at high temperatures the phase boundary is unstable. For 11{332} GB, stacking fault slip occurred at the upper bcc-hcp phase boundary, disrupting the Burgers path phase transition and further destroying the transition region (Fig. 5(e)). For 11{113} GB, dislocations emitted from the lower bcc-fcc phase boundary and piled up at the lower grain fixed end, causing stress concentration and grain cracking (Fig. 5(j)). Additionally, under high temperature effects, 11{113} GB exhibited a brief stress decrease at plastic deformation onset, related to dislocation emission at the GB that divided the phase transition region into two parts (Fig. 5(i)). Finally, when strain reached 10.96%/13.42%, initial cracks formed in the slip band for 11{332} GB or at the lower fixed end for 11{113} GB (Fig. 5(e, j)). In contrast, no phase transition occurred during tensile deformation of bubble-decorated 11{332} and 11{113} GBs, with initial cracks appearing at the grain boundary (Fig. 5(f, k)). Fracture stress was lower than critical stress for Bain/Burgers path phase transitions, leading to brittle fracture and noticeable elongation reduction.

Figure 5. Stress-strain curves and atomic configurations of GBs with holonomic Bain/Burgers path phase transitions. (a) Stress-strain curves of 11{113} and 11{332} GBs with (dotted line) and without (solid line) helium bubbles. Panels (b–e) and (g–j) illustrate atomic configurations of clean 11{332} and 11{113} GBs at different deformation stages, respectively. Blue, red, green, and white spheres represent iron atoms with bcc, hcp, fcc, and other structures, respectively. Panels (f) and (k) illustrate crack initiation atomic configurations of helium bubble-decorated GBs. Blue spheres, red spheres, and green lines represent iron atoms, helium atoms, and ½<111> dislocations/dislocation loops, respectively.

Figure 6 shows fracture processes for three brittle GBs— 3{111}, 9{114}, and

9{221}—with and without helium bubbles. Fig. 6(a) shows that the three clean GBs have similar stress-strain curves. Fig. 6(b–d) presents atomic configurations of the three clean GBs just before fracture, with corresponding stress and strain indicated by stars in Fig. 6(a). Under combined high temperature and stress effects, GB regions in these bicrystals widened and original GB structure units were completely lost, with atomic spatial distribution in the GB region becoming abnormally disordered [**?**]. This GB structural disorder hindered the aforementioned phase transition paths, making atomic disorder the fundamental cause of brittle fracture in clean GBs. Fig. 6(e, f) shows that tensile behavior of bubble-decorated brittle GBs is similar to bubble-decorated ductile GBs, with helium bubbles decreasing both fracture strength and elongation to varying degrees.

Figure 6. Stress-strain curves and atomic configurations of brittle GBs. (a) Stress-strain curves of 3{111}, 9{114}, and 9{221} GBs with (dotted line) and without (solid line) helium bubbles. Panels (b–d) illustrate atomic configurations of clean 3{111}, 9{114}, and 9{221} GBs under ultimate tensile stress, respectively. Blue, green, and white spheres represent iron atoms with bcc, fcc, and other structures, respectively. Panels (e–g) present crack initiation atomic configurations of bubble-decorated 3{111}, 9{114}, and 9{221} GBs, respectively. Blue spheres, red spheres, and green lines represent iron atoms, helium atoms, and ½<111> dislocations/dislocation loops, respectively.

4. Discussion

To further analyze the role of Bain path phase transition in ductile GB plastic deformation, we investigated orientation relationships during bcc-to-fcc Bain path phase transitions (Fig. 7). Fig. 7(a–e) shows crystal plane and crystallographic direction correspondences between bcc and fcc phases for 5{210}, 5{310}, 13{320}, 13{510}, and 11{113} GBs during phase transition. During bcc-to-fcc structure transformation, the <110>α direction in the bcc structure remained parallel to the <121>γ direction in the fcc structure, and the {110}α plane in the bcc structure remained parallel to the {111}γ plane in the fcc structure. Fig. 7(f) presents a schematic diagram of the Bain path phase transition, showing that approximately 40% tensile deformation along the y-axis (<100> crystal direction)—elongating the lattice constant in the y-direction from original a to $\sqrt{2}a$—transforms the original bcc unit cell into an fcc unit cell. The newly formed fcc unit cell has a lattice constant of $2a$ and can therefore store higher strain energy than the original bcc unit cell with lattice constant a. For crystal planes, {111}γ planes in the fcc lattice correspond to {110}α planes in the bcc lattice. For crystal orientations, <112>γ in the fcc lattice corresponds to <110>α in the bcc lattice, and <110>γ in the fcc lattice corresponds to <111>α in the bcc lattice. These crystal plane and direction correspondences during GB phase transition agree with the Bain path phase transition mechanism observed in bulk material [**?**].

Figure 7. Schematic diagram of orientation relationships in Bain path phase

transition from bcc to fcc lattice. (a) 5{210}; (b) 5{310}; (c) 13{320}; (d) 13{510}; (e) 11{113}; (f) correspondence of crystal planes and crystallographic directions between bcc and fcc phases. Blue, green, and yellow spheres represent iron atoms with bcc, fcc, and hcp structures, respectively, in panels (a–e). Solid red spheres represent the original bcc lattice before phase transition in panel (f).

To investigate susceptibility of different GBs to helium embrittlement, we analyzed relationships between ultimate tensile (fracture) strength and failure (fracture) strain with misorientation angle under helium bubble influence (Fig. 8). For comparison, ultimate tensile strength and failure strain for clean GBs are also included in Fig. 8(a, b). Helium bubbles cause failure strain to drop and reduce ultimate tensile strength of individual GBs, consistent with Ref. [**?**] findings. Previous experiments show that ultimate tensile strength of helium-containing GBs relates to misorientation angle [**?**]. Our results in Fig. 8(a) further demonstrate that ultimate tensile strength generally increases with misorientation angle, showing an excellent linear relationship, particularly for <100> tilt axis GBs. Compared with clean GB tensile results, helium bubbles reduce each GB's ultimate tensile strength but do not break the relationship between ultimate tensile strength and misorientation angle.

Fig. 8(b) shows the relationship between failure strain and misorientation angle. The coherent twin boundary 3{112}, with low GB energy and sigma value, exhibited larger failure strain than other bubble-decorated GBs and the lowest strain drop among ductile GBs. Apart from 3{112} GB, fracture strain generally decreased with increasing misorientation angle. Compared with other bubble-decorated GBs, 3{112} GB displayed high ultimate tensile strength while maintaining the largest failure strain. Therefore, we suggest optimizing 3{112} GB distribution in RAFM steel through grain boundary engineering to improve resistance to GB helium embrittlement, similar to related improvements in intergranular damage resistance reported in Refs. [**?**, **?**].

Figure 8. Relationship between (a) ultimate tensile strength and (b) failure strain with misorientation angle for clean (hollow) and bubble-decorated (solid) GBs. Red circles and green squares refer to <110> and <100> tilt axis GBs, respectively.

5. Conclusions

To elucidate the microscopic mechanism of high-temperature GB helium embrittlement and susceptibility of different GB types to helium embrittlement in RAFM steel, we investigated uniaxial tensile processes of ten different clean GBs with two tilt axis types (<110> and <100>) and their corresponding bubble-decorated GBs in bcc iron at 600 K. Tensile behavior reveals that studied GBs fall into two distinct categories: brittle and ductile. Three different plastic deformation mechanisms exist in ductile GBs. The first is Bain path phase transition with lath structure, occurring only in GBs with <100> tilt axis. The second

is deformation twinning, occurring only at the unique twin GB 3{112}. The third is holonomic Bain/Burgers path phase transition, occurring in some GBs with <110> tilt axis. Atomic-scale structural analysis of tensile processes indicates that plastic deformation mechanisms of almost all ductile GBs studied here relate to Bain path phase transition, which plays a vital role in GB plastic deformation. However, helium bubble presence causes all GBs to fail via brittle fracture, decreasing both GB ultimate tensile strength and failure strain. Helium bubbles significantly reduce ductile GB failure strain by inhibiting plastic deformation channels. In helium bubble presence, GB ultimate tensile strength increases with GB misorientation angle. The coherent twin GB 3{112} maintains maximum failure strain and relatively high ultimate tensile strength under helium bubble influence.

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