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Influence of Hydrogen Concentration and Point Defects on the Deformation, Phase Transformation, and Dislocation Evolution in Zirconium: A Molecular Dynamics Study

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Abstract: Hydrogen ingress and irradiation-induced point defects critically influence the mechanical reliability of zirconium-based alloys used in nuclear applications. In this study, molecular dynamics (MD) simulations were employed to systematically investigate the effects of hydrogen concentration, vacancy defects, and self-interstitial atoms (SIAs)—individually and in combination—on the deformation behavior, elastic response, phase transformation, and dislocation evolution of α -zirconium subjected to uniaxial tensile loading. Stress–strain analysis of perfect and defective Zr-H systems revealed that the incorporation of hydrogen up to 5.0% induces only marginal changes in elastic modulus and tensile strength, whereas vacancy and interstitial defects significantly degrade mechanical performance. Vacancies reduce stiffness and promote earlier yielding, while SIAs exert the most pronounced weakening effect, drastically lowering tensile strength and strain at low concentrations and inducing complex deformation behavior at higher concentrations. Temperature and pressure were also shown to strongly modify the onset of yielding and the stability of the hexagonal close-packed (HCP) phase. Common neighbor analysis (CNA) and dislocation extraction algorithm (DXA) evaluations demonstrated that defects accelerate the HCP→“Others” phase transition, modify face-centered cubic (FCC) formation, and promote the nucleation of dislocation loops—especially in systems containing SIAs or high defect densities. Overall, the results highlight the dominant role of point defects, particularly SIAs, in governing the degradation of zirconium’s mechanical integrity, while showing that hydrogen alone exerts comparatively minor influence within the studied

concentration range. These insights provide atomistic understanding essential for predicting the performance of zirconium cladding under irradiation and hydrogen uptake conditions.

Keywords: Hydrogen diffusion in Zirconium alloys; point defects; mechanical properties; Hydrogen-defect interactions; Molecular- Dynamics (MD) simulation; phase transformation; dislocation nucleation; microstructural evolution.

1. Introduction

The mechanical and physical properties of metals and their alloys are considerably influenced by hydrogen ingress, which acts as a common and detrimental impurity in structural materials. In metals with hexagonal close-packed (hcp) structure, such as magnesium alloys, hydrogen diffusion constitutes the rate-limiting factor for the effective storage of solid hydrogen [1]. Additionally, in titanium [2] and zirconium [3] alloys, this diffusion process can lead to a degradation of their mechanical properties. The destructive effects of hydrogen encompass several phenomena, including phase transformations that lead to the formation of flaky or needle-shaped hydrides [4], interactions with structural imperfections that change the plastic properties of materials [5][6][7][8], association with point defects that may promote swelling, and the issue known as hydrogen-induced embrittlement through diverse mechanisms [9][10][11][12].

A significant environment in which materials interact with hydrogen is within a nuclear reactor, where they are subjected to high temperatures, aggressive aqueous coolant, and intense irradiation fluxes. Among the structural materials used in reactors, Zr based alloys (commonly referred to as Zircaloy) are extensively employed as fuel rod cladding, resulting in greater and more direct contact with the coolant water. As a result, α -Zr undergoes an exothermic reaction with water at interface temperatures around 400°C [13][14], leading to oxide layer formation and hydrogen release. Due to zirconium's high affinity for hydrogen, a fraction of the hydrogen generated during corrosion is absorbed into the alloy. Once the hydrogen uptake exceeds the solubility limit, the brittle hydride phases begin to precipitate. This phenomenon compromises mechanical integrity via delayed hydride cracking (DHC) [15][16], diminishes fracture toughness, and ultimately restrict fuel rod lifetime [17]. These processes are also attended by the structural and mechanical variations that arise from irradiation by high-energy neutrons and other particles. Interestingly, radiation is frequently observed to augment the diffusion and permeation processes of hydrogen isotopes in metals [18]. This behavior has been demonstrated under reactor conditions, where the

solubility and diffusivity of hydrogen undergo significant changes due to the emergence of irradiated defects, particularly point defects [19][20]. Notably, the main point defect types generated during the radiation cascade are vacancies and self-interstitial atoms (SIAs) [21]. Point defects interact with dislocation loops and grain boundaries, forming complex defect clusters. These clusters can deteriorate the material's crystal structure, resulting in brittleness, swelling, hardening, and creep [22]. In this context, Zhu et. al. [23] undertook density functional theory (DFT)) investigations of α -Zirconium (α -Zr) across a broad spectrum of vacancy concentrations, ranging from 0.005 to 0.063. Their research elucidated that vacancies exhibit a tendency to aggregate into di-vacancy and tri-vacancy configurations, reducing bulk modulus while increasing shear and Young's moduli. This interaction and resulting changes in mechanical properties highlight the significant impact of point defects and their clusters on the material's overall performance.

Therefore, it's crucial to delve into a comprehensive study of the presence of point defects and hydrogen diffusion, as well as to evaluate the impact of their concentration and interactions on the mechanical behavior of zirconium. Numerous studies have investigated the impact of hydrogen on the mechanical properties of zirconium alloys over several decades [24][25][26][27][28]. For instance, the introduction of hydrogen isotopes (ranging from 5 to 200 wppm) in the Zr-2.5Nb alloy demonstrates a linear decrease in yield strength (YS) and ultimate tensile strength (UTS) with rising temperature. These properties tend to remain stable across various hydrogen concentrations. However, after necking occurs, at temperatures of 25°C and 100°C, hydrogen has a significant impact on these properties, suggesting the presence of hydride embrittlement [29]. Additionally, hydrogen levels exceeding 300 wppm in zirconium alloy claddings significantly reduced fracture load and caused a shift in fracture modes from ductile to brittle, leading to failure of radial hydrides[30].

Despite a robust body of experimental research [31][32][33][34][35], there remains a critical need for predictive, multiscale modeling frameworks that can capture the interactions between defects and impurities, micro-structure evolution, and stress-driven diffusion across high pressure-temperature regimes. This need is further underscored by the notable variability in experimental methodologies across studies, particularly in sample preparation and measurement techniques, which has led to significant discrepancies in the reported hydrogen diffusivity values for zirconium [27][34][36][37]. Recent technological breakthroughs have propelled computational models like

MD simulations and DFT based calculations to the forefront of materials science, particularly for investigating microstructural evolution, behaviors and effects of incorporated elements, and mechanical properties of materials on the atomic scale[38][39]. A large number of researchers have carried out studies to explore the hydrogen diffusion and absorption in Zr alloys. Lee and Lee [40] compared hydrogen diffusion in crystalline and amorphous structures of an alloy of Zr, using MD simulations. Xu et al. [41] used DFT to study hydrogen diffusion, adsorption, and dissociation on Zr(0001) surfaces. Their findings indicated that elevated hydrogen concentrations tend to accumulate below the surface layer, which obstructs H₂ molecule desorption and promotes hydrogen absorption. This phenomenon was linked to reduced surface energy and heightened susceptibility to material embrittlement. Hydrogen diffusion in α -zirconium is anisotropic and directionally dependent. There are disagreements regarding this phenomenon; as outlined by Kearns et al. [36], hydrogen diffuses more rapidly along the $\langle c \rangle$ axis than along the $\langle a \rangle$ axis (i.e., within the basal plane). However, subsequent investigations [42] presented a contrasting view, suggesting that diffusivity along $\langle a \rangle$ may surpass that along $\langle c \rangle$ by more than an order of magnitude. More recently, Zhang et al. [13] employed a combined DFT and accelerated kinetic Monte Carlo (AKMC) approach to simulate anisotropic hydrogen diffusion in α -zirconium and Zircaloy. They found a modest preference for diffusion along the $\langle c \rangle$ crystallographic direction, thereby exhibiting close agreement with the earlier findings reported by Kearns et al. Liyanage [43] developed a method to assess hydrogen diffusivity in hcp Zr through first-principles calculations and kinetic Monte Carlo simulations. They discovered that hydrogen diffusivity in α -zirconium (α -Zr) is nearly isotropic, with its rate increasing along the C-axis. This reduced diffusivity is attributed to lower hopping rates and the formation of hydrogen traps, primarily resulting from elevated activation barriers at the octahedral site under compressive stress.

Further research examined the factors affecting hydrogen penetration behavior in zirconium alloys [40][44]. For instance, calculations conducted by Wang et al. [45] on the diffusion of hydrogen in hcp Zr reveal that the tetrahedral interstitial site (TIS) is the most favorable trapping site for a single H atom, and vacancies can trap up to 8 H atoms without forming H₂. García and Ramunni [46] also found that tetrahedral sites are the most stable for hydrogen accommodation. Moreover, they focused on the influence of Zr alloy composition; adding niobium (Nb) improves hydrogen solubility but makes it harder for hydrogen to diffuse. In this regard, Yu et al.[47] also elaborated on the role of this factor and the effect of stress, via accelerated AKMC, found that

while alloying elements weakly influence diffusion, especially at high temperatures, applied stress significantly alters diffusivity. As previously mentioned, the consequence of hydrogen uptake is the occurrence of hydride precipitation and embrittlement in Zircaloy, which has been extensively analyzed [14][38][48] [49]. Using MD study and applying the MEAM potential, Siripurapu et al. [50] revealed that stress-induced reorientation of zirconium hydrides stems from energy and stress variations across crystallographic directions. Results indicate higher energy and stress along the $[1 \bar{1} 0]$ direction compared to $[111]$, driving hydride realignment perpendicular to applied stress. Meanwhile, Deng et al. [39] employed a modified GTN model, noting that elevated hydrogen concentrations contribute to increased void formation and a heightened risk of brittle failure at low temperatures, reducing plastic deformation while minimally affecting elastic properties. Hydrogen embrittlement also enhances burst stress and plastic strain during accidents such as Loss of Coolant Accidents (LOCA), further complicating the material's behavior under stress. Prior investigations have indicated that the interactions among hydrogen atoms in zirconium are relatively weak [51]. Conversely, substantial interactions between hydrogen and material defects, especially vacancies, have been observed [26]. These interactions significantly influence the deformation governing behavior and mechanical properties of zirconium [52][50]. Maxwell et al. [8] by using MD simulations, revealed that in hydrogen-vacancy of zirconium interactions, the populations of vacancy clusters are influenced by hydrogen concentration, and at high concentrations, with atoms preferentially occupying interstitial sites near vacancies. Building on this, Wimmer et al. [7] introduced a refined EAM potential (BMD19), modeling SIA's effectively and outperforms previous interatomic potentials in describing H-Zr interactions, including binding energy, lattice strain effects, and diffusion barrier energies. Foster and Zhou [21] performed MD simulation, reporting that hydrogen isotopes preferentially cluster around dislocations in α -Zr, particularly under tensile stress, while Christensen et al. [53] conducted an investigation into point defect diffusion and dislocation loop nucleation in both pure and hydrogen-loaded hcp zirconium using ab initio calculations along with classical simulations. Their findings revealed that interstitial hydrogen atoms diffuse isotropically and prevent the collapse of vacancy c-loops, while exerting minimal influence on self-interstitial diffusion and aggregation. Olsson et. al [26] investigates how hydrogen-filled vacancies affect zirconium's mechanical properties through ab initio modeling. The results show that these vacancies decrease surface energy and ductility, while simultaneously increasing unstable stacking fault energy. Furthermore, the presence of hydrogen-filled vacancies

leads to a reduction in both the work of fracture and peak stress. Regarding phase transformations, Mahapatra et al. [54] have investigated the stability and phase transition in Zr nanowire, taking into account size and temperature dependence. Ma et al. [55] also reported that the $\alpha \rightarrow \beta$ phase transition temperature of Zr-4 alloy dropped from 825°C to 550°C after thermo-hydrogen treatment (THT). Higher diffusion coefficients and reduced activation energy in the β -Zr lattice were observed. Thus, the hydrogen-induced phase transition was crucial for low-temperature diffusion bonding of Zr-4 alloys.

In general, the examination of hydrogen and defects interactions within zirconium alloys, involving both experimental research and computational modeling, is imperative for the development of effective methodologies aimed at enhancing the performance and safety of zirconium-based materials across a variety of industrial applications. The current body of literature presents a limited understanding of how hydrogen concentration, along with the presence of point defects, most notably SIAs, influences mechanical properties, phase transformations, and the behavior of dislocations when subjected to stress. These results collectively underscore this gap by emphasizing the significant importance of defects within zirconium. Defects, including vacancies and SIAs, are essential in governing the mechanical behavior of the material, particularly when hydrogen atoms interact with these structural imperfections.

Hence, in the forthcoming study, we generated point defects (including vacancies and SIAs) randomly and considered H atoms in zirconium metal at various concentrations. We dealt with the influence of hydrogen, and point defects, as well as the interactions between H atoms and these defects, on the mechanical properties of zirconium under tensile loading using the MD simulation method.

The organization of this paper is structured in the following manner: **Section 2** provides a comprehensive overview of the computational methods and details pertaining to the MD simulation. In **Section 3**, the mechanical response of perfect Zr and defective Zr-H systems is explored under uniaxial tensile test. The responses to stress-strain, along with the effect of H concentration, defect types and concentrations, temperature, and pressure on phase transformation and length of dislocation are analyzed and reported. Finally, a comprehensive summary of key findings of this study are outlined in **Section 4**.

2. Computational methodologies

To investigate the mechanical behavior of zirconium crystals under uniaxial tensile deformation, MD simulations were performed using the LAMMPS software[56]. The interatomic interactions were described by the embedded-atom method potential developed by Wimmer et al.[7], which has been demonstrated in previous studies to accurately capture zirconium-hydrogen interactions and structural defect behavior.

Simulation boxes with dimensions of $25a \times 16\sqrt{3}a \times 25c$ (containing 40,000 atoms) were constructed, where a and c represent lattice constants of 3.2312 Å and 5.1477 Å, respectively. The coordinate axes were aligned with crystallographic directions such that X, Y, and Z directions corresponded to $[-1\ 2\ -1\ 0]$, $[1\ 0\ -1\ 0]$, and $[0\ 0\ 0\ 1]$ orientations, respectively. Hydrogen atoms, vacancies, and SIAs were randomly introduced into the simulation boxes at concentrations of 0.1%, 0.5%, 1.0%, 2.0%, and 5.0% to achieve uniform distributions. Periodic boundary conditions were applied along all three coordinate directions. Newton's equations of motion were integrated using the velocity-Verlet algorithm[57], while energy minimization was performed using the conjugate-gradient algorithm [58] to eliminate residual forces in initial configurations. Following minimization, all systems underwent thermal and pressure equilibration using the isothermal-isobaric (NPT) ensemble at specified temperatures (300, 400, 500, 600, 800, 1000, 1200, and 1500 K) and pressures (0, 5, 10, 15, 20, 25, and 30 GPa). Systems containing hydrogen and defects were specifically equilibrated at 300 K and ambient pressure. Uniaxial tensile strain was subsequently applied along the Z-direction ($[0001]$) at an engineering strain rate of 10^9 s^{-1} using the NPT ensemble. The simulation results under these controlled conditions were analyzed to extract relevant mechanical property data and deformation characteristics.

3. Results and discussions

To investigate the mechanisms underlying the deformation behavior and elastic response of perfect-Zr, Zr-H, Zr-Vacancy, Zr-SIA, and Zr-H-defects systems, the stress-strain curves, alongside the tensile strength/strain (σ_{TS} and ϵ_{TS}) and modulus of elasticity in z-direction (E_{001}) are calculated. Additionally, the dislocation extraction algorithm (DXA) was implemented in conjunction with common neighbor analysis (CNA) on the deformed simulation boxes to examine the microstructural evolution and phase transformation of these systems under the stretching

process at different strains up to 0.2. Effects of temperature and pressure are also explored on the perfect-Zr.

3.1. Stress-Strain curve of the perfect Zirconium

The stress-strain diagram offers detailed insights into the behavior of materials under varying conditions. The elastic-plastic stress-strain behavior for perfect Zirconium (Zr) at 300 K and 0 GPa pressure, under uniaxial tensile loading along [001] direction, is presented in Figure 1. The observed linear characteristics of the curves indicate an elastic response up to a defined strain. This is where Hooke's law can be employed, allowing for the calculation of the elasticity modulus, or Young's modulus. However, as further strain is applied, the stress-strain relationship becomes non-linear, signaling the onset of plastic deformation. This rise in stress persists until it attains the tensile strength (σ_{TS}). The yield strength denotes the maximum level of stress that a material can sustain without experiencing permanent deformation. The computed values of E_{001} , σ_{TS} , and ϵ_{TS} for perfect Zirconium at 300 K and 0 GPa were determined to as 99.53 GPa, 10.022 GPa, and 12.4% respectively. These findings exhibit strong concordance with established literature values: the elastic modulus aligns with reported ranges of 96-99.9 GPa [59][60][61], while both the tensile strength (9.48-10.5 GPa [62][63]) and yield strain (10.8-12.6% [62][63]) fall within documented benchmarks. This strong correspondence validates the current simulation methodology and interatomic potential for accurately capturing zirconium's mechanical response.

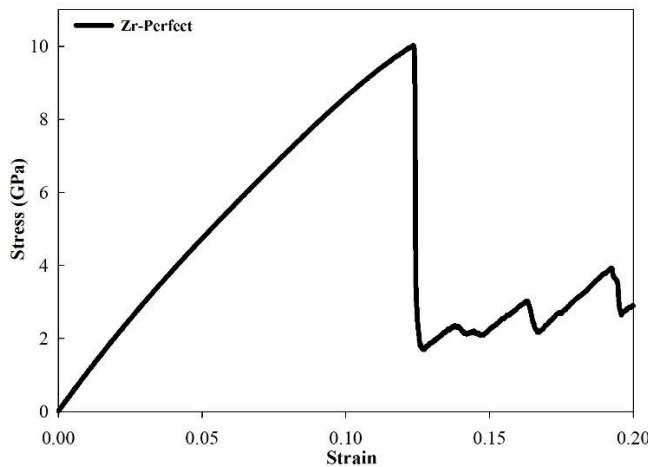


Figure 1 The stress-strain curve of perfect Zirconium at 300 K and 0 GPa

3.2. Phase evolution of the perfect Zirconium under various strains

Figure 2 shows snapshots of the simulation box under the common neighbor analysis (CNA) method and atomic microstructural changes during stretching at various strains. The HCP structure undergoes a transformation into the two alternate structures, resulting in a decrease in the number of HCP structures and an increase in the remaining two configurations. Similar identification of HCP, FCC, and other predicted crystallographic phases based on CNA for α -Zr has been reported by Foster and Zhou [21]. As demonstrated in Figure 2(a-e), at strains less than 0.124, elastic deformation occurs, with atoms maintaining their characteristic HCP arrangement, thereby exhibiting no permanent alterations to the system's shape or structural integrity, a finding that is also confirmed by Figures 1 and 3. As strains surpass 0.124, signifying the onset of the plastic stage, the stress begins to decline as the crystalline structure of Zirconium undergoes a transformation. According to Figure 3, upon reaching the yield point at $\epsilon=0.124$, the crystal structure experiences substantial transformations, deviating from the conventional HCP arrangement and disordered formations within the perfect Zirconium are revealed, which are labeled as the “Others” phase. At this point, the Zirconium structure has ceased to exist as a single crystal. A comparable evolution in structure has been reported in previous molecular dynamics simulations of HCP-Zr. An et al. [64] observed the formation of intersecting BCC bands within the parent HCP matrix at a strain of 0.10.

Upon a thorough examination of the simulation snapshot at a strain of $\epsilon=0.126$, which is slightly higher than the onset of the plastic stage, it was observed that Zirconium undergoes another phase transition. This transition leads to the formation of small phases (green points at Figure 2) that are closer to the FCC structure and are primarily located at the boundaries of the HCP- “Others” phase. When the strain exceeds 0.17, the number of atoms with an FCC structure becomes equal to the number with an irregular structure. The phase transition can persist until the HCP structure completely disappears, and all the crystal structure transforms into different forms at higher applied strains. However, we only conducted our calculations up to a strain of 0.2, and the ratio of HCP to other phases remains higher. It's important to note that this change in phase results in a rise in the level of disorder, or entropy, within the system. As a result, the plastic phase of the system (from strain of 0.124 and above) turns irreversible, in contrast to the elastic phase (at strains below 0.124). The growth of the irregular structure disrupts the crystal structure. These

disarrangements lead to the creation of various dislocation loops at strains exceeding $\epsilon = 0.124$ (illustrated at Figure 4).

Dislocations are one-dimensional lattice defects present in crystalline solids that significantly influence the mechanisms of plastic deformation. The distribution and interactions of dislocations play a pivotal role in determining key mechanical properties, including strength, ductility, and hardness. The analysis of dislocation is critical for comprehending the behavior of materials when subjected to stress. The analysis of dislocations is essential for gaining insights into the behavior of materials under stress. To perform this analysis on Zr during the stretching process, the dislocation extraction algorithm (DXA) was employed [65]. Figure 4 illustrates the distribution of dislocations in ideal zirconium metal under tensile strength conditions. The snapshots indicate that no defects are detected within the tensile strain range of 0 to 0.122. At a strain of 0.124, corresponding to the yield point of the structure, the nucleation of dislocation loops is observed. This behavior is also evident in Figure 3, where the HCP phase disappears and the “Others” phase emerges. The formation of dislocation loops can be attributed to the disruption of the local atomic arrangements associated with the structural transformation. As the tensile strain increases further, dislocation loops of varying lengths become increasingly apparent, indicating the progressive accumulation of dislocations within the material. A similar trend was reported in previous molecular dynamics simulations of HCP-Zr using a machine-learning interatomic potential, in which the HCP phase fraction decreased while the FCC phase fraction increased with increasing tensile strain [66]. The dislocation lengths as a function of tensile strain for a perfect Zr sample were analyzed utilizing OVITO, with results presented in Figure 5. The data presented in this figure indicates that the primary dislocation loops or segments are predominantly associated with the total line length configuration. In contrast, a smaller portion of the dislocations is related to the $1/3 \langle 11-20 \rangle$ direction. Within the elastic region, there are no dislocation loops, and the HCP atom ratio, as shown in Figure 3, remains invariant, leading to a flattening of the curves in this domain. Then, the dislocation lengths exhibit a pronounced increase and the ratio of HCP atoms drop at a strain of 0.124, which corresponds to the point (yield stress) at which the stress-strain curve (Figure 1) demonstrate a marked deterioration.

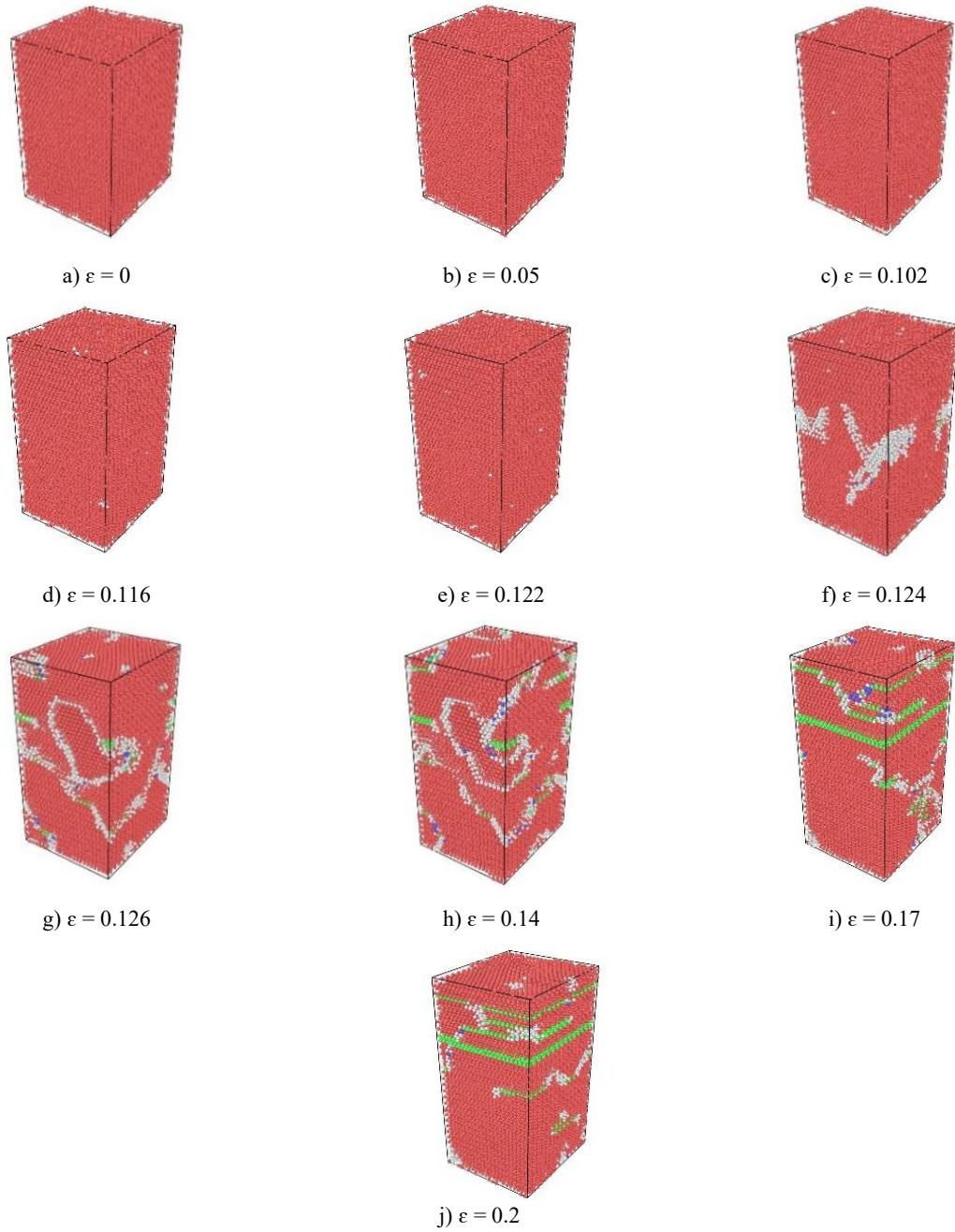


Figure 2 The atomic microstructures of Zr during the stretching process at various strains (with red, white, green, and blue points representing HCP, “Others”, FCC, and BCC structures)

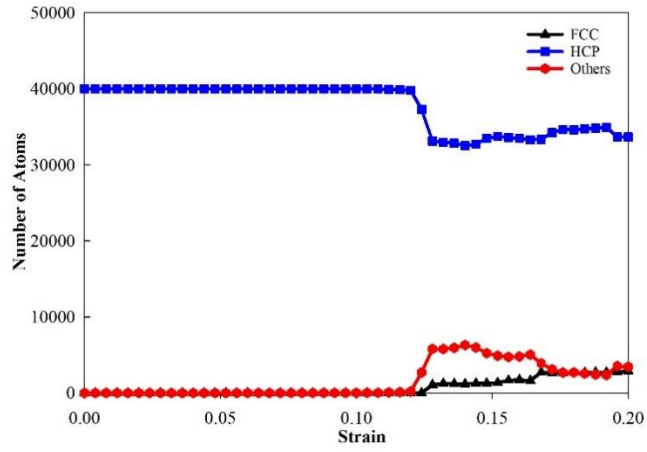


Figure 3 Phase transition of pristine Zr

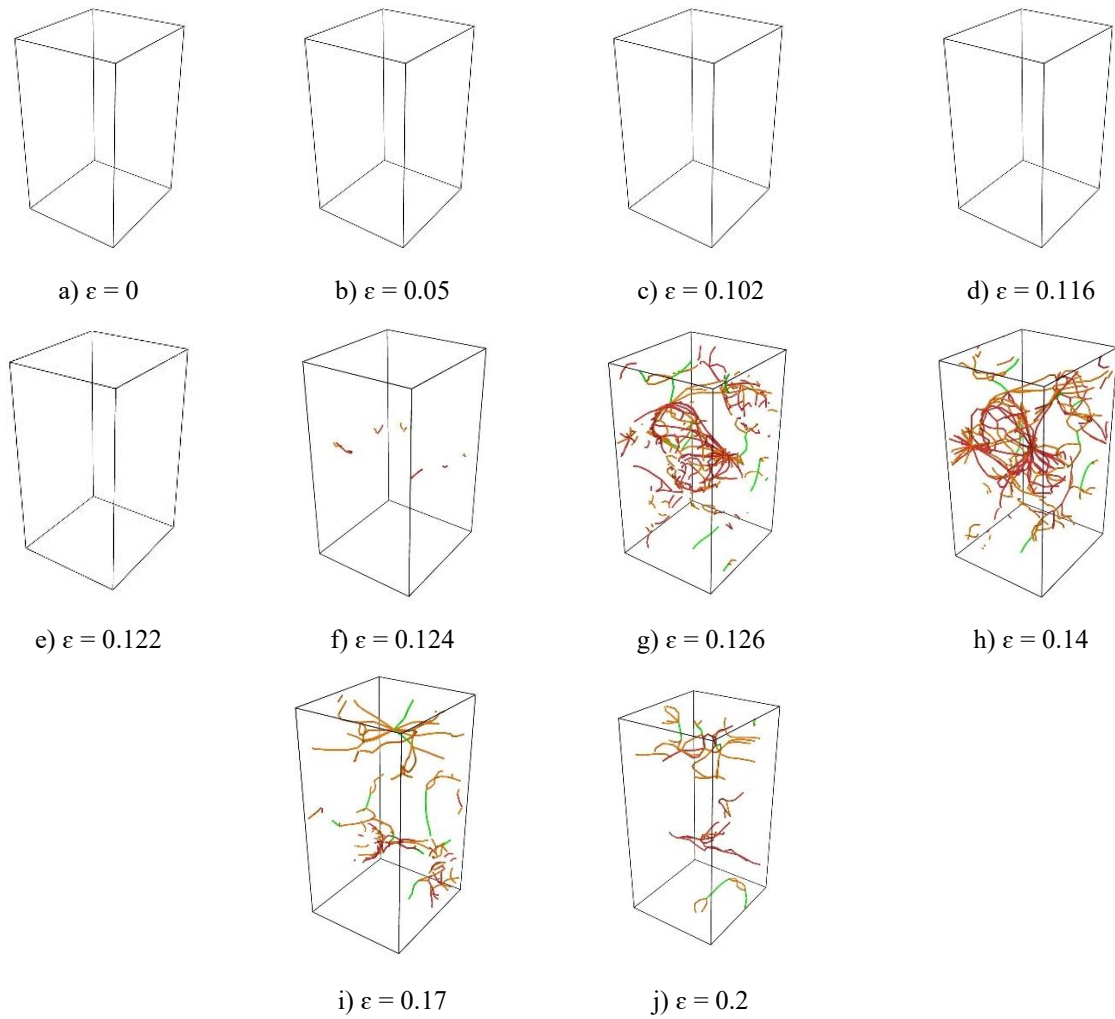


Figure 4 The microstructure evolution of a pristine Zr under tensile strain condition

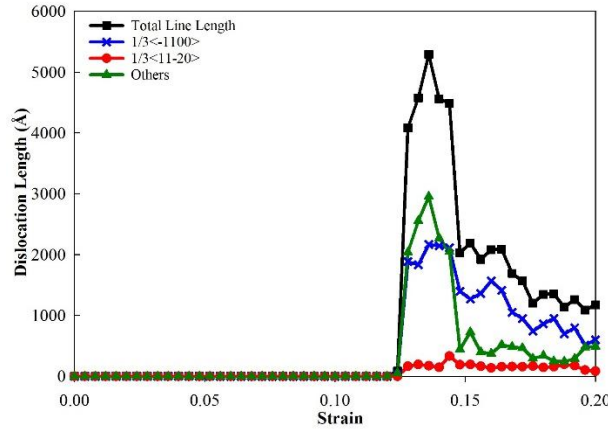


Figure 5 Lengths of dislocations in a pristine Zr as a function of tensile strain

3.3. Effect of temperature

3.3.1. Effect of temperature on the mechanical properties of perfect Zirconium

In this section, simulations were performed to investigate the influence of temperature on the mechanical properties of zirconium. Given its critical role in determining material strength, temperature variations were applied to single-crystal Zr, and the stress-strain response was analyzed across a range from 300 K to 1500 K, as illustrated in Figure 6(a). Young's modulus, which is defined by the slope of the linear elastic portion of the stress-strain curve, shows a clear dependence on temperature. The results demonstrate a consistent decrease in Young's modulus with increasing temperature, as evidenced by the reduction in both the height and slope of the stress-strain curves within the elastic region. Moreover, increasing temperature leads to a decrease in both the yield stress and yield strain, indicating a reduction in the tensile strength of the material. These trends are consistent with the findings reported by Islam and Haque [67], and An et al. [64]. Both studies similarly showed that increasing temperature destabilizes the HCP structure and promotes an earlier onset of phase transformation, which contributes to the observed deterioration in the mechanical response at elevated temperatures.

This finding is further supported by Figure 6(b), which shows how tensile strength varies with temperature. It is clear from this figure that temperature significantly influences the decline in tensile strength, tensile strain, and elastic modulus. Following the elastic region, the plastic region comes next, and as the strain continues to increase, further fracture takes place. Also, increased temperature accelerates the fracture of Zr, consistent with the findings of Barik and Sarangi [68]. At elevated temperatures, the intermolecular force between atoms diminishes, allowing them to

more readily depart from their equilibrium positions. Consequently, at identical strain levels, the stress experienced by Zr decreases, and the elastic modulus diminishes as the temperature rises, as indicated in Figure 6(b). Elevated temperatures contribute to a rise in lattice defects and nucleation and dislocations of atoms, which increases the likelihood of the system approaching its yield limits. Consequently, this leads to reduced yield strengths and elastic moduli at higher temperatures when compared to those at lower temperatures.

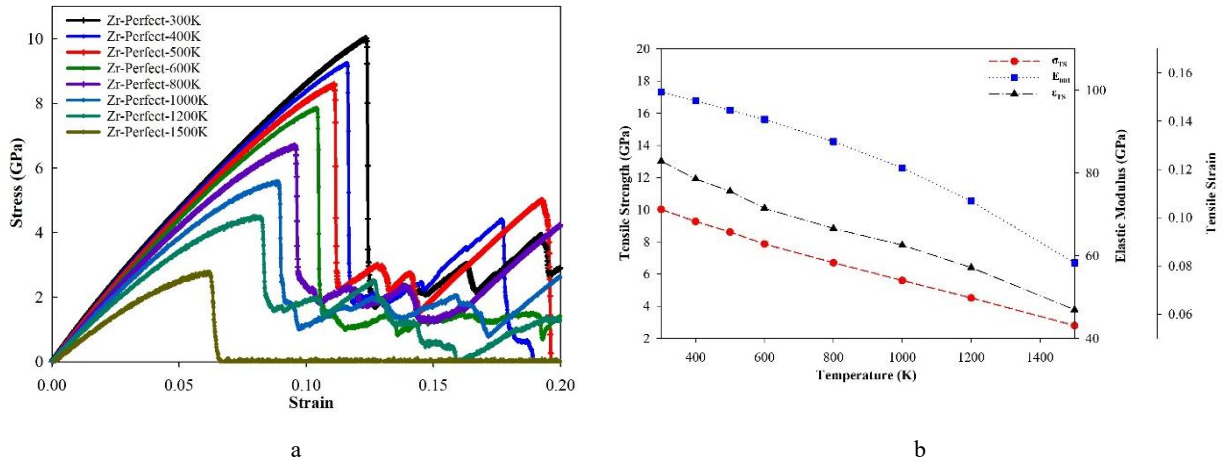


Figure 6 a) The stress–strain curves b) Evolutions of the tensile strength/strain (σ_{TS} / ϵ_{TS}) and elastic modulus (E_{001}) of the perfect zirconium at various temperatures spanning from 300 K to 1500 K.

3.3.2. Effect of temperature on the phase transition of perfect Zirconium

The common neighbor analysis (CNA) technique was used to illustrate the structural phase transition occurring during the tensile process and the fractions of three structures (HCP, FCC, and other structures) at various temperatures, and the findings are shown in Figure 7. At temperatures spanning from 300K to 600K, the HCP structure has the same initial number of atoms; However, as temperatures rise beyond this range, the number of atoms decreases, and the HCP phase begins to transition into disordered phase of "Others", even without applying any strain. Raising the temperature results in an unstable of HCP structure and an earlier occurrence of the yield strain. Indeed, as the temperature increases, the "Others" phase rise proportionally with decrease of HCP phase. This observation underscores the influence of temperature on the kinetic energy of the crystal and the degree of structural disorder. The FCC phase exhibits a fluctuating trend with rising temperature up to 800K. At this temperature, when the strain exceeds 0.16, the number of atoms exhibiting

FCC structures surpasses those with “Others” configurations. Ultimately, this number gradually decreases until the FCC phase vanishes, resulting in only the “Others” phase remaining in the crystal structure at 1500 K. At the temperature of 1200K, the HCP and "Others" phases are in equilibrium at the yield strain. It is worth noting that the growth rate of the "Others" phase and the simultaneous disappearance rate of the HCP phase are more pronounced at temperatures between 1200 and 1500 K. This figure shows that with rising temperatures, the yield strength point shifts to lower strain levels, which aligns with the stress–strain diagrams of Figure 6(a). At $T = 1500$ K, strains higher than 0.075 cause the disappearance of all HCP and FCC phases, leading to the collapse of the perfect zirconium crystal structure, which transforms completely into "Others.". In comparison to the current study, An et al. [64] noted the vanishing of the HCP phase at a lower temperature. In their simulations, the HCP phase nearly disappeared at a strain of around 0.10 and a temperature of 900 K. This discrepancy may be attributed to differences in interatomic potential, criteria for phase identification, loading conditions, and the pathways for phase transformation.

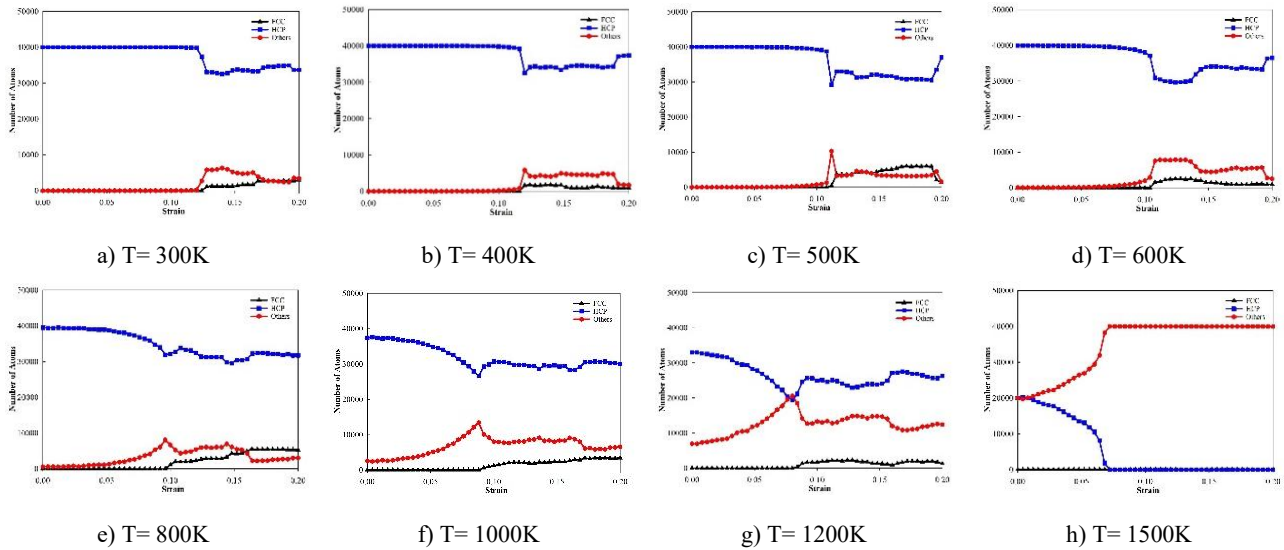


Figure 7 Effect of temperature on the phase transition of a perfect zirconium during stretching process at various strains

3.3.3. Effect of temperature on microstructure evolution of perfect Zirconium under tensile strain

The temperature-dependent evolution of the pure Zr microstructure, as revealed by DXA analysis, is presented in Figure 8. Primary dislocation loops are generated at strain levels corresponding to the tensile strength at each temperature, in agreement with the stress–strain

responses. With increasing temperature, the onset of dislocation nucleation shifts to lower strain values, which is consistent with the earlier appearance of the yield point observed in Figure 6. This trend indicates that elevated temperatures reduce the energy barrier for dislocation nucleation, thereby promoting an earlier transition of the material into the plastic deformation regime. Nevertheless, despite the facilitated nucleation of dislocations at higher temperatures, their length does not increase monotonically. Instead, the dislocation length attains a maximum at 600 K and subsequently decreases with further temperature increase [64], eventually reaching zero at 1500 K. The pronounced dislocation length observed at 600 K can be rationalized by the concurrent effects of enhanced thermal activation and preserved microstructural stability. At lower temperatures, such as 300 K, limited atomic mobility restricts dislocation glide and expansion following nucleation, resulting in relatively short dislocation loops. In contrast, at 600 K, the available thermal energy is sufficient to significantly enhance atomic diffusion and dislocation mobility, thereby facilitating dislocation glide, growth, and the formation of extended and stable dislocation loops. Importantly, as shown in Figure 7, the HCP phase remains the dominant structural component at this temperature, while the fraction of the disordered “Others” phase remains comparatively low. This structural integrity provides a coherent crystalline framework that supports sustained dislocation propagation. At temperatures exceeding 600 K, increased thermal agitation leads to progressive lattice instability and structural disorder. This behavior is evidenced in Figure 7 by the rapid increase in the fraction of the “Others” phase accompanied by a substantial reduction in the HCP structure. Under these conditions, although dislocations nucleate at lower strain levels, the loss of crystalline coherence and the prevalence of disordered atomic environments enhance dislocation annihilation, fragmentation, and loss of line continuity. As a result, the effective dislocation length decreases with increasing temperature, and at 1500 K, the complete dominance of the “Others” phase corresponds to the absence of well-defined dislocations within the fully disordered crystal structure. Overall, 600 K represents an optimal temperature regime in which thermal activation is sufficiently high to promote dislocation mobility and growth, while the crystal lattice retains adequate structural order to sustain extended dislocation loops. This combined effect accounts for the maximum dislocation length observed at 600 K, whereas lower temperatures suppress dislocation mobility and higher temperatures favor deformation mechanisms governed by structural disorder and phase transformation.

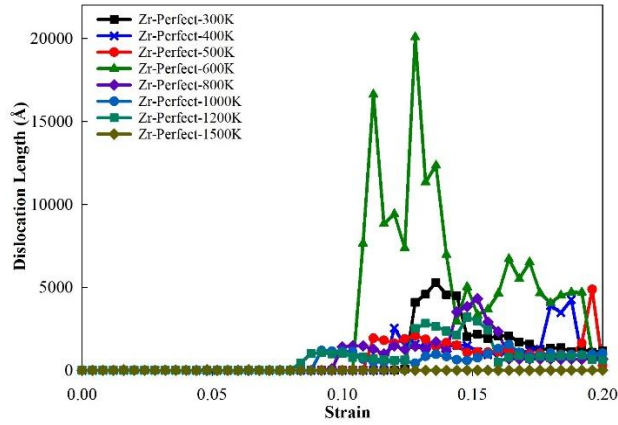


Figure 8 Effect of temperature on dislocation analysis of a perfect zirconium as a function of tensile strain

3.4. Effect of pressure

3.4.1. Effect of pressure on the mechanical properties of perfect Zirconium

Figure 9 illustrates the stress–strain responses and mechanical properties of pure zirconium subjected to hydrostatic pressures ranging from 0 to 30 GPa. Although the overall shapes of the stress–strain curves remain similar, notable differences are observed in their slopes and yield points, which occur at different strain levels. With increasing pressure, the slope of the elastic region systematically increases, indicating an enhancement of the Young’s modulus of pure Zr. This behavior arises from the reduction in interatomic spacing under hydrostatic compression, which strengthens interatomic interactions and steepens the interatomic potential. As a result, the elastic stiffness of the material increases, rendering zirconium more resistant to elastic deformation and requiring higher stress levels to achieve a given strain. In addition to the elastic response, the yield behavior of zirconium is also significantly influenced by hydrostatic pressure. Increasing the pressure up to approximately 25 GPa leads to an increase in the yield strength, indicating enhanced resistance to the onset of plastic deformation. This effect can be attributed to the restriction of dislocation motion under pressure. Hydrostatic compression reduces the available free volume within the crystal lattice and increases lattice friction, thereby raising the energy barrier for dislocation nucleation and glide. Consequently, the initiation of plastic deformation is shifted to higher stress levels, and the material exhibits increased strength. However, when the pressure is further increased from 25 to 30 GPa, a reduction in the yield strength is observed, as shown in Figure 9(b). This non-monotonic behavior suggests a transition in the dominant deformation mechanism at very

high pressures. In this pressure range, elevated internal stresses and lattice instabilities may facilitate dislocation nucleation, activate additional slip systems, or induce localized structural disorder within the crystal lattice. Such effects can lower the critical stress required for the onset of plastic deformation, despite the continued increase in elastic stiffness. The decrease in yield strain (ϵ_{TS}) observed between 20 and 30 GPa, as illustrated in Figure 9, further supports this interpretation. While increasing pressure enhances the elastic modulus and resistance to elastic deformation, excessively high pressures promote stress concentration and microstructural instabilities that accelerate the initiation of plasticity at lower strain levels. Therefore, the mechanical response of zirconium under hydrostatic pressure reflects a competition between pressure-induced elastic stiffening and the activation of pressure-assisted plastic deformation mechanisms at higher pressures.

Overall, the application of hydrostatic pressure significantly strengthens the elastic mechanical properties of zirconium. Nevertheless, at very high pressures, changes in lattice stability and deformation mechanisms lead to a reduction in both yield strength and yield strain, a behavior that is clearly captured in the stress–strain characteristics presented in Figure 9.

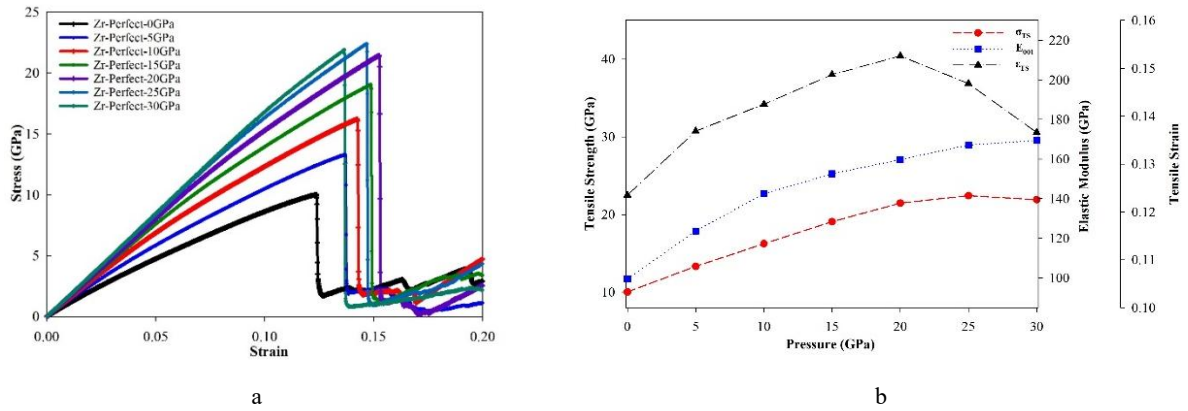


Figure 9 a) The stress–strain curves b) Evolutions of the tensile strength/strain (σ_{TS} / ϵ_{TS}) and elastic modulus (E_{001}) of the perfect zirconium at different pressures from 0 to 30 GPa

3.4.2. Effect of pressure on the phase transition of perfect Zirconium

Figure 10 demonstrates how external pressure influences the phase transition of zirconium structures, as revealed by CNA. As also shown in Figure 9, during the elastic stage, an increase in pressure up to 20 GPa postpones the onset of the yield strain and the transition of the HCP phase.

However, at pressures exceeding 20 GPa, this transition occurs at lower strains. Upon reaching the plastic stage, both the "Others" and FCC curves start to emerge as strain increases, but this occurs only up to a pressure of 20 GPa. At higher pressures and after attaining equilibrium, the amount of the HCP phase significantly decreases until it is eliminated at 30 GPa, resulting in a complete HCP → "Others" phase transition. This transformation demonstrates how higher pressure leads to a greater number of disordered atoms forming within the crystal. It is crucial to highlight that the transformation rate of the HCP phase to the "Others" phase is significant at pressures between 15 and 20 GPa.

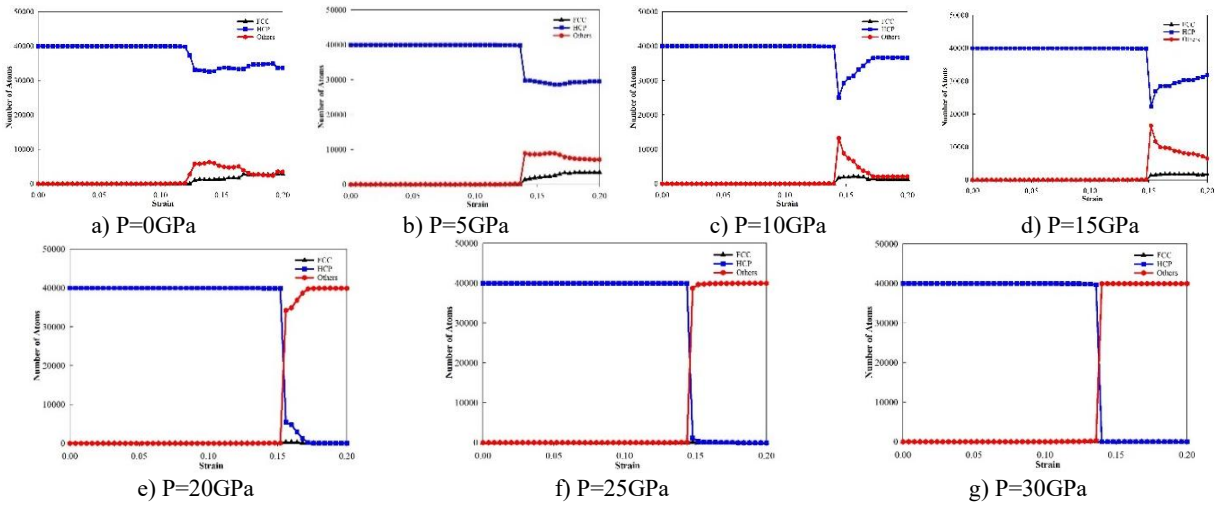


Figure 10 Effect of pressure on phase transition of perfect zirconium during stretching process at various strains

3.4.3. Effect of pressure on microstructure evolution of perfect Zirconium under tensile strain

Figure 11 presents the impact of pressure on the evolution of dislocation lengths during the tensile deformation process. The formation of dislocation loops is observed to be pressure-dependent. At pressures up to 15 GPa, the first dislocation loops nucleate at a strain corresponding to the yield point, with higher pressures delaying their formation to higher strain levels. This trend, however, is only valid for pressures below 20 GPa. At higher pressures, ranging from 20 to 30 GPa, no discernible dislocation loops are formed. This absence suggests a transition in the deformation mechanism, potentially due to the emergence of more complex defect structures—such as volumetric defects—that are not readily detectable through dislocation analysis alone. Furthermore, the initial dislocations that do form are replaced by new configurations during the plastic phase, underscoring how increased hydrostatic pressure alters the failure mechanisms of the crystal structure after the elastic limit is surpassed. Regarding dislocation length, increasing pressure

generally has no significant effect, with one notable exception: at 5 GPa, a substantial increase in total dislocation length is observed, indicating a unique regime of plastic activity at this specific pressure.

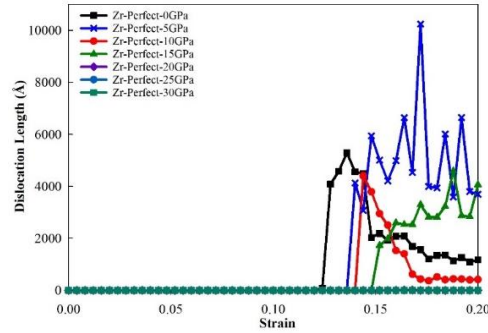


Figure 11 Effect of pressure on dislocation analysis of a perfect zirconium as a function of tensile strain

3.5. The effect of Hydrogen, Defect Types and their concentrations on mechanical behavior of Zirconium

The presence of hydrogen atoms, as well as structural defects including vacancies and self-interstitial atoms, exerts a substantial impact on the mechanical properties of zirconium [28][69][70]. To investigate the mechanical characteristics of Zirconium under these specific conditions, an analysis of tensile deformation was conducted. The stress-strain curves, alongside the computed tensile strength, tensile strain, and elastic modulus values for the Zr-H, Zr-V, Zr-SIA, Zr-H-V, and Zr-H-SIA systems, are depicted in Figures 12-18. The values pertain to hydrogen, vacancy, and SIA concentrations of 0.1%, 0.5%, 1.0%, 2.0%, and 5.0%, and are assessed in comparison to the characteristics of perfect Zr.

Considering the results, for all systems analyzed, it is observed that mechanical parameters exhibit a decline in response to increasing concentrations of defects and hydrogen. For example, in the Zr-Vacancy 5.0% system, the elastic modulus was measured at 78.7 GPa, with the tensile strength and tensile strain recorded at 5.18 GPa and 0.065 GPa, respectively. These findings signify reductions of 21%, 48%, and 47% when compared to pure Zr. It's noted that 5.0% inclusion of H into Zr results in 2%, 4.3%, and 2.4% reductions in the parameters of interest, which can fairly be neglected. Likewise, the Zr-SIA system exhibited reductions of 2%, 64%, and 69% in the same mechanical parameters. Based on these observations, it can be inferred that, at similar concentrations, the interstitials weaken the Zr's strength far more dramatically than hydrogen and vacancy do. However, the variations of elastic modulus are mostly influenced by the concentration

of vacancies. As regards, it is evident in the slopes of the stress-strain curves in the elastic region, showing that an increase in vacancy concentration significantly reduces Young's modulus. These findings are consistent with those of our prior study and the research conducted by Zhu et al. [23][28]. Figure 14 further demonstrates that SIAs detrimentally impact the mechanical behavior of zirconium, with an effect even more pronounced than that of vacancy defects. At high concentrations, these defects can compromise the structural integrity of the zirconium crystal and cause a severe reduction in its mechanical strength. The increase of H incorporated into Zr does not alter the shape of the stress-strain curves, which maintain a similar slope and approximately the same Young's modulus. In contrast, vacancies affect the maximum stress levels, while interstitials significantly alter the curves, resulting in a wavelike pattern [52]. Generally, the values of tensile strength and tensile strain exhibited a marginal decrease as hydrogen concentration increased; however, a minor increase in these parameters was observed at hydrogen content levels ranging from 0.5% to 1.0%. In general, Figure 12 shows no significant variation in the σ_{TS} , ϵ_{TS} , and E_{001} across the entire range of hydrogen concentrations[39]. Consequently, the content of hydrogen appears to exert a negligible influence on the mechanical properties measured[29]. It implies that throughout the entire range of hydrogen concentrations, from 0.1% to 5.0% H, the tensile deformation and elastic moduli remain largely unaffected by the precipitation of hydrides within the matrix.

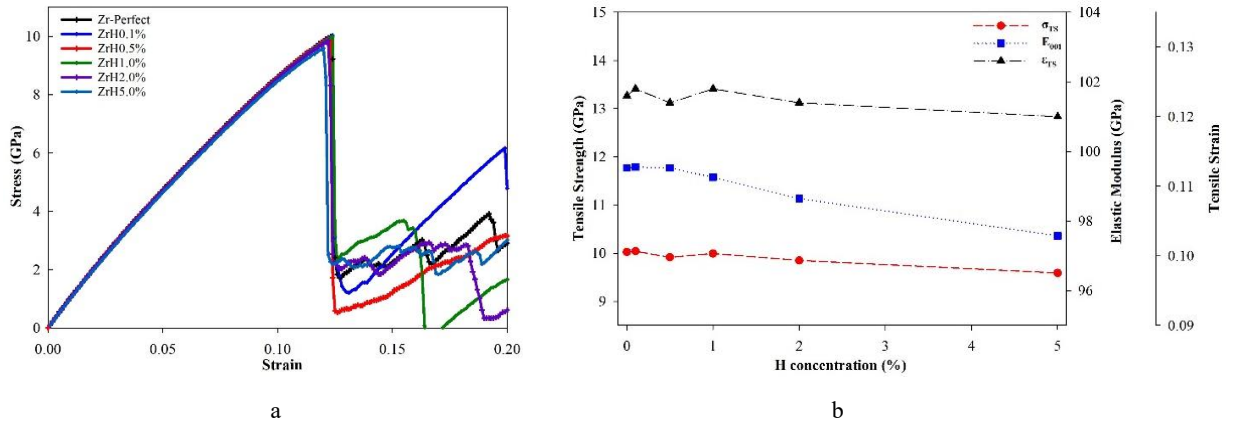


Figure 12 a) stress-strain curve and b) mechanical properties (σ_{TS} , ϵ_{TS} , and E_{001}) for Zr-H systems as a function of H concentration in comparison of perfect Zr

According to Figure 13(a), the presence of vacancies altered the form of the stress-strain curve. As the concentration of vacancy increases, the linear elastic region, yield stress and strain

progressively diminish while the non-linear plastic region expands. This suggests a transition toward ductile failure. In fact, Zirconium breaks down at lower strains with increasing vacancy concentration. These findings are also explicitly illustrated in Figure 13(b). The reduction in yield stress is more noticeable than the elasticity, which can also be seen from the slight variations in the slopes of the stress-strain curves. Generally, the findings indicate that vacancy defects considerably decrease the mechanical properties of zirconium.

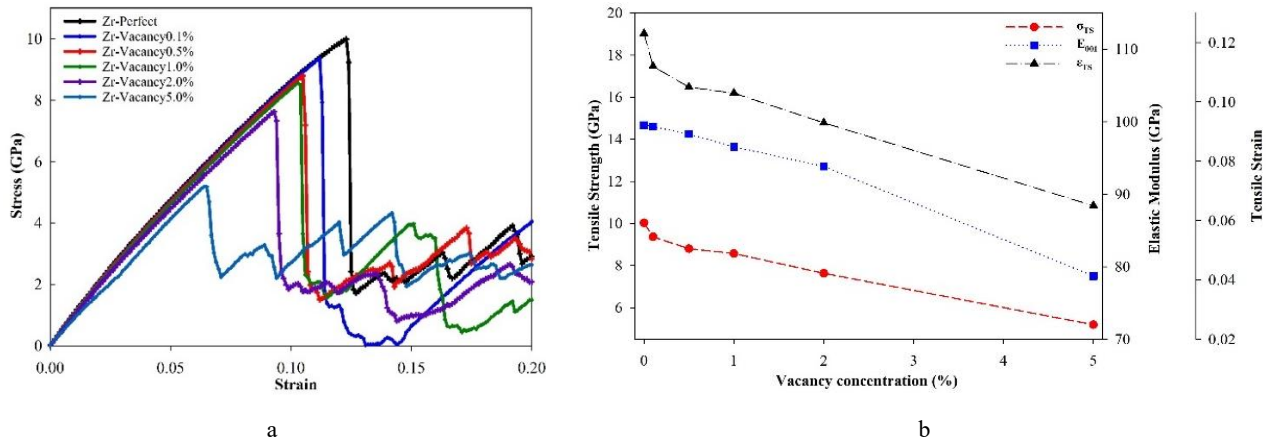


Figure 13 a) stress-strain curve and b) mechanical properties (σ_{TS} , ϵ_{TS} , and E_{001}) for Zr-V systems as a function of vacancy concentration in comparison of perfect Zr

Analysis of the Zr-SIA systems reveals a complex influence of SIA concentrations on mechanical properties. At low concentrations (up to 2.0%), SIAs induce a drastic reduction in tensile strength and strain compared to other defect scenarios, a trend clearly reflected in the diminished yield stress and strain observable in Figure 14(a). This pronounced decrease underscores that self-interstitial defects degrade tensile strength more significantly than either vacancy defects or the presence of hydrogen. The results consistently indicate that while various structural point defects generally diminish the mechanical properties of zirconium, SIAs exert a particularly severe adverse impact. However, the mechanical response becomes less straightforward at higher SIA concentrations. While concentrations above 1% lead to an apparent increase in the measured maximum stress, this occurs at a point different from the calculated yield stress and is accompanied by significant noise in the stress-strain curve, as evidenced in Figure 14(a). Furthermore, Young's modulus (E_{001}) shows an atypical upward trend within the 1-2% SIA concentration range. Beyond the 2.0% threshold, the mechanical properties generally reach a plateau, and Figure 14(b) demonstrates that the influence of SIAs becomes negligible at these

higher concentrations. The substantial lattice distortion under uniaxial strain at elevated SIA concentrations renders the stress-strain data fundamentally unreliable. Therefore, the apparent increase in maximum stress is more accurately interpreted as an artifact of severe lattice distortion rather than a genuine strengthening effect. In summary, while low concentrations of SIAs are profoundly detrimental to mechanical strength, their influence saturates and the associated data becomes unreliable at higher concentrations due to extreme crystal lattice disruption.

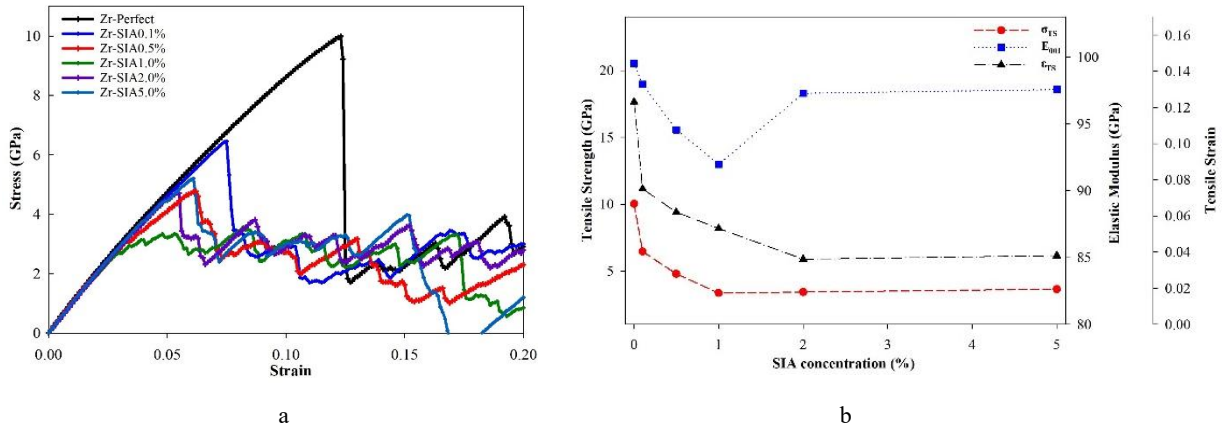


Figure 14 a) stress-strain curve and b) mechanical properties (σ_{TS} , ϵ_{TS} , and E_{001}) for Zr-SIA systems as a function of SIA concentration in comparison of perfect Zr

To achieve better results and facilitate the analysis of the behavior of Zr, the concurrent impact of hydrogen atoms, vacancies, and self-interstitial atom (SIA) defects on mechanical behavior of Zr, along with their interactions with one another, was also evaluated. As such, the Zr structures were examined for a hydrogen content of 1.0% while varying the concentrations of vacancy and SIA defects from 0% to 5.0%. In the next two cases, conversely, a constant defect density of 1.0% was considered, and the concentrations of H were varied within the same 0% to 5.0% range. The results of these investigations are illustrated in Figures 15-18. This data is presented to enable a comparison with the ZrH-1.0% and Zr-defects1.0% systems. Figure 15 illustrates the impact of vacancy concentration on the elastic moduli and strength of Zr-H1.0%-V systems. Similar to the trend observed in Zr-V systems, an increase in vacancy concentration leads to a consistent degradation of zirconium's mechanical resistance. For example, when zirconium containing 1.0% H is subjected to a 5.0% vacancy concentration, its mechanical parameters decrease to $\sigma_{TS} = 4.93\text{GPa}$, $\epsilon_{TS} = 0.063$, and $E_{001} = 77.6\text{GPa}$. These values represent a reduction of 50.8%, 48.7%, and 22%, respectively, compared to perfect Zr. Crucially, the decline is nearly equivalent when

compared to the ZrH-1.0% system, with reductions of 50.6%, 49.1%, and 21.8%. This confirms that the strength degradation is primarily a function of the vacancy concentration itself. A comparison of the trends in Figures 13 and 15 confirms this interpretation, as both exhibit nearly identical behavior. This consistent pattern strongly suggests that the presence of hydrogen does not significantly alter the detrimental impact of vacancies on the structure; hydrogen atoms neither meaningfully mitigate nor exacerbate the mechanical degradation induced by vacancies. Consequently, the mechanical integrity of zirconium, in this context, demonstrates a notable insensitivity to hydrogen content, with vacancy concentration being the dominant factor controlling the loss of mechanical resistance.

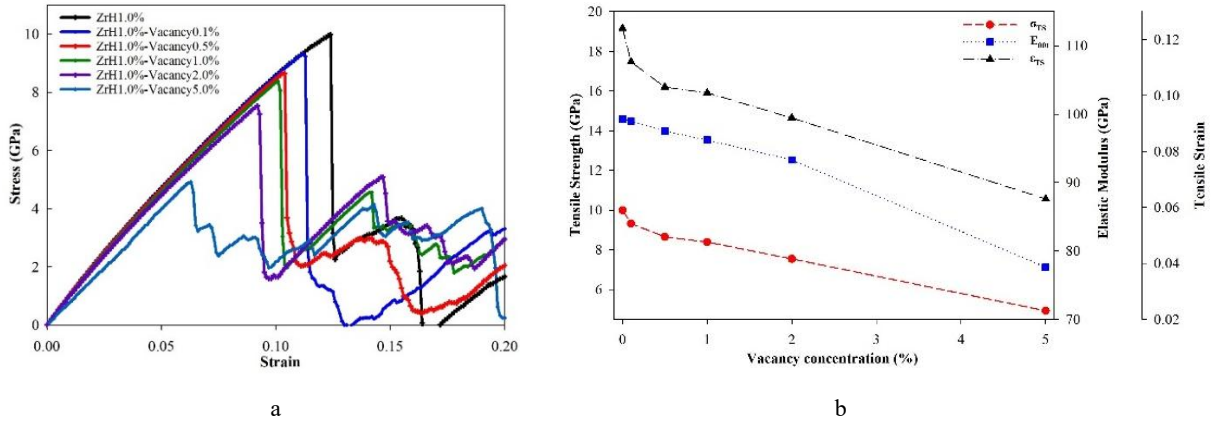


Figure 15 a) stress-strain curve and b) mechanical properties (σ_{TS} , ϵ_{TS} , and E_{001}) for Zr-H1.0%-Vacancy systems as a function of vacancy concentration in comparison ZrH1.0%

To investigate the impact of SIA concentration on the mechanical properties of Zr-H1.0%-SIA systems, stress-strain curves along with tensile stress/strain values and elastic modulus were determined and are presented in Figure 16. As observed in Figure 16(b), the Zr-H1.0%-SIA systems exhibit behavior remarkably similar to the Zr-SIA systems, particularly in their differential response at low versus high SIA concentrations. At low SIA concentrations (up to 1.0%), a significant degradation of mechanical properties occurs, especially in tensile strength and strain. In contrast, at higher concentrations (1.0% to 5.0%), a slight increase in these properties is observed. However, consistent with previous findings, this apparent enhancement in maximum stress and Young's modulus does not indicate genuine crystal strengthening. Rather, it represents an artificial effect arising from severe lattice distortion. Consequently, while low SIA concentrations are profoundly detrimental to mechanical strength, their influence saturates at

higher concentrations, where the associated data become unreliable due to extreme crystal lattice disruption. Nevertheless, the presence of SIAs still causes a decrease in the mechanical properties of Zr-H1.0% systems. The values obtained for tensile stress and strain, and elastic modulus in the Zr-H1.0%-SIA2.0% system are 4.51GPa, 0.054, and 92.73 GPa, respectively. These values represent reductions of 55%, 56.1%, and 6.8% compared to pristine Zr, and 54.9%, 56.5%, and 6.6% compared to the Zr-H1.0% system, confirming that SIAs consistently diminish mechanical properties regardless of hydrogen presence. The similar curve shapes between Figures 16 and Figure 14 provide further confirmation that hydrogen has negligible influence on how point defects affect zirconium's properties. Therefore, despite the complex concentration-dependent behavior, the presence of SIAs unequivocally reduces the mechanical performance of Zr-H1.0% systems, with hydrogen playing an insignificant role in modifying this defect-mediated degradation.

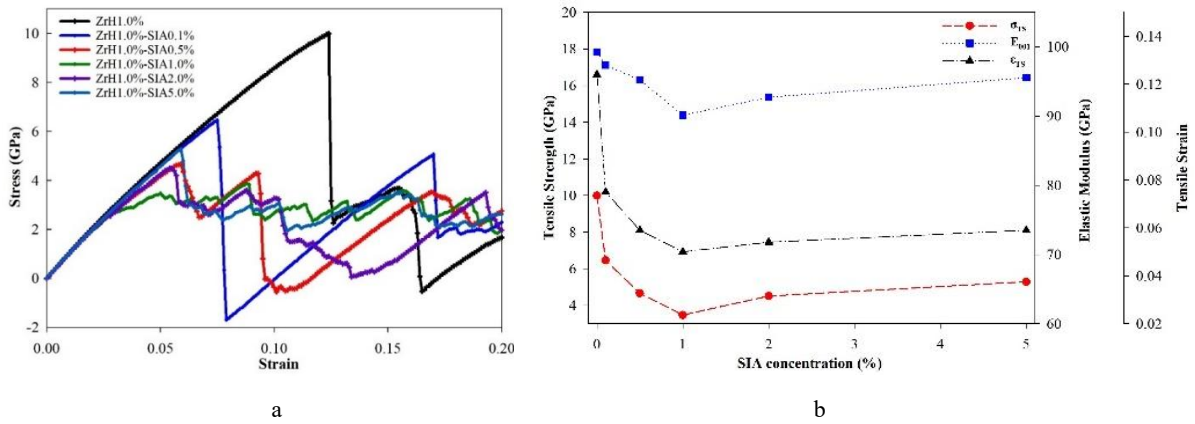


Figure 16 a) stress-strain curve and b) mechanical properties (σ_{TS} , ϵ_{TS} , and E_{001}) for Zr-H1.0%-SIA systems as a function of SIA concentration in comparison ZrH1.0%

Figure 17 investigates the interactive effects of H concentration on the structural characteristics of ZrH systems containing a fixed 1.0% vacancy concentration. The results demonstrate that increasing the H concentration in these systems leads to a slight reduction in mechanical properties. This observed reduction, however, is notably minimal when placed in a comparative context. The degradation is significantly less severe than in scenarios where vacancy concentration varies under constant hydrogen content. Furthermore, the extent of property reduction is almost equivalent to the case where hydrogen is present alone in the Zr lattice without any vacancy defects. These comparative findings lead to a critical conclusion: a 1.0% vacancy concentration does not play a significant role in either neutralizing or amplifying the mechanical parameters of ZrH systems.

The vacancy defects appear to exist independently in the lattice without forming substantial interactive complexes with H atoms that would meaningfully alter the mechanical response. This suggests that at this specific concentration threshold, vacancies and hydrogen influence the mechanical properties through largely independent mechanisms rather than synergistic interactions. The mechanical behavior is thus dominated by the individual contributions of each defect type, with hydrogen exerting its characteristic embrittling effect regardless of the presence of these specific vacancy concentrations.

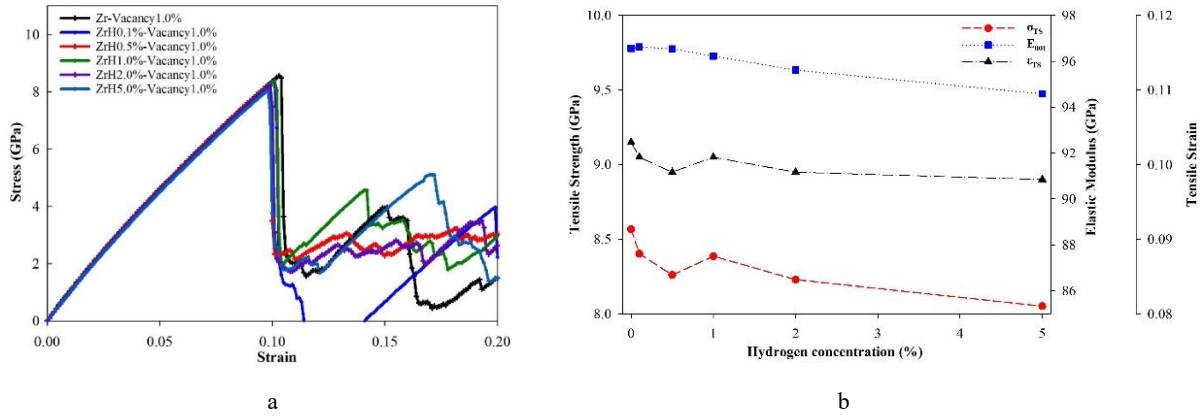


Figure 17 a) stress-strain curve and b) mechanical properties (σ_{TS} , ϵ_{TS} , and E_{001}) for Zr-H-Vacancy1.0% systems as a function of H concentration in comparison of Zr-Vacancy1.0%

Figure 18 depicts the stress-strain curves for Zr-H-SIA systems with 1% SIA defect. In this case, the presence of 1.0% SIA with variable H atoms causes the stress-strain curves to deviate from their normal pattern. The strong interactions between the SIAs and H atoms led to these inaccurate and messed up results. Therefore, we chose not to include a diagram of the mechanical parameters, and this figure is provided solely to complete our review.

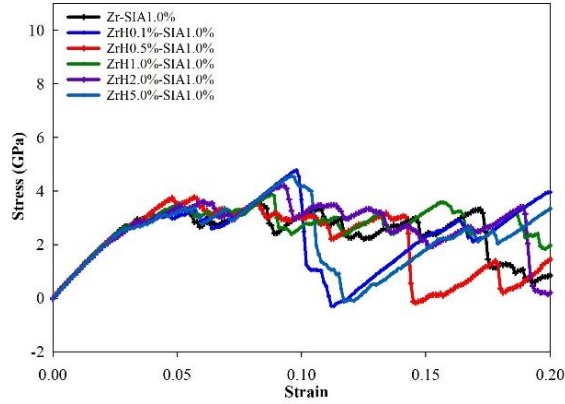


Figure 18 stress-strain curve for Zr-H-SIA1.0% systems as a function of H concentration in comparison of Zr-SIA1.0%

3.6. Effect of Hydrogen Concentration, Defect Types, and their densities on phase transition

Figures 19-25 depict the phase transition of Zr systems under tensile strain, analyzing three structural categories involving H atoms, point defects, and their combinations across a concentration range of 0.1% to 5.0%. The analysis reveals that systems containing H and/or defects initially lack a perfect HCP structure and instead contain a significant fraction of an "Others" phase. This "Others" phase fraction increases with rising H and vacancy concentrations even within the elastic region, with the first significant phase transition consistently occurring at strain levels corresponding to the end of the elastic region as shown in Figures 12-18. However, the structure featuring SIAs has the least fraction of the "Others" phase, and the number of atoms in the existing phases shows no observable variation during stretching. In other words, a crystal with an interstitial defect experiences a slight transition to the "Others" and FCC phases. A significant portion of FCC atoms is found in the initial stages of plastic deformation.

In systems containing only H atoms, it is observed that the number of HCP atoms decrease as the hydrogen content increases [71]. The more incorporation of H atoms within the pure HCP Zr crystal structure leads to a disruption of local symmetry, which in turn causes the neighboring Zr atoms to deviate from HCP coordination. This facilitates a phase transition from HCP to the "Others" phase, with the FCC phase emerging subsequently at higher strains beyond approximately 0.12. A pure HCP structure is only maintained up to a strain of about 0.12 in systems with very low hydrogen content around 0.1%. When examining vacancy effects, data from Figure 20 indicates that increasing vacancy concentration lowers the critical strain required for the initial

transition into both the "Others" and FCC phases, with the disordered "Others" phase forming in greater quantity than the FCC phase at this transition point.

Structures with SIAs exhibit distinctly different behavior by retaining the highest initial fraction of the primary HCP phase in the elastic region compared to other defect types. The impact of SIAs on phase stability remains minimal, with the initial HCP fraction showing little variation during stretching. However, at high concentrations around 5.0% and elevated strains, a unique phenomenon occurs where the FCC phase transition ceases entirely. This behavior can be attributed to the formation of interstitial clusters under high SIA density, where tensile strain reducing density along the [0001] direction potentially allows some interstitial atoms to relocate into proper HCP sites [72] - explaining the observed increase in HCP atoms at a strain of 0.16 for the 5.0% SIA concentration. The comparative analysis clearly demonstrates that vacancies and hydrogen act synergistically to destabilize the HCP phase, leading to a corresponding decline in its fraction. In stark contrast, SIAs have a fundamentally different impact on phase changes and can even promote HCP stability at high concentrations through a unique reordering mechanism. This comprehensive examination underscores the distinct roles these different defect types play in zirconium's structural evolution under mechanical strain, providing crucial insights for predicting material behavior in engineering applications.

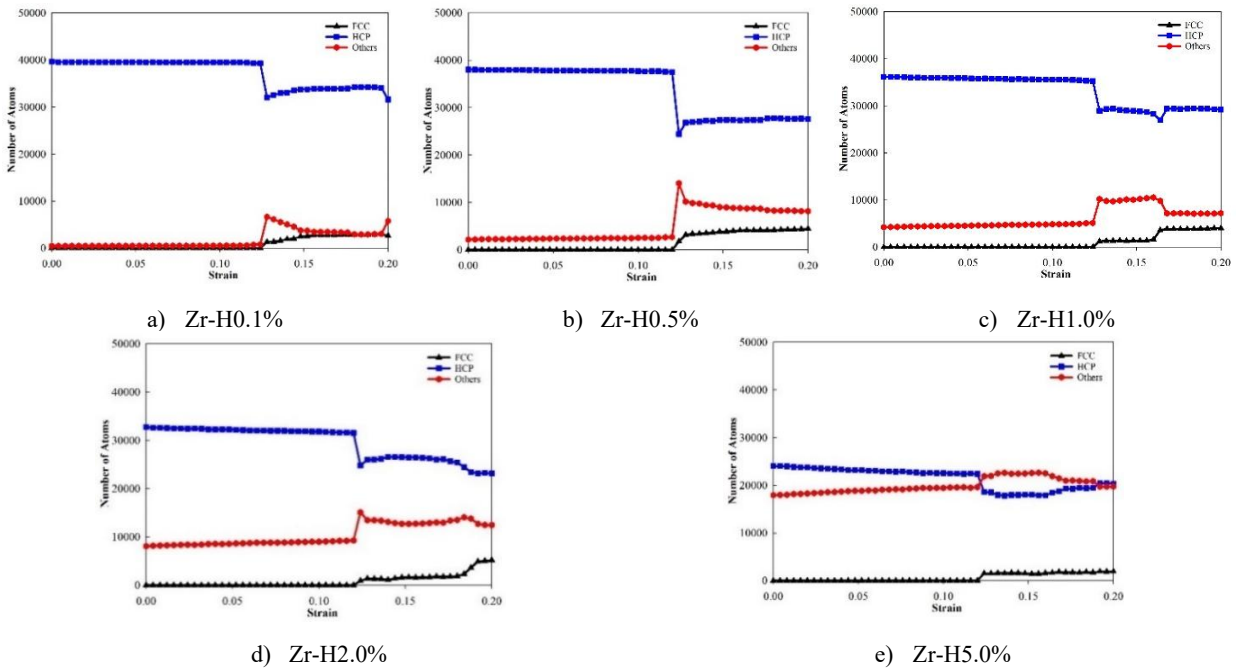


Figure 19 Effect of H concentration on the phase transition of Zr during stretching process at various strains

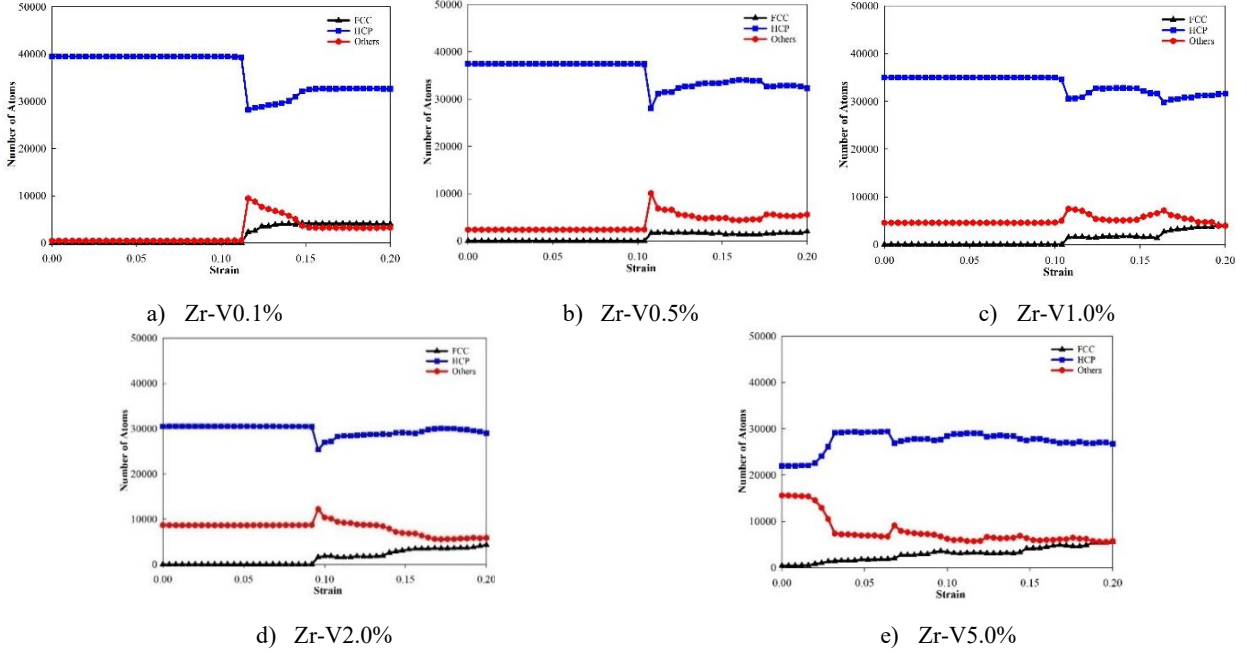


Figure 20 Effect of vacancy concentration on the phase transition of Zr during stretching process at various strains

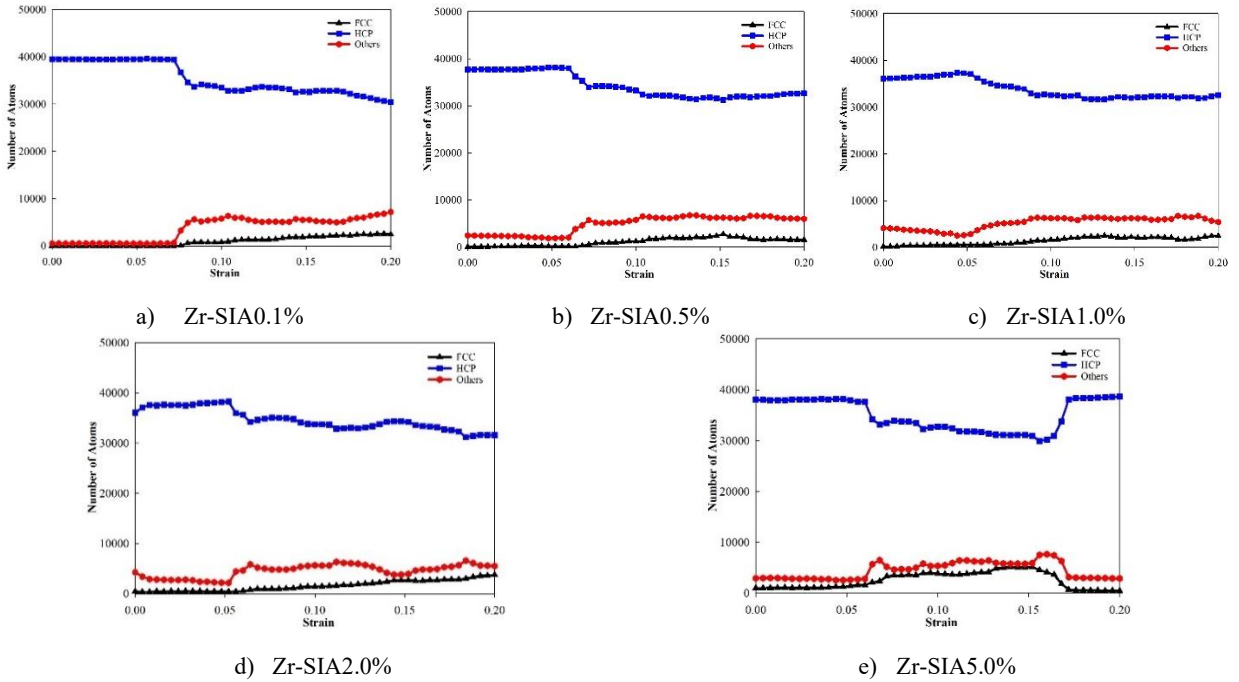


Figure 21 Effect of SIAs concentration on the phase transition of Zr during stretching process at various strains.

Figure 22 reveals a significant synergistic degradation effect between vacancy defects and hydrogen on the stability of the primary HCP phase in Zr systems. The data demonstrate that increasing vacancy density in hydrogen-charged Zr (ZrH1.0%) leads to a more substantial reduction of the HCP phase within the elastic region compared to systems containing only

hydrogen or only vacancies. This amplified effect suggests that vacancies and hydrogen cooperate in disrupting the HCP lattice, potentially through a mechanism where vacancies serve as hydrogen trapping sites that subsequently amplify local lattice strain and facilitate HCP destabilization.

While the general trend of phase evolution in ZrH-V systems mirrors that observed in Zr-V systems without hydrogen, a crucial distinction emerges in the post-yield behavior. In the ZrH1.0%-V5.0% system, a distinct phase transition is initiated at approximately $\varepsilon = 0.2$, whereas in the hydrogen-free Zr-V5.0% system, the phase fractions stabilize without undergoing a similar transformation. This delayed transition in the hydrogen-containing system indicates that hydrogen, when combined with a high vacancy concentration, fundamentally alters the material's deformation pathway. The H atoms, likely mobilized by the increasing strain and interacting with the vacancy-rich microstructure, appear to enable a transformation that is suppressed in their absence. This observation underscores that the combination of hydrogen and vacancies creates a unique defect environment that not only accelerates initial HCP degradation but also unlocks deformation mechanisms inaccessible to either defect acting alone, highlighting the critical importance of defect interactions in determining the mechanical and microstructural response of zirconium alloys.

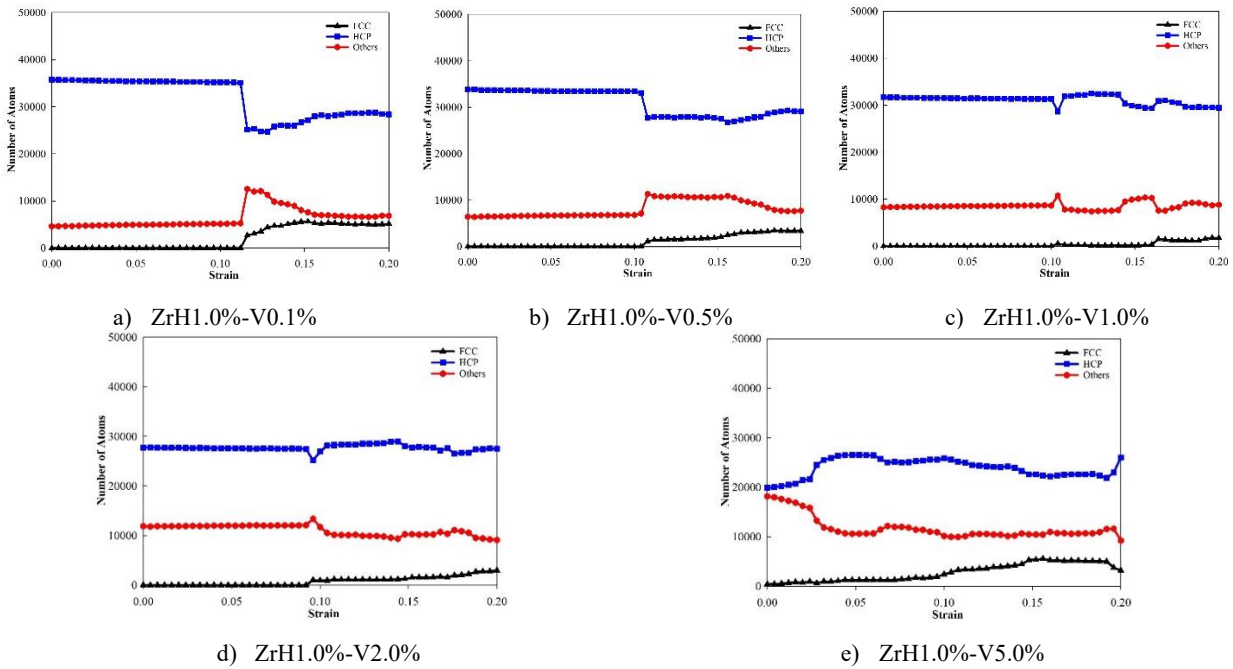


Figure 22 Effect of vacancy concentration on the phase transition of ZrH1.0%-Vacancy system during stretching process at various strains

Figure 23 reveals a complex, non-monotonic relationship between SIA concentration and phase stability in ZrH1.0% systems under tensile strain. A key finding is the strain-induced phase transformation, which initiates at a consistent critical strain value irrespective of SIA concentration. This suggests that the nucleation of new phases is triggered by a global mechanical instability, likely the onset of widespread plastic deformation, rather than being directly governed by the initial defect concentration itself. The evolution of the HCP phase population demonstrates a particularly intriguing trend: it decreases gradually as the SIA concentration rises to 2.0%, but then exhibits a significant recovery at the highest concentration of 5.0%. This rebound implies a saturation threshold is crossed, where the high density of SIAs may lead to the formation of interstitial clusters or dislocation structures that paradoxically restore a degree of local order, effectively stabilizing the HCP configuration against transformation. The presence of 1.0% hydrogen is shown to have only a marginal influence on the initial HCP and "Others" phase fractions, indicating that hydrogen plays a secondary role to the dominant effect of SIAs in the initial microstructural state. However, in the plastic region, a clear positive correlation emerges between SIA concentration and the fraction of the FCC phase. This indicates that while SIAs may stabilize the HCP structure at very high concentrations initially, they simultaneously facilitate the nucleation and growth of the FCC phase once plastic flow commences, likely by providing preferential sites for phase transformation and enhancing atomic mobility through the locally strained lattice. This dual role of SIAs—as both potential stabilizers and facilitators of phase change—highlights their complex and concentration-dependent influence on the deformation microstructure.

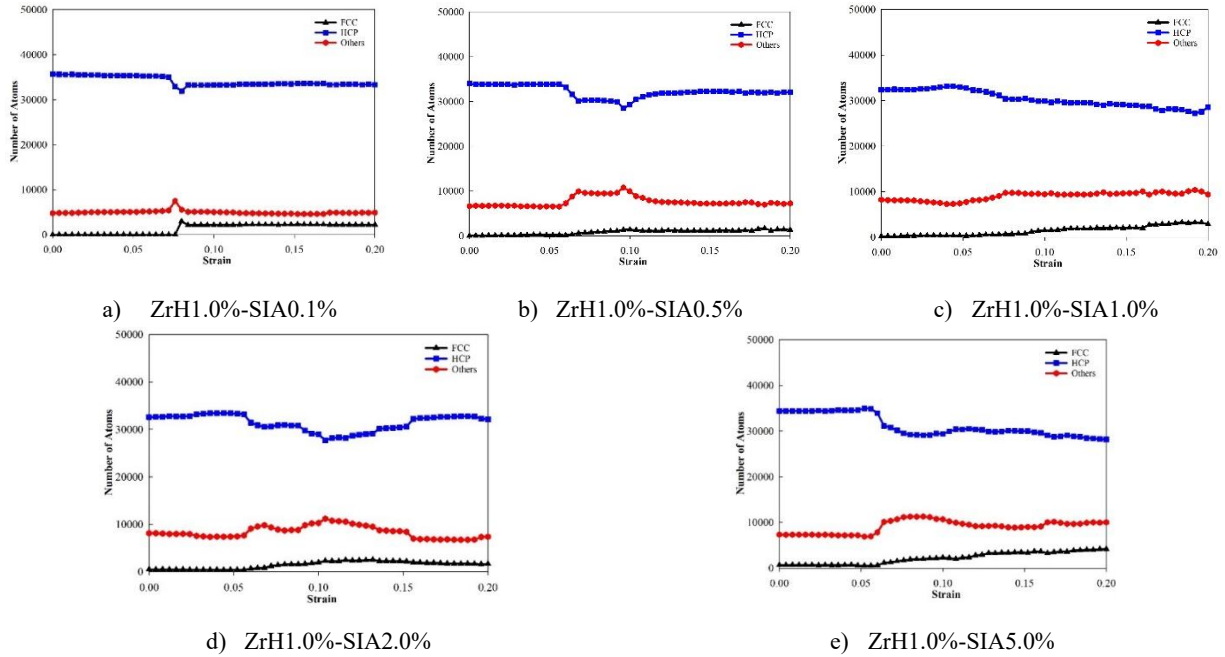


Figure 23 Effect of SIA concentration on the phase transition of ZrH1.0%-SIA system during stretching process at various strains

As demonstrated in Figure 24, the initial phase composition in the ZrH-Vacancy1.0% systems mirror that of the ZrH1.0%-Vacancy systems, suggesting that the concurrent presence of low concentrations (1.0%) of both vacancy defects and hydrogen does not produce a significant synergistic effect on the initial atomic distribution. However, a critical distinction emerges at the elevated H concentration of 5.0%, where a complete annihilation of the FCC phase is observed, and the HCP and "Others" phases subsequently reach an approximate equilibrium. This phenomenon can be attributed to two primary, interconnected mechanisms. Firstly, the high density of vacancy defects acts as potent trapping sites for H atoms, effectively sequestering them and reducing their mobility and availability to facilitate the formation of the FCC phase. Secondly, the aggregation of vacancies introduces substantial local lattice strains and disrupts the crystalline periodicity, which collectively destabilizes the FCC structure—a phase that requires a relatively ordered atomic arrangement—while concurrently enhancing the relative stability of the more tolerant HCP and disordered "Others" phases. These findings reveal a competitive interaction where, beyond a critical defect density, vacancies effectively suppress the hydrogen-mediated formation of the FCC phase by both immobilizing the hydrogen species and distorting the lattice, thereby steering the system's phase evolution toward an equilibrium dominated by the HCP and amorphous-like structures.

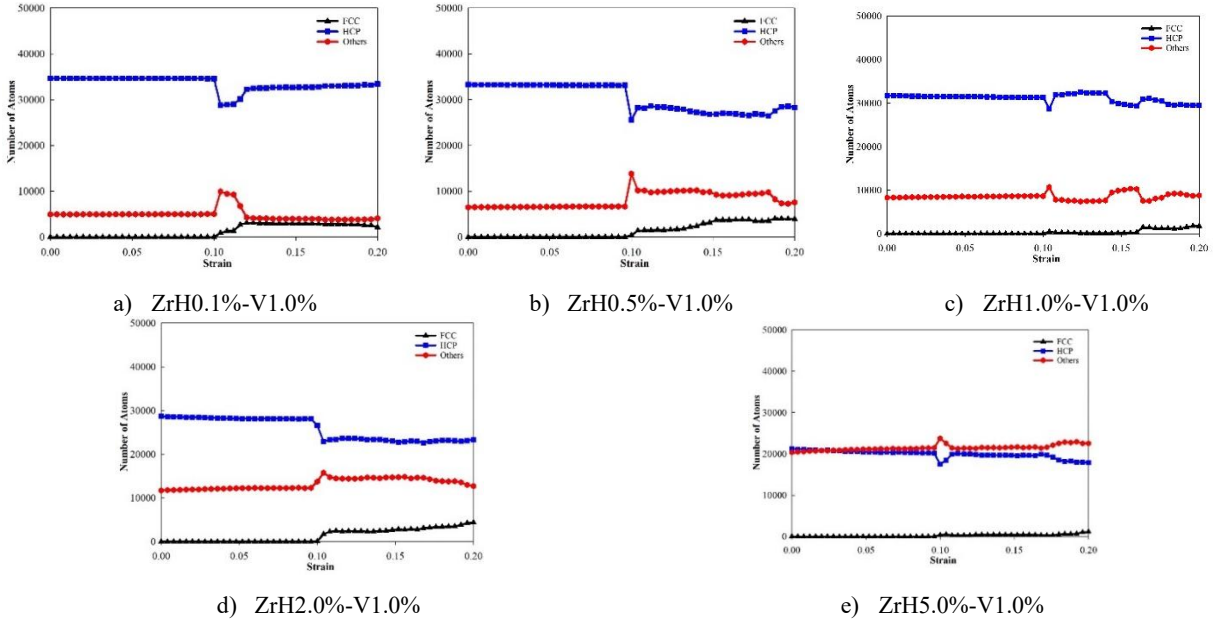


Figure 24 Effect of H concentration on the phase transition of ZrH-Vacancy1.0% system during stretching process at various strains

As can be seen in Figure 25, the phase stability behavior of zirconium systems reveals a fundamental contrast when comparing the effects of SIA concentration versus H concentration. In ZrH1.0%-SIA systems, the phase composition remains remarkably stable; the population of atoms in the HCP and disordered ("Others") structures shows no significant variation with increasing SIA content. This indicates that SIAs, up to a certain concentration, do not inherently destabilize the crystalline matrix. In stark contrast, ZrH-SIA1.0% systems demonstrate a strong hydrogen-dependent response. As the H concentration increases, a continuous redistribution of atoms occurs, characterized by a systematic decrease in HCP atoms and a corresponding rise in the "Others" phase. This trend culminates in an equilibrium state at 5.0% H, where the populations of HCP and "Others" phases become equal, suggesting that hydrogen acts as a potent driver of disordering.

A key finding across all systems is that within the elastic deformation regime, no obvious HCP to non-HCP phase transition is activated by the presence of hydrogen, vacancies, or interstitials—except at the highest defect concentration of 5%. This implies that the lattice can accommodate a certain threshold of defects without undergoing a fundamental structural change under elastic strain. However, the resistance to phase transformation is significantly compromised in the plastic regime for systems containing 1.0% hydrogen combined with varying defect concentrations (ZrH1.0%-V and ZrH1.0%-SIA). These systems demonstrate a markedly lower resistance to the HCP-to-disordered structure transformation compared to their defect-free or single-defect

counterparts. This synergistic weakening effect underscores that the combination of hydrogen with point defects creates a potent pathway for microstructural degradation, significantly reducing the phase stability of zirconium under mechanical load.

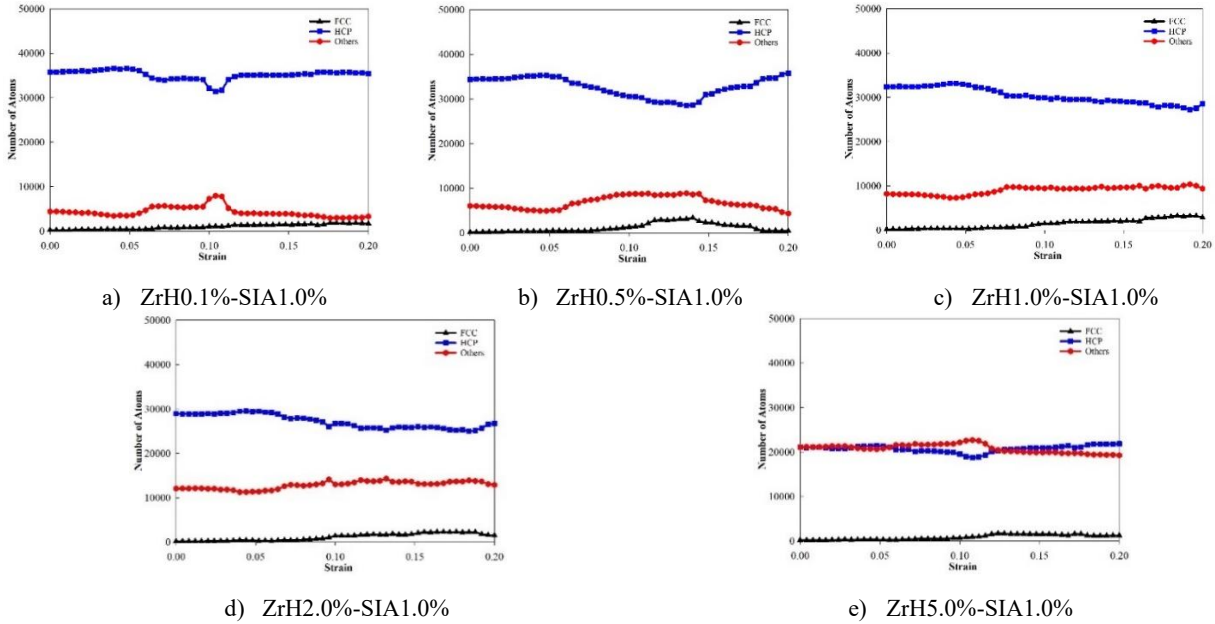
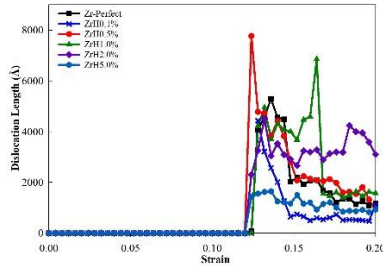


Figure 25 Effect of H concentration on the phase transition of ZrH-SIA1.0% system during stretching process at various strains

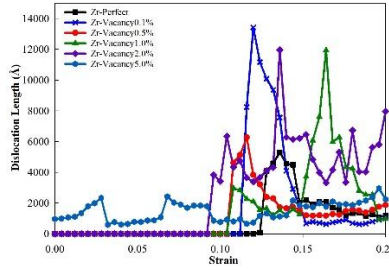
3.7. Effect of Hydrogen Concentration, Defect Types, and their densities on Dislocation Behavior

Figure 26 plots the dislocation length as a function of tensile strain for both ZrH, defective Zr systems, and defective Zr-H systems with defect densities ranging from 0.1% to 5.0%. In all Zr-H-defect systems, dislocations nucleate at a strain corresponding to their respective yield points. With increasing vacancy concentration, however, dislocation loops emerge at progressively lower strain levels, which align with the corresponding reduction in yield strain. Notably, in systems with a high defect density of 5.0%, dislocation loops are present even in the initial, unstrained state. A similar trend is observed in structures containing self-interstitial atom (SIA) defects, with the key distinction that the formation of pre-existing dislocation loops begins at a lower concentration threshold of 1.0%. The data reveal a clear distinction in dislocation behavior based on defect type and concentration. In perfect Zr crystals and low-defect systems like Zr-Vacancy1.0%, dislocation loops form predominantly within the plastic region. In contrast, systems with higher defect densities—including Zr-SIA and Zr-H1.0% at concentrations of 1.0% and above, as well as Zr-V5.0%, Zr-H1.0%-V5.0%, and Zr-SIA1.0% with variable H—already contain dislocation loops

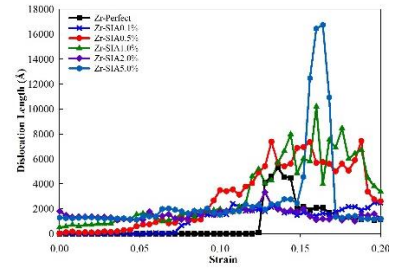
in their initial structure, and these pre-existing loops elongate significantly at higher strains. The density of dislocation loops increases markedly in the plastic region across all systems, coinciding with the partial transformation of the HCP structure into the "Others" phase. Among all tested configurations, the longest dislocation loops form in the presence of 5.0% SIAs. Furthermore, in Zr-H-V1.0% systems, an increase in hydrogen concentration generally leads to longer dislocation loops, with the exception of the system containing 1.0% H. Consistent with previous studies [48], the initiation of dislocation formation occurs earlier and at lower strain magnitudes in hydrided and defective structures compared to perfect zirconium. This accelerated dislocation activity, particularly the extensive loop formation in Zr structures with 5.0% SIAs (Figure 26(c)), indicates that interstitial defects have a more detrimental impact on structural integrity than either vacancy defects or hydrogen alone. A critical observation is the marked increase in dislocation length at the strain level where the stress-strain curves exhibit a rapid decline. This correlation suggests that the nucleation of a significant number of dislocations signifies the onset of plastic deformation, a transition that occurs simultaneously with a measurable decrease in the HCP phase fraction.



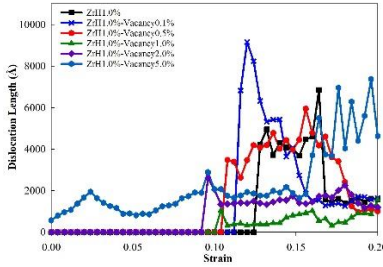
a) ZrH



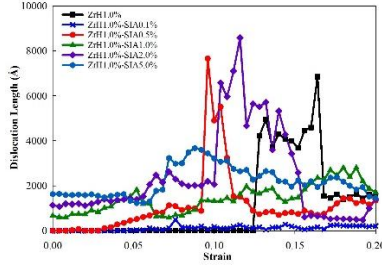
b) Zr-V



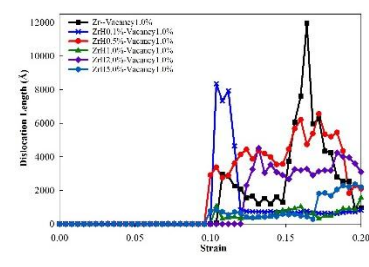
c) Zr-SIA



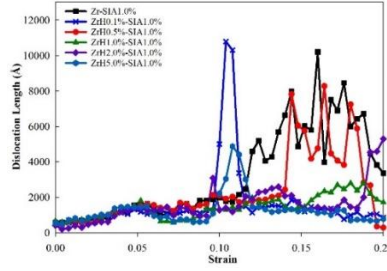
d) ZrH1.0%-V



e) ZrH1.0%-SIA



f) ZrH-V1.0%



g) ZrH-SIA1.0%

Figure 26 Effect of hydrogen and point defects on dislocation lengths of zirconium-based systems as a function of tensile strain

Conclusion

This study employs MD simulations to investigate the mechanical behavior and microstructural evolution of zirconium under uniaxial tensile loading, with a systematic focus on three key factors: hydrogen content, point defects (vacancies and self-interstitial atoms), and variations in temperature and pressure. The work begins by evaluating the stress–strain response and elastic properties of defect-free zirconium, and then examines the effects of gradually increasing hydrogen concentrations (0.1%, 0.5%, 1.0%, 2.0%, and 5.0%) as well as vacancy and SIA defect densities in the same 0.1%–5.0% range—both individually and in combination. Detailed structural analyses using CNA and DXA were performed to identify phase transitions, the onset of plasticity, and the nucleation and growth of dislocation loops. The central objective of the study is to determine whether hydrogen or structural point defects play the dominant role in degrading zirconium’s mechanical integrity, and to clarify how these factors influence phase stability and dislocation behavior under applied stress. The key conclusions can be presented as follows:

- Hydrogen additions across the full range of 0.1%–5.0% cause only minor changes in Young’s modulus, tensile strength, and overall stress–strain behavior of zirconium.
- Vacancy defects (0.1%–5.0%) significantly reduce mechanical performance, decreasing stiffness and shifting the onset of plasticity to lower strains.
- SIAs at concentrations of 0.1%–2.0% impose the strongest weakening effect, drastically lowering tensile strength and strain; at 5.0% SIA, the structure becomes highly disordered.
- High SIA densities (especially at 5.0%) generate the longest and most numerous dislocation loops, indicating severe structural disruption.
- Combining 1.0% hydrogen with vacancies or SIAs does not mitigate or amplify the defect-induced degradation; behavior remains primarily defect-controlled.

- Increasing temperature destabilizes the HCP phase, reduces elastic modulus, and shifts the yield point to smaller strains.
- Hydrostatic pressure increases stiffness but, at 20–30 GPa, destabilizes the HCP phase and accelerates the formation of disordered structures.
- Vacancies and SIAs both promote earlier HCP → “Others” phase transitions, with SIAs showing the strongest influence across the 0.1%–5.0% defect range.
- Defective systems—especially those containing SIAs $\geq 1.0\%$ —exhibit early dislocation nucleation and longer loop propagation, corresponding to rapid post-yield softening.
- Overall, the mechanical deterioration of zirconium is governed primarily by point-defect populations (0.1%–5.0%) rather than hydrogen concentration, even at the highest hydrogen levels tested.

Declarations

Ethical Approval

This study does not involve any research on human participants, human data, or human tissue, nor does it involve any research on animals. Therefore, ethical approval was not required for this work.

Consent to Participate

This research did not involve human subjects; hence, consent to participate is not applicable.

Consent to Publish

Not applicable.

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Competing Interests

The authors declare that they have no competing financial or non-financial interests in relation to the work described in this paper.

Data Availability

The data generated and/or analyzed during the current study are not publicly available due to the large volume of simulation data and computational restrictions. However, the data supporting the findings of this study are available from the corresponding author upon reasonable request.

Author Contributions

A. A. conducted all the numerical calculations, analyzed the results, and wrote the main manuscript text. S. R. contributed to analyzing the results and writing the main manuscript text. Gh. A. supervised and oversaw the entire project, and also contributed to analyzing the results and writing the main manuscript text. All authors reviewed and approved the final manuscript.

Declaration of Generative AI and AI-assisted Technologies in the Writing Process

During the preparation of this work, the author(s) used AI tools in order to improve the linguistic clarity, grammar, and stylistic fluency of the English text. After using this tools, the author(s) reviewed and edited the content as needed and take(s) full responsibility for the content of the publication.

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