Hydrogen-Induced Transformation of Dislocation Core in Fe and Its Effect on Dislocation Mobility

Md. Shahrier Hasan, Hadia Bayat, Colin Delaney, Christopher Foronda, and Wenwu Xu

Abstract In this research, we employ atomistic simulations to scrutinize the impact of hydrogen (H) on dislocation mobility in iron (Fe). Our study uncovers two critical aspects: Firstly, hydrogen atoms serve to stabilize the edge dislocation core, thereby elevating the shear stress threshold needed for dislocation mobilization. Secondly, hydrogen's influence on dislocation mobility is velocity-dependent; it enhances mobility at low velocities by diminishing lattice resistance but hampers it at high velocities due to increased viscous drag. These nuanced findings illuminate the multifaceted relationship between hydrogen atoms and dislocation mechanisms. They offer valuable insights for the development of materials with enhanced mechanical properties and contribute to strategies for mitigating hydrogen-induced material degradation.

Keywords Hydrogen embrittlement · Dislocation mobility · Atomistic modeling

Introduction

Metals and alloys are indispensable structural materials as they have the desirable combination of strength and ductility required for structural applications [1–4]. Moreover, metals and alloys allow for substantial plastic deformation before failure, making them ideal for manufacturing. This essential property of metals and alloys, however, can be negatively impacted by a phenomenon: hydrogen (H) embrittlement [5–7].

Hydrogen embrittlement is a phenomenon where metals and alloys crack or fail before reaching their fracture strength after being exposed to H. Since H atoms are much smaller than most metallic atoms, H atoms permeate through the metallic systems and can occupy interstitial and defective regions. Despite extensive research,

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the mechanism behind H's detrimental effect on metals remains debated. A cohesion-based theory, the H-enabled decohesion (HEDE), posits that H facilitates crack formation and growth in polycrystalline metals by promoting decohesion at crack tips. Another explanation about HEDE suggests that H accelerates formation of vacancies, weakening the metal [8]. It is worth noting that while HEDE is theoretically robust, experimental evidence is inconclusive. The above mechanisms explain brittle fractures, they do not account for ductile fractures, the primary failure mode in metals and alloys. Ductile failure begins with the microvoid formation near the second phase particle or precipitate in metals and alloys, followed by void coalescence and growth culminating in ductile failure. The hydrogen-enabled localized plasticity (HELP) mechanism proposes that H affects plastic deformation in metals. According to the HELP mechanism, the presence of hydrogen eases dislocation motion, reduces dislocation–dislocation interaction known as hydrogen shielding and promotes dislocation nucleation locally softening the material. This theory gains support from observation showing reduced dislocation pile-up distances in metals like steels and aluminum with higher H concentration.

Atomistic modeling is an effective tool to investigate a variety of phenomena where atomistic description of the material has a significant effect [9–13]. This research aims to examine how varying H concentrations influence dislocation core velocity in single crystal iron under shear loads. The following sections outline our Methodology, Results, and Discussions, and finally, Conclusions are drawn from the results to further our understanding of the atomistic mechanism responsible for H embrittlement.

Methodology

Periodic array of dislocation (PAD) [14] model is used to model edge dislocation inside of a single crystal BCC Fe model. Periodic boundary condition (PBC) was used in the boundary along X- and Z-directions, and shrink-wrapped boundary condition was used along the Y-direction to be used as a traction boundary. A convergence analysis with energy minimization is performed to find the minimum dimensions of the PAD model with no significant periodic effect. The dimension for the PAD model was determined to be 61[111] × 40[−110] × 12[−1−12] with 9480 atoms in pure Fe model. An edge dislocation with 1/2[111] burger vector is introduced at the center of the XZ plane by adding the upper half plane above the dislocation line with the Atomsk software tool [15]. The schematic diagram of this PAD model with the edge dislocation is shown in Fig. 1a.

The widely used Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software is then used to perform a series of molecular dynamic simulations [16]. In the PAD model, at the traction boundary along Y-direction, atoms that are six atomistic layers deep from the upper and lower regions were marked to be frozen from thermal activation. For pure metal Fe, EAM potential is used by Proville et al. that is specifically developed for simulating thermally activated glide

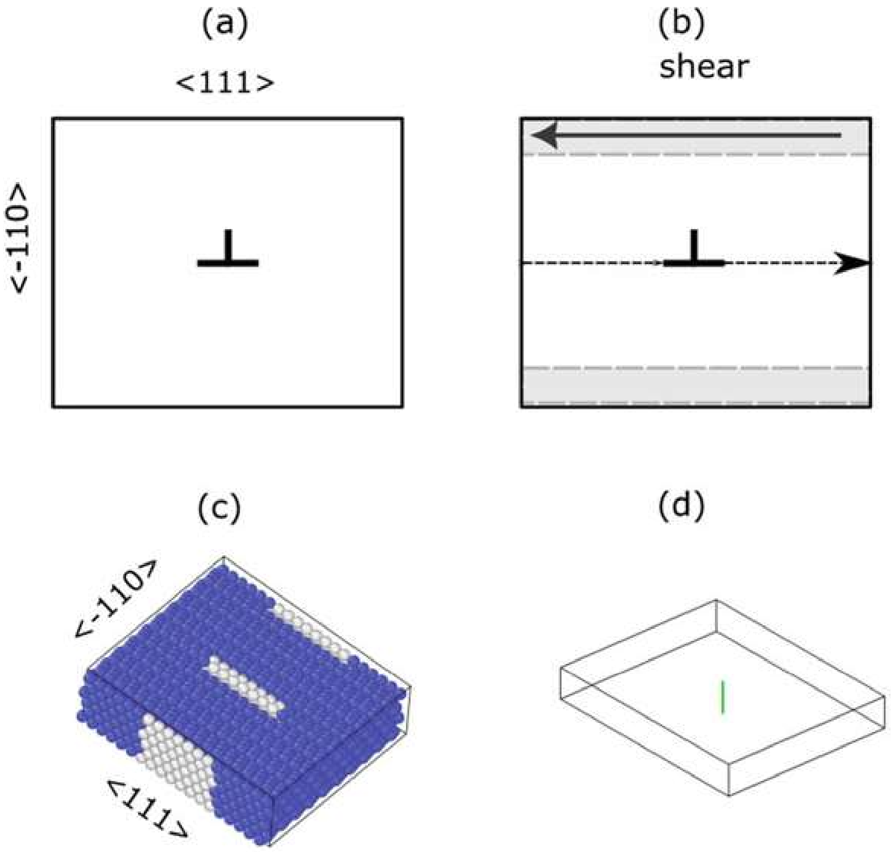

Fig. 1 Schematic diagram and atomistic PAD model of pure metal Fe: **a** and **b** show schematic diagram of dislocation in PAD model at rest and under shear, respectively. **c** shows the atomistic PAD model where blue and white atoms represent matrix and dislocation core atoms, respectively. **d** shows line representation of the dislocation

of dislocations [17]. The PAD model is then equilibrated at 300 K temperature for 10 picoseconds (PS) which was found to be sufficient to relax the pure Fe model. Care is taken not to include the frozen atoms in the equilibration process. After the equilibrated configuration is obtained, a shear stress is applied on the upper traction boundary along Y. Total shear force is equally distributed among the upper frozen atoms. Shear stress varies from 0.1 GPa to 1.5 GPa for the PAD model keeping the temperature fixed at 300 K and shear simulation time at 150 PS.

Open Visualization Tool (OVITO) is used to analyze the time-series data from molecular dynamic simulation [18]. To identify the local crystal structure, OVITO has two different tools based on distinct algorithms, namely Common Neighbor Analysis (CNA) [19] and Polyhedral Template Matching (PTM) [20]. In the presence of strong thermal fluctuations and strain, the PTM method is determined to be a more reliable tool for structural identification. With the help of PTM, the atoms with native BCC crystal structure can be distinguished from dislocation core atoms with unmatched crystal structure as can be seen from Fig. 1c. The atoms that make up the dislocation core are marked and average position of the collection of dislocation core atoms is recorded at each time step. This average position of dislocation core atoms is plotted against time to calculate the edge dislocation velocity in pure Fe. To investigate the H effect on edge dislocation velocity, the PAD model is randomly incorporated with varying number of H atoms. After creating models with varying concentration of H, the simulation process of equilibration, shear, and dislocation velocity calculation is performed on each model.

Results and Discussion

The effect of H on the edge dislocation core at zero temperature is previously reported by Wang et al. where Peierls stress, shear modulus, and dislocation core energy are computed at various H concentrations [21]. Edge dislocation core energy is reported to show a steady decrease with the increase of H concentration from 0 to 0.08 at%. In the present work, the effect of edge dislocation core configuration is computed at room temperature (300 K). Furthermore, to model H effect on Fe, the EAM potential developed by Wen [22] is used here as opposed to the Mendelev [23] potential as the former takes H–H interaction into account in addition to H-Fe interaction.

In the atomistic model, dislocation core atoms are identified using the PTM method. The dislocation core energy then can be computed as the model is allowed to be equilibrated for 100 ps. Dislocation core atoms are at a higher energy compared to the rest due to the lattice mismatch. Figure 2a, b shows that the addition of H affects the energy distribution of the core, and Fig. 2c shows that H atoms also affect the average energy of the core atoms. During equilibration, the average dislocation core energy of pure Fe remains constant but for the models with H atoms, dislocation core energy progressively reduces. This result shows the H atoms stabilize the dislocation core of Fe and the rate of stabilization directly correlates to the H concentration. Atomistic visualization reveals that the H atoms occupy the dislocation core interstitial position, reducing the lattice mismatch at the edge dislocation core which explains the reduction in core energy. The continuous reduction in core energy also confirms the progressive accumulation of H atom at the dislocation core.

The effect of this H induced stabilization of dislocation core on the mobility of dislocation is studied by analyzing the MD simulation result of application of shear load on the equilibrated models. The applied shear stress in the simulation varied from 500 to 1500 MPa, whereas the H concentration varied from 0.25 to 1.00%. Table 1 shows the shear stress and H concentration at which the edge dislocation was able to mobilize. In pure Fe, the dislocation was observed to be able to move at 50 MPa shear stress. However, with as little as 0.25% presence of H, the dislocation is rendered immobile below 900 MPa shear stress. At 1.00% H concentration, edge dislocation can only move at and above 1200 MPa applied shear.

At the applied shear and H concentration where dislocation can move, dislocation velocity is calculated from the slope of average dislocation core position against time curve. Figure 3 shows how dislocation velocity changes with the increasing applied shear in pure Fe model. It can be noted that at lower applied shear stress, the

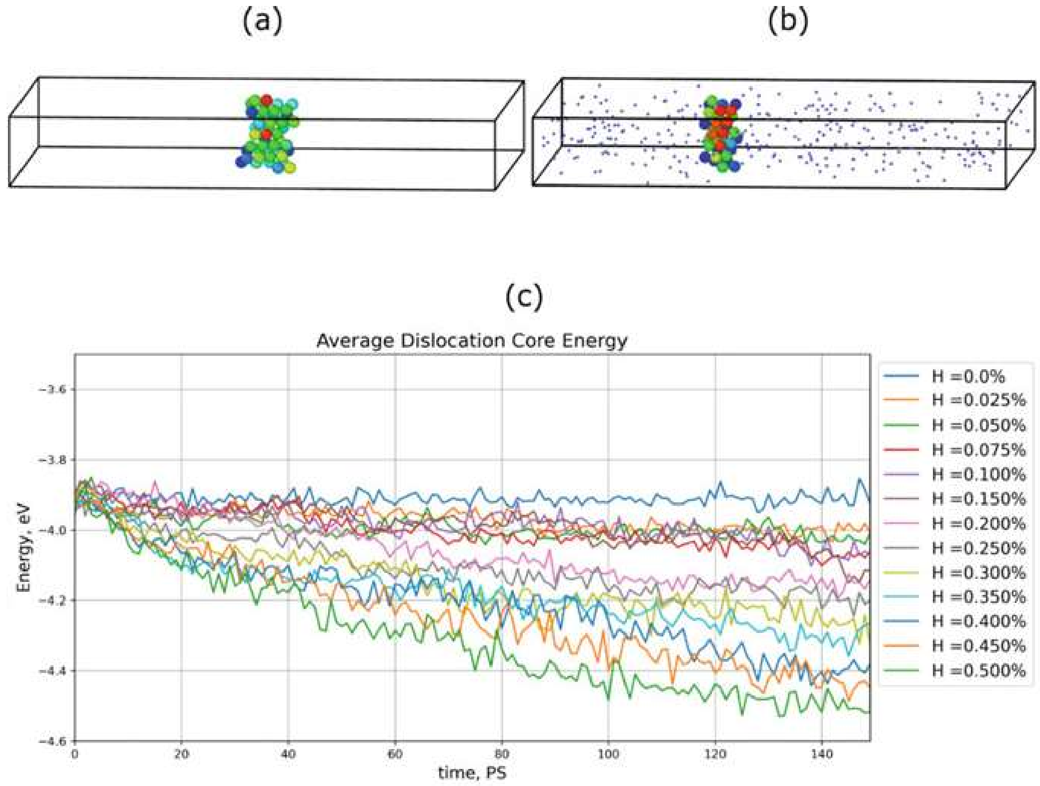

Fig. 2 H effect on dislocation core. **a** and **b** show the relative energy distribution in the edge dislocation core with and without H atoms respectively. The average energy of the dislocation core with increasing H concentration is shown in (**c**)

Table 1 Effect of H concentration on the mobility of the Fe edge dislocation

Atom% H	50 MPa	100 MPa	300 MPa	600 MPa	900 MPa	1200 MPa	1500 MPa
0.00	m	m	m	m	m	m	m
0.25	s	s	s	s	m	m	m
0.50	s	s	s	s	m	m	m
0.75	s	s	s	s	m	m	m
1.00	s	s	s	s	s	m	m

dislocation core movement is non-linear but as with the increase of applied shear, core movement becomes nearly linear. At low applied shear, atomistic lattices resist the core movement which becomes insignificant with the increase of applied shear. This observation justifies the linear approximation to calculate dislocation velocity.

Even a small concentration of H dramatically modifies the dislocation core behavior as observed from Table 1. Figure 4 shows the effect of H concentration on dislocation velocity. While increase of H concentration increases the shear stress level required to mobilize an edge dislocation core, it also eases the initial lattice resistance, enhancing the dislocation velocity compared to dislocation core in pure

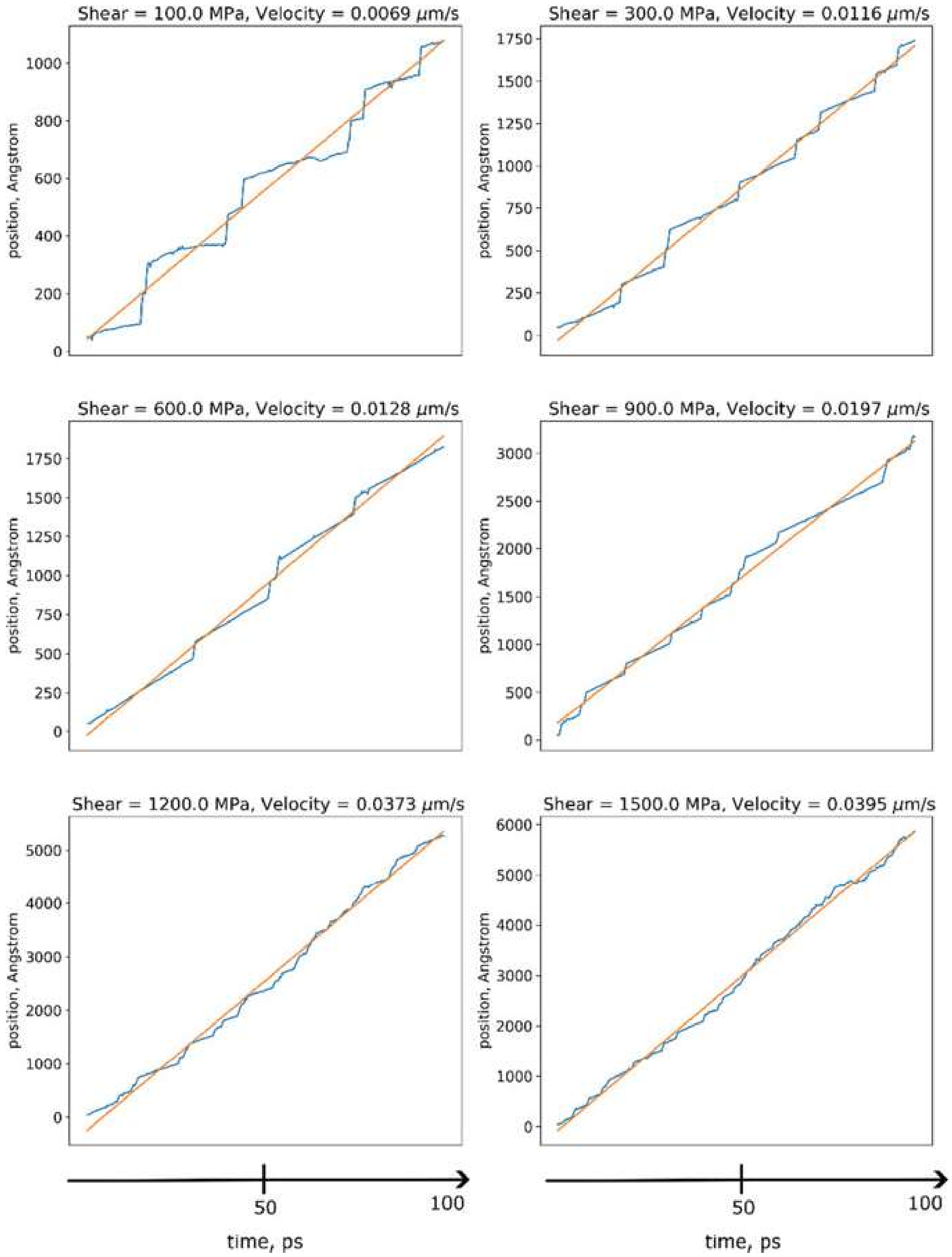

Fig. 3 Dislocation velocity with varying applied shear stress in pure Fe

Fe. However, since at higher shear stress level (>900 MPa) lattice resistance does not play a significant part, this enhancement also becomes insignificant. Above 900 MPa shear stress, increasing H concentration starts to impede dislocation velocity. This can be explained by the fact that under high shear and larger dislocation velocity,

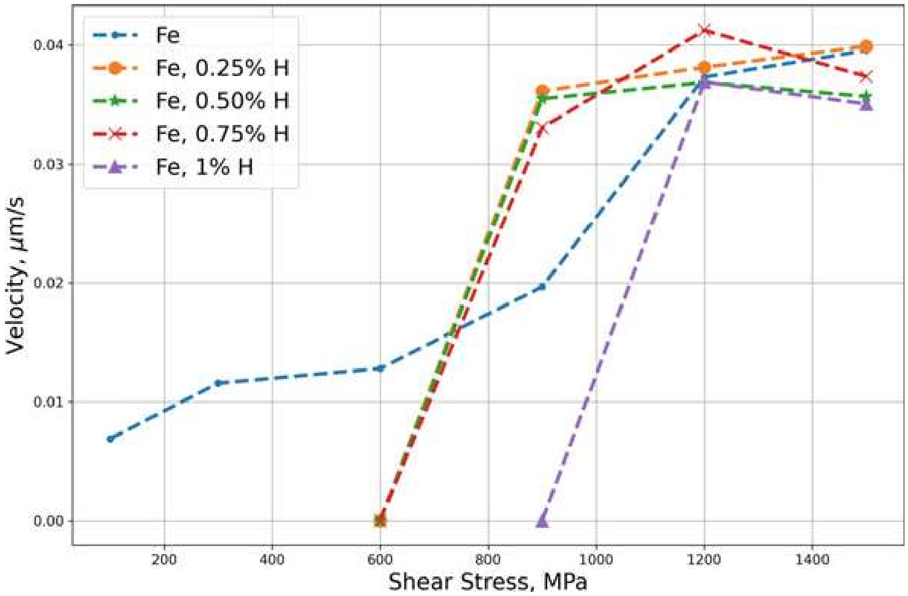

Fig. 4 Effect of H concentration on Fe dislocation velocity

lattice resistance is already small, and thus, H atoms only add to the viscous drag of the dislocation movement.

Conclusions

In conclusion, this study delves into the nuanced effects of hydrogen (H) on dislocation mobility within iron (Fe). Our key findings reveal a dual role for hydrogen atoms in influencing this process. First, H atoms serve to stabilize the edge dislocation core in Fe, thereby elevating the level of shear stress necessary to mobilize the dislocation. Secondly, H atoms exhibit a velocity-dependent impact on dislocation mobility: They facilitate it at low velocities by reducing lattice resistance but act as an impediment at high velocities by increasing viscous drag. These insights offer a deeper understanding of the complex interactions between hydrogen and dislocation behaviors, setting the stage for future research in this critical area.

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Data Availability The raw/processed data required to reproduce these findings cannot be shared at this time as the data also forms part of an ongoing study.

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