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Lattice Distortion-Induced Mechanical Asymmetry and Coupled Magnetic-Electronic Responses in a Model bcc Fe-Si Alloy: A Combined Experimental and First-Principles Investigation

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Abstract

Dislocations and defect clusters critically influence the mechanical, magnetic, and electronic properties of body-centered cubic (bcc) iron, which is the foundational matrix for reactor pressure vessel (RPV) steels and low-activation ferritic alloys. Yet, the underlying mechanisms driving load-dependent asymmetry in these extreme-environment structural materials remain unclear. Here, we integrate experimental characterizations with first-principles density functional theory (DFT) calculations to elucidate dislocation-induced lattice distortions in bcc Fe. Transmission electron microscopy and electron backscatter diffraction on a rolled Fe-Si model alloy reveal dense dislocation networks and heterogeneous residual stress fields. Informed by these microstructural heterogeneities, simplified DFT simulations of supercells with varying local atomic displacements (15–45% along the [001] crystallographic direction) demonstrate pronounced mechanical asymmetry: distortions enhance compressive stiffness but induce early tensile instability, with softening scaling to distortion magnitude. Electronic analysis shows defect-suppressed density of states near the Fermi level and reduced magnetic moments, weakening interatomic bonds under tension. These effects position dislocations as stabilizers under compression but initiators of tensile failure. Our findings provide atomic-scale insights into defect-controlled asymmetry in iron-based materials, guiding microstructural engineering for improved strength, magnetic stability, and electronic performance in structural steels and soft magnetic devices.

Full Text

Preamble

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Abstract

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Here, we integrate experimental characterizations with first principles density functional theory (DFT) calculations to elucidate dislocation induced lattice distortions in bcc Fe. ransmission electron microscopy and electron backscatter diffraction on a rolled Fe Si model alloy reveal dense dislocation networks and heterogeneous residual stress fields. Informed by these microstructural heterogeneities, simplified DFT simulations of supercells with varying local atomic displacements (15 45% along the [001] crystallographic direction) demonstrate pronounced mechanical asymmetry : distortions enhance compressive stiffness but induce early tensile instability, with softening scaling to distortion magnitude. Electronic analysis shows defect suppressed density of states near the Fermi level and reduced magnetic moments, weakening interatomic bonds under tension. These effects position dislocations as stabilizers under compression but initiators of tensile failure. Our findings provide atomic scale insights into defect controlled asymmetry in iron based materials, guiding microstructural engineering for improved strength, magnetic stability, and electronic performance in structural steels and soft magnetic devices.

Keywords

Local lattice distortion; Mechanical asymmetry; Magnetic electronic response; Tensile instability; Density functional theory; Fe Si model alloy

1. Introduction

based materials have been extensively used in industry due to their abundance, low cost, and excellent mechanical and magnetic properties . High content structural steels, exhibit a desirable combination of high strength, good ductility, and ferromagnetism [2,3] . For instance, iron based shape memory alloys (e.g., Fe Si) have shown great promise as cost effective smart materials for civil structural reinforcement . At room temperature, body centered cubic (bcc) Fe exhibits ferromagnetism with high saturation magnetization and low magnetocrystalline anisotropy, making it widely applicable in soft magnetic systems Moreover, due to its limited slip systems, bcc iron demonstrates high yield strength and pronounced temperature sensitivity especially at low temperatures resulting in mechanical behaviors distinct from face centered cubic (fcc) structures . In nuclear engineering, bcc iron based alloys are extensively utilized as structural components in reactors. Under long term neutron ir radiation, the accumulation of high density dislocation loops and defect clusters severely degrades their macroscopic performance, leading to irradiation hardening and embrittlement.

During processing (e.g., rolling, forging) and service, plastic deformation introduces various crystal defects especially dislocations that significantly affect material performance. An increase in dislocation density leads to work hardening, enhancing yie ld strength and hardness while compromising ductility. Dislocations also strongly influence magnetic and transport properties. For instance, dislocation induced stress fields can pin magnetic domain walls, causing Barkhausen noise and increasing coercivity . Quantitative studies have revealed that coercivity in ferrites correlates positively with dislocation density approximately proportional to its square root while the initial magnetic permeability decreases with increasing dislocation density . Moreover, dislocations act as electron scattering centers, thereby elevating residual resistivity and reducing electrical conductivity . First principles calculations have further demonstrated that atomic charge distribution, electronic states, and spin po larization in the vicinity of dislocations differ significantly from those in the defect free matrix , indicating that dislocation defects critically alter local electronic structures and magnetic moment distributions.

Conventional mesoscale theories, such as continuum elasticity theory and dislocation dynamics, are capable of describing long range elastic interactions and the collective motion of dislocations. However, these frameworks exhibit significant limitations in capturing atomic scale behaviors near dislocation cores. For example, multiscale simulations have shown that the influence zone of a dislocation core may extend up to 7 11 times the Burgers vector , which far exceeds the 1 3 times estimated by classic al continuum models. Moreover, the core energy exhibits strong dependence on the applied strain, and nontrivial configurational forces can emerge in the vicinity of the dislocation core, extending over tens of nanometers . These findings highlight that traditional models often neglect such atomistic effects, making it difficult to accurately capture the impact of defects on local material properties.

In recent years, first principles methods particularly density functional theory (DFT) been widely employed to investigate the effects of dislocations on material properties . Numerous DFT studies have elucidated the atomic structures of dislocation cores, Peierls barriers, and their interactions with other defects across various metallic systems, revealing both stable and metastable configurations that were previously unantic ipated . In ferromagnetic iron, DFT calculations indicate that the at omic configuration of dislocation cores differs markedly between ferromagnetic and disordered paramagnetic states. For example, the energy difference of a 1/2 screw dislocation core between the two magnetic states is relatively small, yet noticeable variations in atomic volume and magnetic moment are observed . These findings suggest that defect structures can substantially alter local magnetic moment distributions and electronic states. Furthermore, DFT allows for the direct calculation of local de nsity of states (DOS) and magnetic moment distributions in the vicinity of defects, enabling exploration of multiphysical effects such as magneto phonon coupling on electronic and magnetic behaviors Nevertheless, current research still lacks a systematic analysis of multiphysical couplings.

Most DFT studies are constrained to idealized dislocation configurations, such as shear displaced supercell models, which are inadequate for capturing the response s of real dislocation networks under complex stress conditions . Particularly in terms of magneto mechanical coupling, existing atomic scale simulations often fail to incorporate the localized magnetoelastic stress fields induced by dislocations into the system . This omission limits our understanding of how dislocations simultaneously affect mechanical behavior, magnetic response, and electronic transport. Therefore, it is imperative to integrate high precision computations with multiscale simulations to

systematically investigate Fe supercells containing dislocation like perturbations of varying magnitude under tensile and compressive strains. Such a combined approach can reveal their stress responses, thermodynamic stability, magnetic moment evolution, a nd electronic structure transformations.

In engineering iron based materials such as rolled steels and odel bcc Fe based alloy dislocation accumulation and residual stresses are unavoidable during processing and service. These defect rich regions often dominate mechanical reliability, particularly under tensile or cyclic loading conditions. However, the role of dislocation ced lattice distortions in governing tensile instability and failure initiation remains insufficiently clarified. Addressing this issue is essential for defect engineerin g and reliability oriented design of structural and functional iron based materials.

In this study, we first performed experimental characterizations on odel bcc Fe based alloy samples to establish the relationship between microstructural features and residual stresses.

Subsequently, first principles calculations were employed to construct Fe supercell models containing dislocation like distortions of varying magnitudes. These m odels were subjected to both tensile and compressive strains to evaluate their stress strain responses, structural stability, local magnetic behavior, and electroni c structure characteristics. By comparing the simulation results under different combinations of defect severity and loading conditions, this work aims to systematically elucidate the mechanisms by which realistic dislocation structures affect the coupled mechanical, magnetic, and electronic properties of iron based materials.

2.1 Experimental Procedures

odel bcc Fe based alloy specimens produced by a domestic steel manufacturer were selected as the experimental materials to investigate the correlation between microstructural defects and macroscopic properties.

Its chemical composition (wt%) is shown in Table 1 .

The samples were mechanically ground using a sequential series of SiC abrasive papers with grit sizes of 120, 200, 500, 1000, and 2400, until a final thickness of approximately 50 m was achieved. Circular disks with a diameter of 3 mm were then punched from the polished sheets. To prepare transmission electron microscopy (TEM) specimens, a double jet electro polishing technique was employed using a 4% nitric acid ethanol solution. Dislocation structures were characterized by a Fischione M3000 TE M operating at 200 kV in annular dark field mode. based alloy (wt%).

For electron backscatter diffraction (EBSD) analysis, samples were ground sequentially using 120 to 2400 grit papers, followed by fine polishing with a 2.5 m diamond suspension.

Electrochemical polishing was then performed in a solution of 5% perchloric a cid in ethanol at 30 V and 50 mA for 10 seconds. After ultrasonic cleaning in ethanol and air drying, the specimens were examined using a JSM 7900F field emission scanning electron microscope (FE SEM) equipped with a Hikari XP EBSD detector to characterize grain structure and phase distribution.

After EBSD characterization, the samples were lightly reground and etched in a 4% nitric acid ethanol solution for approximately one minute. The grain morphology was subsequently observed using an Axio Observer optical microscope. These multi scale microst ructural characterizations provided crucial insights int o the grain topology and dislocation density, serving as a reference for subsequent theoretical modeling

Residual stress measurements were performed using an X350A X ray diffraction (XRD) residual stress analyzer (iXpic Inc., Canada). Nine measurement points (labeled 1 9, see Figure 1 [Figure 1: see original paper]) were marked on the surface of the odel bcc Fe based alloy sheets. Residual stresses were measured in both the rolling (longitudinal) and transverse (perpendicular to rolling) directions. The instrument is capable of probing residual tensile or compressive stresses within a depth range of approximately m from the surface.

To ensure the stability and reliability of the results, each point was measured three times and the average value was used. Given that the thickness of the steel sheets is significantly smaller than their in plane dimensions, the study primarily focused on plane residual stress variations (i.e., longitudinal and transverse directions), and did not consider through thickness stress distributions.

Schematic illustration of the odel bcc Fe based alloy specimen geometry and the locations selected for residual stress measurements.

2.2 Computational Details

First principles calculations were performed within the density functional theory (DFT) framework. The bcc Fe crystal was modeled using supercells incorporating atomic displacement perturbations simulating dislocation like distortions. Specifically, the central Fe atom coordinate along the [001] crystallographic direction was adjusted to create three defect models Defect 1: body center Fe atom shifted downward by 15% along the [001] direction Defect 2: body center Fe atom shifted downward by 30% along the [001] direction Defect 3: body center Fe atom shifted downward by 45% along the [001] direction displacements simulate local asymmetric distortions under thermal or mechanical perturbations without introducing vacancies or impurities, facilitating analysis of local stress fields and electronic state perturbations induced by dislocations.

Atomic configurations of pristine and defect containing bcc Fe supercells used in first principles calculations.

The present study employs first principles calculations based on Density Functional Theory (DFT) to systematically optimize and analyze the physical properties of three defect containing crystal models. Specifically, the CASTEP module was utilized to perfo rm self consistent calculations for each defect model under various compressive strain states, obtaining the total energy, stress tensor, and atomic magnetic moments under spin polarized conditions. Additionally, the evolution of electronic density of stat es (DOS) and band structures was comprehensively analyzed under both tensile and compressive loading to elucidate the response mechanisms of the crystal's electronic structure and magnetic behavior under strain.

The calculations employed the revised Perdew Burke Ernzerhof (RPBE) exchange correlation functional within the generalized gradient approximation (GGA) [19,20] to accurately describe electron exchange correlation effects. Ultrasoft pseudopotentials were used to treat ion electron interactions, with a plane wave cutoff energy set at 330 eV. The Brillouin zone was sampled using the Monkhorst Pack scheme with an 11 × 11 × 11 k point grid to ensure computational accuracy.

The geometry optimization was deemed converged when the total energy change was less than 1\$×10^{-5}\$ eV/atom, the maximum atomic displacement was below 0.001 Å, residual stress was under

0.05 GPa, and Hellmann

Feynman forces were less than 0.03 eV/Å. The Brody Fletcher Goldfarb Shanno (BFGS) algorithm was employed for efficient minimization of the potential energy surface. Spin polarization effects were explicitly considered throughout all calculations to accurately evaluate the physical properties of th e three defect containing crystals.

Although the present models do not represent explicit dislocation cores, the imposed atomic displacements capture the essential local lattice distortions and stress asymmetry induced by high density dislocation networks commonly observed in heavily deforme d engineering steels.

3. Results and Discussion

3.1 Microstructural Characterization and Residual Stress

Microstructural characterization of rolled odel bcc Fe based alloy (a) TEM image showing dense dislocation networks; (b) EBSD (c) Kernel average misorientation (KAM) map indicating local lattice distortion; (d) Grain orientation and grain boundary distribution. based alloy samples. The TEM dark field image in Figure 3 Figure 3: see original paper reveals a dense network of dislocations, which inevitably form and accumulate during plastic deformation processes such as smelting and rolling.

These microscale defects lead to localized stress concentrati ons inside the material, contributing significantly to the heterogeneous distribution of internal residual stresses. The EBSD phase map in defects and stress fields have influenced grain growth. These observations underscore the necessity of studying the nature of microstructural defects to understand their impact on macroscopic material properti

Transverse Longitudinal Residual stress/MPa Residual stress/MPa Transverse Longitudinal Measure Point Measured residual stresses in the rolling and transverse directions of the odel bcc Fe based alloy sheet. based alloy sheets after rolling. As illustrated in Figure 4 Figure 4: see original paper, although the material appears macroscopically intact, a highly heterogeneous residual stress field has developed internally due to uneven plastic deformation, temperature gradients, and phase transforma tions introduced during rolling. Figure 4(b) reveals that residual stresses in the transverse direction (perpendicular to rolling) generally exceed those along the longitudinal (r olling) direction, which correlates with anisotropic strains induced by the rolling process. Negative values in the figure indicate compressive stresses; the measured residual stresses are predominantly compressive and associated with initial stress concen trations caused by cold rolling hardening. Overall, dislocation defects exert significant influence on the internal stress state of the material, spanning from microscale to mesoscale.

3.2 First

principles analysis Valence electron density distributions on the (011) plane for pristine and defect containing bcc Fe models.

Figure depicts the valence electron density isosurfaces on the (011) plane for pristine and defect containing bcc Fe models, illustrating local bonding electron cloud distributions. The perfect crystal exhibits highly symmetric electron clouds with uniform bondi ng electron density in all directions, characteristic of typical metallic bonding. As the dislocation distortion magnitude increases from Defect 1 to Defect 3, this symmetry is progressively disrupted. Notably, in the Defect 3 model, electron densi ty near the dislocation core is significantly enhanced, while regions far from the dislocation become electron deficient. This indicates localized stress concentrations induced by dislocations, where shortened interatomic distances cause increased electron cloud overlap and

bonding strength, whereas elongated directions exhibit weakened bonding. These findings qualitatively reveal the inhomogeneous electronic structure and bonding induced by dislocation defects, providing a microscopic basis to interpret subsequent changes in mechanical properties, magnetism, and electronic states.

Original Defect 1 Defect 2 Defect 3 Stress/GPa Stress/GPa Original Defect 1 Defect 2 Defect 3 Strain Strain Stress strain responses of pristine and defect containing bcc Fe crystals under compression and tension.

Figure presents the stress strain responses of pristine and defect containing Fe crystals under different loading conditions. The left panel shows results under compression (strain $\epsilon = 0$ 0.10), where compressive stress increases with strain for all models. Notab ly, the stiffness in compression is significantly enhanced as the dislocation distortion increases; at $\epsilon = 0.10$, the compressive stress for Defect 3 reaches approximately 187.5 GPa, more than 40% higher than the pristine model' s

131.5 GPa. This suggests

that the pre existing distorted structures provide additional resistance against deformation under compression, effectively strengthening the local stiffness phenomenon akin to "pre compression structural hardening." Conversely, the right panel displays the tension ($\epsilon = 0$ 0.05) stress strain curves, where defect models exhibit markedly reduced peak stresses: the pristine crystal attains a maximum stress around 15.4 GPa, whereas Defect 3 reaches only about 1.3 GPa, nearly losing its elastic response capaci ty. Taken together, these results reveal a pronounced mechanical asymmetry induced by dislocation defects, characterized by "enhanced compression resistance but weakened tensile strength." It should be noted that while the pristine ideal crystal exhibits linear and symmetric elastic behavior at infinitesimally small strains (< 0.01), the inherent anharmonicity of the interatomic potential naturally leads to a divergence between tensile and compressive responses at larger finite strains (0.05). However, the introduction of local lattice distortions (Defects 1 3) dramatically exacerbates this baseline asymmetry. nonlinear mechanical behavior is significant in multiscale mechanical responses and offers microscopic insights into microcrack initiation and propagation mechanisms.

Original Defect 1 Defect 2 Defect 3 Original Defect 1 Defect 2 Defect 3 Strain Strain Evolution of average atomic magnetic moments as a function of applied compressive and tensile strain for different defect containing models.

Figure illustrates the evolution of atomic magnetic moments in the different models under compressive and tensile strains.

For the pristine crystal, the total magnetic moment of the simulation cell (containing 2 Fe atoms) decreases from approximately 4.49 (i.e., ~2.25 atom) to 3.41 with increasing compressive strain , indicating magnetic weakening under compression. This trend can be explained by the Stoner model: compression reduces the lattice constant, broadens the d orbital bandwidth, lowers t he density of states at the Fermi level, and thus diminishes ferromagnetic exchange stability. In contrast, the magnetic moment variation in defect models is more drastic; for Defect 3 at $\epsilon = 0.10$, total netic moment drops to about 1.96 , significantly lower than the pristine crystal, suggesting severe disruption of local spin order due to defect induced electronic perturbations. The severity correlates with defect magnitude.

Under tensile strain, the pristine crystal' s total magnetic moment increa ses from 4.49 to 5.25 , reflecting increased Fe spacing that enhances magnetic moments. However, defect models show limited magnetic moment enhancement; for example, Defect 3 reaches only about 4.40 in total . This indicates that dislocation structures weaken the external strain' s ability to modulate magnetic moments, implying that materials' magnetostrictive or magnetic field responses are highly sensitive to dislocation density.

Original Defect 1 Defect 2 Defect 3 Energy/eV Energy/eV Original Defect 1 Defect 2 Defect 3 Strain Strain Total energy variation with applied strain for pristine and defect containing bcc Fe crystals.

Figure illustrates the variation of total energy with strain for different models, serving as an indicator of thermodynamic stability. Under increasing compressive strain, the total energy continuously rises, indicating that the system is driven away from its or iginal ground state. At 0.10, the pristine crystal' s total energy increases by approximately +8.24 eV, whereas Defect 3

shows a more significant rise of about +13.42 eV. This demonstrates that higher magnitudes of distortion considerably elevate the strain energy density, making the system more prone to instability or deformation softening. Under tensile strain, total energ y also increases but with a smaller increment; for Defect 3 at $\epsilon = 0.05$, the energy increase is about +3.52 eV. From a thermodynamic perspective, dislocation defects reduce the crystal' s stability under external loads, particularly favoring structural reco nstructions or localized collapses under compression. Furthermore, such energy states can trigger redistributions of electronic states, thereby influencing the material' s electronic and magnetic properties.

Original -0.04GPa Original -0GPa Density of States(electrons/eV) Density of States(electrons/eV) s Down p Down d Down f Down Total Up Total Down Energy/eV Defect 1 -0GPa Density of States(electrons/eV) Density of States(electrons/eV) s Down p Down d Down f Down Total Up Total Down Energy/eV Defect 2 -0GPa Density of States(electrons/eV) Density of States(electrons/eV) s Down p Down d Down f Down Total Up Total Down Energy/eV Defect 3 -0GPa Density of States(electrons/eV) Density of States(electrons/eV) s Down p Down d Down f Down Total Up Total Down Energy/eV Original -0.08GPa Density of States(electrons/eV) s Down p Down d Down f Down Total Up Total Down Energy/eV Defect 1 -0.08GPa Density of States(electrons/eV) s Down p Down d Down f Down Total Up Total Down Energy/eV Defect 2 -0.08GPa Density of States(electrons/eV) s Down p Down d Down f Down Total Up Total Down Energy/eV Defect 3 -0.08GPa Density of States(electrons/eV) s Down p Down d Down f Down Total Up Total Down Energy/eV s Down p Down d Down f Down Total Up Total Down Energy/eV Defect 1 -0.04GPa s Down p Down d Down f Down Total Up Total Down Energy/eV Defect 2 -0.04GPa s Down p Down d Down f Down Total Up Total Down Energy/eV Defect 3 -0.04GPa s Down p Down d Down f Down Total Up Total Down Energy/eV Evolution of the electronic density of states (DOS) under compressive strain for pristine and defect containing bcc Fe crystals.

Density of States(electrons/eV) Density of States(electrons/eV) s Down p Down d Down f Down Total Up Total Down Energy/eV Density of States(electrons/eV) Density of States(electrons/eV) s Down p Down d Down f Down Total Up Total Down Energy/eV Density of States(electrons/eV) Density of States(electrons/eV) s Down p Down d Down f Down Total Up Total Down Energy/eV Density of States(electrons/eV) Density of States(electrons/eV) s Down p Down d Down f Down Total Up Total Down Energy/eV Density of States(electrons/eV) s Down p Down d Down f Down Total Up Total Down Energy/eV Density of States(electrons/eV) s Down p Down d Down f Down Total Up Total Down Energy/eV Density of States(electrons/eV) s Down p Down d Down f Down Total Up Total Down Energy/eV Density of States(electrons/eV) s Down p Down d Down f Down Total Up Total Down Energy/eV s Down p Down d Down f Down Total Up Total Down Energy/eV s Down p Down d Down f Down Total Up Total Down Energy/eV s Down p Down d Down f Down Total Up Total Down Energy/eV s Down p Down d Down f Down Total Up Total Down Energy/eV Evolution of the electronic density of states (DOS) under tensile strain for pristine and defect containing bcc Fe crystals.

Figures and 1 depict the evolution of total electronic density of states (DOS) under compressive and tensile strains, respectively. Under compression (Figure), the pristine crystal exhibits continuous and distinct DOS peaks and valleys near the Fermi level, characteristic of metallic behavior, which slightly weakens with increasing strain. The introduction of dislocation defects significantly perturbs and reduces the DOS at the Fermi level; as the defect severity increases, the DOS near Ef gradually diminishes, and the bandwidth narrows. Notably, Defect 3 exhibits a DOS collapse reminiscent of an energy gap, indicating disruption of electron transport pathways.

Under tensile strain (Figure), DOS peaks near the Fermi level generally increase for all models, with the pristine crystal showing pronounced DOS enhancement, reflecting strain induced orbital delocalization and elevated carrier concentration. However, in Defect 3, DOS profiles remai

irregular with discrete states, indicating stronger electron localization. Overall, dislocations introduce localized scattering centers in the electronic structure, diminishing metallicity and rendering electronic transport properties more sensitive and no nlinear to applied strain.

Original-0.04GPa Original-0GPa Energy/eV Energy/eV Defect 1-0GPa Energy/eV Energy/eV Defect 2-0GPa Energy/eV Energy/eV Defect 3-0GPa Energy/eV Energy/eV Original-0GPa Energy/eV Energy/eV Original-0.08GPa Energy/eV Defect 1-0.08GPa Energy/eV Defect 2-0.08GPa Energy/eV Defect 3-0.08GPa Energy/eV Original-0.04GPa Energy/eV Defect 1-0.04GPa Defect 2-0.04GPa Defect 3-0.04GPa Band structure evolution of pristine and defect containing bcc Fe crystals under compressive strain.

Original-0.02GPa

Defect 1-0GPa Defect 1-0.02GPa Defect 1-0.04GPa Energy/eV Energy/eV Energy/eV Defect 2-0GPa Defect 2-0.02GPa Defect 2-0.04GPa Energy/eV Energy/eV Energy/eV Defect 3-0GPa Defect 3-0.02GPa Defect 3-0.04GPa Energy/eV Energy/eV Energy/eV Band structure evolution of pristine and defect containing bcc Fe crystals under tensile strain.

Figures 1 and 1 further reveal changes in the electronic band structures for the different models. In the pristine crystal under compressive strain, bands continuously cross the Fermi level without any gap, displaying symmetric and closely packed band structures indicati ve of a highly ordered lattice. With the introduction of defects, band structures exhibit pronounced perturbations: some bands shift away from Ef, resulting in asymmetry near the Fermi surface. In highly defective models (Defect 2 and Defect 3), certain ba nds show splitting or flattening, indicating the formation of localized quasi bound states induced by lattice distortions. Under tensile strain (Figure 1), the pristine crystal' s bandwidth slightly increases, with denser bands near the Fermi level enhancing conductivity. However, despite some band expansion in defect models under tension, Defect 3 still displays several flat or isolated bands, suggesting t hat electron propagation is hindered by local potential wells. These band structure characteristics co rroborate DOS evolution, demonstrating how dislocation defects restrict electron mobility and fundamentally reduce carrier transport performance.

4. Discussion

The present integrated experimental and first principles study elucidates the critical role of dislocation induced lattice distortions in governing tensile instability and failure initiation in body centered cubic (bcc) iron based materials. Unlike defect free lattices that exhibit nearly symmetric elastic behavior, dislocation rich regions display pronounced mechanical asymmetry, with enhanced compressive strengthening but severe tensile softening. This section discusses the underlying mechanisms and their implications for failure prevention in iron based structural materials.

Dislocation Induced Mechanical Asymmetry: Compression Strengthening vs. Tensile

Vulnerability Experimental observations confirm that rolling introduces dense and heterogeneous dislocation networks, accompanied by anisotropic residual stress distributions (Figures 3 and 4). These microstructural heterogeneities generate non uniform local stress stat es, which serve as the physical basis for the dislocation like lattice distortions modeled in the DFT supercells.

Stress strain responses (Figure) reveal that pre existing distortions markedly enhance compressive stiffness providing additional resistance through closer atomic packing and increased electronic overlap while dramatically reducing tensile load bearing capacity due to bond stretching an d stress concentration. This asymmetry explains why heavily deformed iron based materials often exhibit high compressive strength but limited tensile ductility and fracture resistance under service conditions.

Tensile Instability as a Precursor to Microcrack Nucleation and Failure Initiation The most significant finding is the severe tensile softening in defect containing models (Figure 6 [Figure 6: see original paper]), where increasing distortion magnitude leads to early elastic instability and rapid stress degradation. From a failure mechanics perspective, dislocation ch regions act as mechanically weak zones that promote localized strain accumulation and premature bond rupture under tensile loading.

In polycrystalline steels, external tensile stresses are unevenly accommodated due to grain orientation, residual stresses, and defect clustering. High dislocation density zones are therefore preferential sites for microcrack nucleation, providing root cau ses for brittle or quasi brittle failure initiation. This mechanism has direct implications for structural reliability, particularly under tensile dominant or cyclic loading, where progressive dislocation accumulation further reduces tensile stability.

Electronic and Magnetic Contributions to Bond Weakening and Tensile Softening Electronic structure analyses provide microscopic insight into the origins of tensile vulnerability. In pristine bcc Fe, tensile strain enhances the density of states (DOS) near the Fermi level, stabilizing metallic bonding. However, dislocation distortion s significantly suppress DOS at E_F and reduce atomic magnetic moments, indicating weakened interatomic cohesion.

This electronic degradation diminishes the lattice' s ability to redistribute stress under tension, accelerating elastic instability. The observed magnetic moment reduction serves as a sensitive indicator of deteriorated bonding rather than an isolated magn etic phenomenon. Thus, the coupled lattice electronic magnetic response constitutes a fundamental mechanism driving dislocation induced tensile failure in ferromagnetic iron.

Implications for Failure Prevention and Microstructural Design in Structural Steels These results highlight the dual role of dislocations: beneficial for compressive load bearing but detrimental to tensile performance and fracture resistance. Controlling excessive dislocation accumulation through optimized processing or alloying offers a practical strategy to improve tensile stability, delay microcrack initiation, and enhance overall structural integrity. schematically summarizes the dislocation driven mechanical asymmetry and its linkage to failure initiation. Dislocation networks create pre distorted zones that stabilize under compression but manifest early tensile instability, manifesting as preferentia l sites for crack nucleation. Incorporating such defect effects into microstructural design is essential for developing reliability iron based materials subjected to complex loading.

Overall, this work demonstrates that dislocation induced distortions are central to tensile

failure mechanisms in bcc iron, providing mechanistic guidance for failure mitigation in structural and functional ferromagnetic alloys.

Experimental Observationas First principles

analysis

Microstructure

- Dislocation non - uniformity - Crystallographic anisotropy - Stress difference
- mechanical properties asymmetry - Reduced magnetism - Electronic degradation

Dislocation Defects lead to the generation of micro stress Defects affect crystal constitutive relations Compress Tensile schematically summarizes the coupling between dislocation induced lattice distortions and the resulting mechanical asymmetry in bcc iron, integrating the experimental observations and first principles insights obtained in this study. . Conclusion:

In this study, we have demonstrated the profound impact of dislocation induced lattice distortions on the mechanical, magnetic, and electronic properties of ferromagnetic bcc iron through a synergistic experimental and computational approach. Experimental characterizations of rolled odel bcc Fe based alloy uncover heterogeneous dislocation networks and residual stresses, while DFT calculations reveal that these defects lead to mechanical asymmetry: enhanced compressive stiffness contrasted with tensile softening and instability. Magnetically, dislocations r educe atomic moments and dampen strain modulation; electronically, they depress the density of states at the Fermi level and flatten bands, signaling reduced carrier mobility and bond strength.

These multiphysics couplings highlight dislocations' dual role bolstering compression but precipitating tensile failure explaining behaviors in deformed steels. For materials design, controlling defect density offers pathways to tune properties: high dislocations for coercivity in permanent magnets, low for permeability in soft magnets, or optimized distributions in shape memory alloys and advanced iron based alloys for structural and functional applications Overall, our integrated findings bridge microstructural defects to macroscopic performance, paving the way for defect engineered iron based materials with superior mechanical reliability and magnetoelectronic functionality. . References Sun W, Wang S, Yu Z, et al. Characteristics and application of iron based materials in heterogeneous Fenton oxidation for wastewater treatment: a review[J]. Environmental Science:

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