



Full Length Article

Al-driven magnesium alloy functionality *via* manifold structuring and disorder

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Abstract

Magnesium alloys have had wide, historic industrial and societal impact, Mg-Al-Zn (Magnesium-Aluminum-Zinc) ones in particular for their lightweight structural applications due to a high strength:weight ratio, good castability and machinability. Yet, there is limited comprehensive atomistic-level insights resolving the effects of alloying and porosity on structural and mechanical evolution, especially under load. Herein, we investigated the mechanical behavior of Mg-Al-Zn alloys under uniaxial tensile loading using computational molecular dynamics simulations. A range of alloy compositions (0–18% total Al and Zn) and porosity levels (0–3%) were modeled to assess their influence on strength, phase stability, and mechanisms of structural deformation. Results show that increasing Al and Zn content accelerates the transformation from the hexagonal close-packed (HCP) crystalline phase to more ductile non-HCP phases (eg. FCC), leading to reduced tensile strength and fracture strain at higher alloying levels. In particular, pronounced declines in HCP content immediately preceded fracture, followed by post-fracture stabilization, with intermediary amorphisation observed. Moderate alloying improves mechanical performance, yet excessive additions (>4%) introduce structural instability. Porosity further compromises strength by acting as a stress concentrator, promoting early dislocation activity that correlates with localized phase transformation through atomic diffusion. Metallic/alloy grain-refinement and dislocation analyses revealed that porous alloys undergo more heterogeneous deformation, with earlier dislocation onset and reduced elastic modulus with respect to non-porous systems. In contrast, non-porous alloys exhibit more uniform grain evolution and delayed failure. Overall, the result trends highlight the critical interplay between alloying content and porosity in governing phase transformation, deformation behavior, and mechanical performance. This work provides insight and inroads into the rational design and optimization of alloys with tailored porosity and alloying content for specific applications requiring enhanced mechanical performance, with forward vision to the characterization by advanced operando techniques (e.g., neutron scattering, positron annihilation).

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Keywords: Mg-Al-Zn alloy; Mechanical properties; Dislocations; Phase transition; Grains; Molecular dynamics; Neutron scattering; Mg alloy.

1. Introduction

As-cast magnesium (Mg) metal offers potential lightweight applications due to its low density, yet is limited by its poor strength [1]. The mechanical properties of magnesium can be improved by physical and processing methods, such as microstructural refinement and thermal treatment [2]. This

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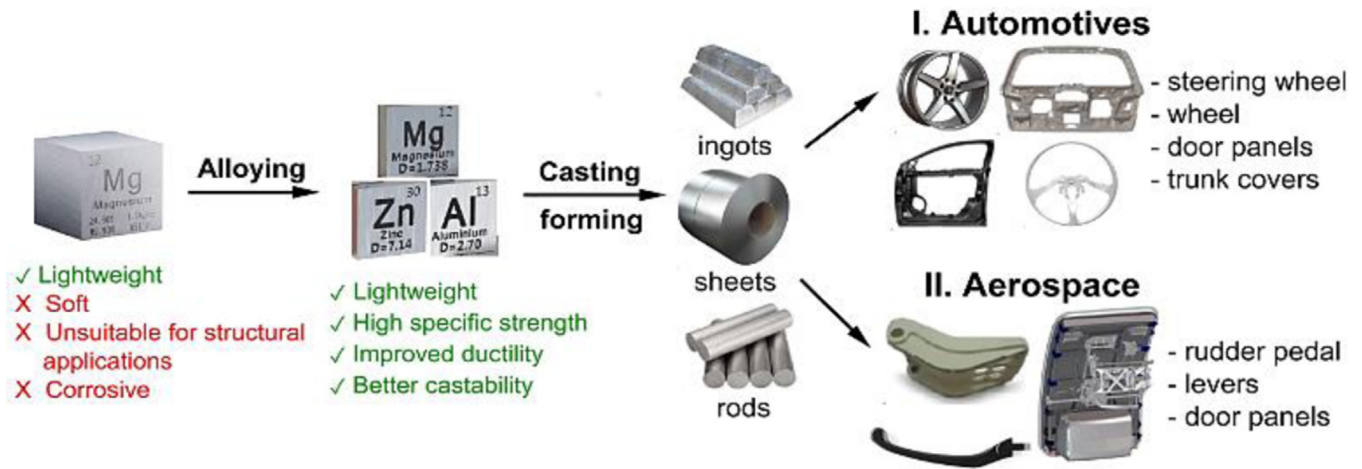


Fig. 1. Alloying with Al and Zn enhances mechanical properties of magnesium metal. Mg-alloys can be cast into ingots, sheets and rods, which are typically used in aerospace and automotive industries.

can also be achieved through chemical or metallurgical approaches, such as alloying [3–5]. The desirable properties of Mg-alloys make them versatile for a variety of applications, while their light weight and high specific strength make them a key alloy in the automotive industry; the latter comprising ~70% of global Mg-alloy demand [6]. For similar reasons, Mg-alloys are also often utilized for aerospace applications to reduce the weight of components in air/space-crafts [7] (Fig. 1). Further, the biocompatibility and biodegradability of Mg-alloys, along with their density and elastic moduli similar to that of bone, have contributed to their ever-expanding applications, including as biomedical implants [8].

Apart from indirectly facilitating the reduction of CO₂ emissions in the transportation industry through weight reduction as a cost-effective strategy for decreasing fuel consumption, Mg-alloys have high inherent sustainability. Magnesium metal is highly recyclable: very low energy is required for recycling, at only 5% of the primary production [9]. Further, apart from the small fraction employed in biomedical applications, magnesium can be recycled indefinitely without property degradation [10], translating to cost & resource savings and raising sustainability. Yet, magnesium metal's structural application is limited due to poor ductility [11], primarily due to its hexagonal close-packed (HCP) crystal structure which offers limited slip systems and restricts plastic deformation [12,13]. To improve mechanical properties, Al and Zn are among the most widely studied magnesium alloying elements due to high abundance, recyclability and strong solid-solution strengthening effect [14–17]. The Mg-Al-Zn system is known to form multiple intermetallic phases, such as the α -Mg phase, MgZn₂, β -Mg₁₇Al₁₂ and their eutectic mixtures. The β phase (Mg₁₇Al₁₂) is the second most prevalent phase in Mg-Al-Zn alloys [18], with indication that it may block dislocation motions at grain boundaries, thereby potentially enhancing grain boundary strength and influencing corrosion resistance [18,19]. Consequently, the presence of the β -phase plays a dominant role in determining the overall

performance of Mg-alloys. Microalloying can further refine α -Mg grains and enhance mechanical performance [20], while Al improves tensile strength & hardness, and the addition of Zn promotes formation of MgZn₂ phases that also contribute to hardening [21]. Extensive efforts have been made to rationalizing the effects of Al and Zn on the strengthening and deformation behavior of Mg-alloys [22–25]. Yet, there is insufficient information to understand these behaviors with respect to varying composition, and hence further study is suggested to clarify the effect of multi-component Mg alloys [26].

While alloying offers significant potential for enhancing mechanical properties, microstructural features such as porosity also play a critical role in performance. Typically, materials exhibit their highest strength when porosity is close to zero [27]. Whilst high pressure die-casting (HPDC) is the leading process in fabricating Mg-alloy components, it inevitably introduces pores as the predominant defect due to gas-segregation and solidification-shrinkage [28]. Porosity is known to be one of the most detrimental factors controlling mechanical behavior in cast light alloys [29] with evidence showing that an Mg alloy with lower volume porosity leads to higher ultimate strength and elongation [30], and that a higher initial porosity increases the rate of formation of subsequent pores — leading to more rapid material deterioration and failure [31]. Studies on high-porosity Mg-scaffolds have shown that increasing pore size reduced yield strength while increasing elasticity [32]. Pore distribution also plays a critical role in mechanical behavior, as previous studies have concluded that the areal distribution of pores was more influential to mechanical properties than the total volume porosity. Specifically, systems with a higher overall porosity may withstand greater stresses compared to those with lower porosity, yet with higher pore concentration in fracture-prone regions [33,34]. These aspects highlight the importance of understanding and characterizing pore morphology, and its effect on mechanical properties.

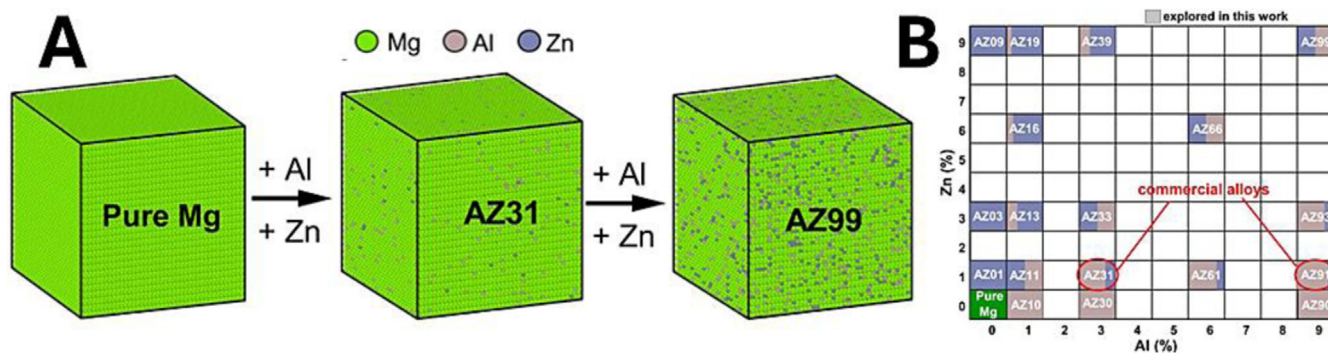


Fig. 2. [A] A “select and substitute” approach is employed, where pure Mg is replaced with Al and Zn atoms to achieve the required alloy composition. The nomenclature of alloys is given by AZXY where X = at%, Al and Y = at% Zn. [B] Compositions studied in this work, represented by filled, labelled boxes.

Resolving the atomistic basis of alloying and microstructure on fracture toughness and stress-strain behavior of Mg-alloys has yet to be fully explored, particularly with computational modeling. Although elemental composition is known to be crucial to alloy properties, full empirical characterization of all combinations of structure, porosity and phase composition in Mg-Al-Zn alloying would be resource and cost-intensive. Modern computational techniques allow these to be explored *in silico*, through simulation and subsequent comparative analyses & interpretation. The use of molecular dynamics (MD) approaches and advanced methods provide insight into phenomena such as phase transitions and atomic-level dynamics that are difficult, or (near-)impossible, to be obtained through traditional empirical techniques [35]. To date, there has been limited work presenting comprehensive atomistic-level insight into the combined effects of alloying, nano- through mesoscale (dis-)order and porosity on the mechanical properties of Mg-alloys. This work aims to resolve the fundamental contributions of structure, alloying and porosity to the manifold fracture toughness observed in Mg-Al-Zn ternary alloys, *via* MD simulation with subsequent in-depth analyses and nano-through mesoscopic interpretation.

Following the composition ranges commonly used in industrial Mg-alloy fabrication [36], this work considered Mg-Al-Zn compositions with Al and Zn concentrations ranging from 0 to 9 atomic percentage of each element (at.%). By integrating the effects of alloying and porosity at the atomic scale, this work offers novel insights into the mechanisms that govern strength and ductility in Mg-Al-Zn alloys, with broad applications in aerospace, (infra-)structural, biomedical, and lightweight structural systems and applications.

2. Methodology

2.1. Atomistic models of Mg-Al-Zn alloys

The AtomsK [37] software was used to construct an initial simulation box of “Pure Mg-metal” with a HCP structure and unit cell parameters $a = b = 3.17 \text{ \AA}$ and $c = 5.14 \text{ \AA}$, as obtained from Materials Project (mp-153)

[38] (Fig. S.1). Consistent with prior work demonstrating that 1,000,000 atoms provides representative strain-induced material behaviour in metallic systems [39], a simulation box size of approximately 1,000,000 atoms was adopted (Fig. S.2), corresponding to dimensions of approximately $30 \text{ nm} \times 30 \text{ nm} \times 30 \text{ nm} = 27,000 \text{ nm}^3$ (Fig. 2A). Alloy systems of interest are then created by replacing the relevant percentage of Mg atoms with Al and Zn using the “select and substitute” function in AtomsK (Fig. 2B). Compositions are reported in atomic percent (at.%) rather than weight percent (wt.%), providing a procedurally-pragmatic representation for MD simulations, or simple “atom counting/ratioing.” This approach aligns with the study’s focus on atomic-scale mechanisms, where the number and nature of constituent atoms dictate the underlying interatomic interactions. In this work, we refer to a “Zn limit,” typically up to $\sim 1\text{--}2\%$ Zn—a concentration near the solubility threshold of Zn in Mg at room temperature [40]. This limit aligns with typical experimental and industrial Mg-alloy compositions [41–46].

2.2. Incorporation of porosity

To explore the effect of porosity on mechanical properties, all Mg-Al-Zn alloys, including Pure Mg (AZ00), were modeled with porosity (p) = 0, 1, 2 and 3% , with $p \sim 1\text{--}3\%$ corresponding to the typical upper-levels seen in real-world fabricated alloys; the higher (p) = 2–3% models allowing for exploration of the effect at extremes of industrial porosity. The principal porosity descriptors explored are pore quantity and pore size. For the $p = 2\%$ and 3% porosity systems, two models were created for each as follows: one with fewer, larger pores and the other with more, smaller pores, with both corresponding to an overall constant porosity-volume, or “free volume” (V_f). This allowed for exploration of the isolated effects of size relative to quantity at constant V_f . Parameters of models explored in this work are listed in Table 1, with visual representation in Fig. 3C. Pores were created by producing 3D models of “holes in a cube” to represent pores in a solid alloy system using the SALOME (version 9.8.0) software [47] (Fig. S.3). The models were then mapped onto the

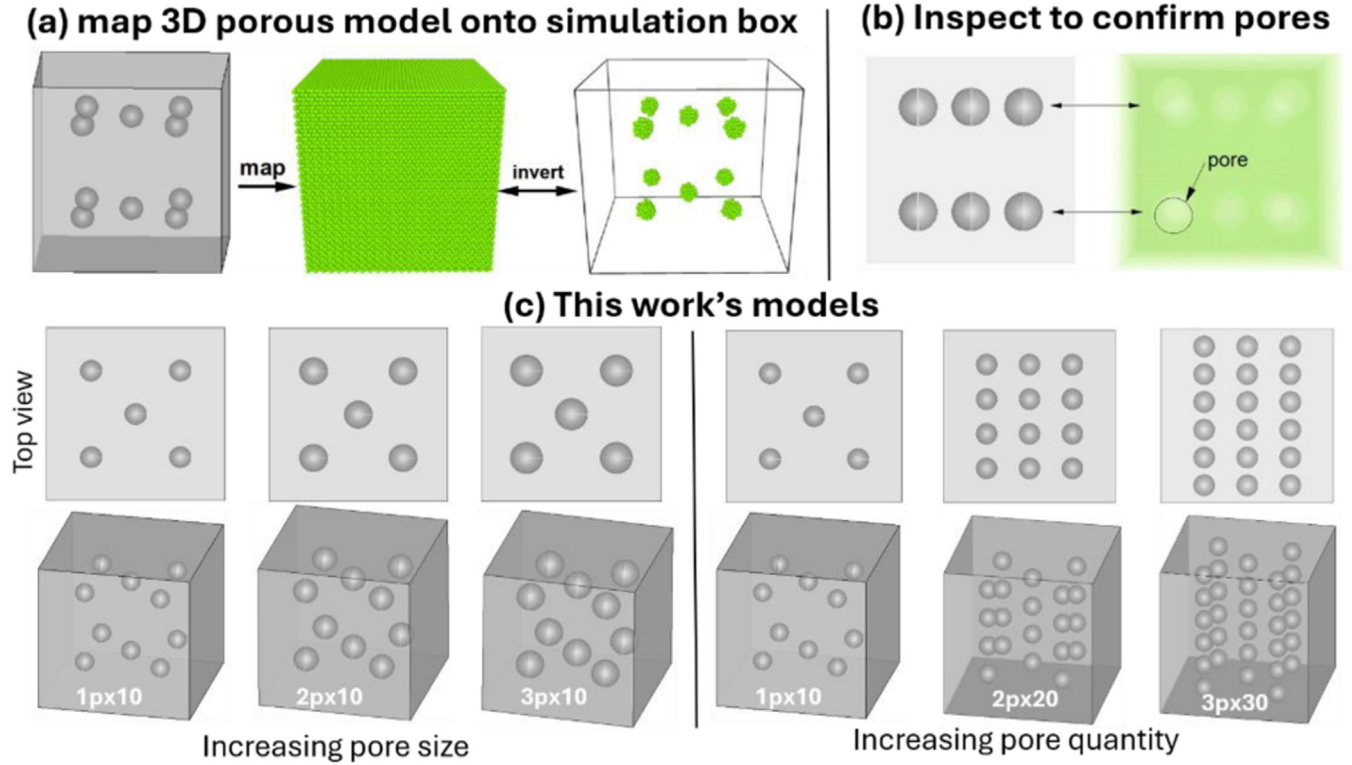


Fig. 3. A) 3D models of “pores in a box” is mapped onto a simulation box to obtain porous alloy models. B) The presence and geometric distribution of pores is confirmed *via* visual inspection. C) The porous models investigated in this work, ranging in both size and quantity for porosity (p) = 1–3%.

Table 1
Porosity models explored in this work and their corresponding parameters.

Model name	Porosity (%)	No. of pores	Pore cluster size (no. of atoms/pore)
1px10	1	10	1000
2px10	2	10	2000
2px20	2	20	1000
3px10	3	10	3000
3px30	3	30	1000

alloy simulation boxes to create pores by removing clusters of key atoms (eg. comprising the pore areas) from the alloy (Fig. 3A). Pores are confirmed to have been successfully mapped (Fig. 3B), evidenced through tracking of atomic composition for all models to ensure consistency, subsequent to pore removal, with all models remaining within >99.98% of the intended composition of each element type.

2.3. Interatomic potential model

The Modified Embedded Atom Method (MEAM) potential was used to model interaction between Mg, Al and Zn atoms. The parameters in this work were based off that reported by Doyl E Dickel et al. [48], developed specifically for Mg-Al-Zn alloys. Whilst EAM is often used for simulating alloys, this work implements MEAM due to its incorporation of angular contributions which is important in anisotropic systems, such as in this work where models are based on Mg's HCP

crystal structure. The MEAM potential is a semi-empirical many-body potential based on DFT methods, and is typically utilized for modeling metallic, covalent and mixed systems. It takes on the general form (1):

$$E_{\text{MEAM}} = \sum_i \left[\underbrace{F_{\tau}(\bar{\rho}_i)}_{\text{embedding}} + \frac{1}{2} \sum_{j \neq i} \underbrace{\phi_{\tau\tau}(R_{ij})}_{\text{pair interaction}} \cdot \underbrace{S_{ij}}_{\text{screening}} \right] \quad (1)$$

The embedding function (2) represents the energy cost to insert atom i of element type τ at a site with background energy density ρ_i :

$$F_{\tau}(\bar{\rho}_i) = A_{\tau} \cdot E_{\tau}^0 \cdot \frac{\bar{\rho}_i}{\rho_{\tau}^0} \cdot \ln \left(\frac{\bar{\rho}_i}{\rho_{\tau}^0} \right) \quad (2)$$

where A_{τ} is an element dependent parameter, E_{τ}^0 is the cohesive energy of a reference structure, ρ_i is the total background electron density at site of atom i , and ρ_{τ}^0 is the equilibrium background electron density of the reference structure. Term ρ_i is the combination of partial electron densities of a spherically symmetrical term $\rho_i^{(0)}$ and three angular terms $\rho_i^{(1-3)}$. The pair interaction term (3) accounts for the energy per atom given as a function of the nearest neighbor (NN) distance.

$$E_{\tau\nu}^u(R_{ij}) = -E_{\tau\nu}^0 \cdot \left[1 + a^*(R_{ij}) + \delta_{\text{lv}} \cdot \frac{R_{\tau\nu}^0}{R_{ij}} \cdot a^*(R_{ij})^3 \right] \cdot e^{-a^*(R_{ij})} \quad (3)$$

where $a^*(R_{ij}) = \alpha_{\tau\nu}^0 \cdot \left[\frac{R_{ij}}{R_{\tau\nu}^0} - 1 \right]$

The parameters $E_{\tau\nu}$, $R_{\tau\nu}$, $\alpha_{\tau\nu}^0$ and $\delta_{\tau\nu}$ are obtained from reference structures, where in this work's case, $\tau\nu = \text{Mg-Mg}$, Al-Al , Zn-Zn and their combinations: Mg-Al , Mg-Zn and Al-Zn . The pair interaction is calculated by consideration of only the first nearest neighbor (1NN) interaction, else by considering partial contributions from 'next nearest' atoms; for example 2nd and 3rd neighbors (2NN or 3NN, respectively). This work uses a potential that considers 1NN and 2NN interactions. The screening function S_{ij} is a product of all screening factors S_{ijk} , which represents the screening effect of a third atom k on the interaction between atoms i and j . This ensures only physically meaningful atomic interactions are included by reducing interactions that are "screened" (shielded, eg. electronically - by the atom's electrons) by nearby atoms. For the total screening function S_{ij} , values of $S_{ij} = 1$ means atoms i and j are within the cut-off distance whilst $S_{ij} = 0$ means atoms i and j are completely screened or outside the cut-off.

2.4. Computational simulation

The open-source software LAMMPS [49] (version 3Mar20) was used to simulate tensile loading on Mg-Al-Zn alloys. The alloys were first equilibrated under the NPT ensemble with a target temperature and pressure of 300 K and 0.0 bar, respectively. The time step was set to 2 fs and the equilibration process lasted for 25,000 steps (50 ps). Satisfactory equilibration was defined when the temperature stabilized to 300 K. The alloy was then subjected to tensile loading in the x -direction. The initial simulation box length in the x -direction was defined as L_0 , and the length after the tensile loading was defined as L_x . The strain was then calculated as $(L_x - L_0)/L_0$. The strain rate was set to 0.01 ps^{-1} , representing a relatively high strain rate to capture deformation mechanisms in the relevant simulation time covered by MD techniques. The loading process was conducted over 15 ps ($7500 \times 2\text{fs}$ steps). At a strain rate of 0.01 ps^{-1} this produced a total applied strain of $\varepsilon = 0.15$ (15%); sufficient to capture the alloy's mechanical response through to failure.

2.5. Mechanical properties

The mechanical properties tracked in this work are Young's modulus of elasticity (E), representing material stiffness [50] and ultimate tensile strength (UTS), representing the maximum stress the material can bear (Fig. S.4a). Values of E were estimated from the stress-strain response up to 2% strain, taken as an assumed elastic region where the stress-strain curves are linear. The mechanical property values were derived as percentage changes with each porosity level ($p = 1\%$, 2% , 3%) relative to the non-porous model ($p = 0\%$) to assess the influence of porosity on alloy stiffness and strength.

2.6. Radial distribution functions

The Radial Distribution Function (RDF) provides insight into the local atomistic structure and bonding. The probability

($g(r)$) of finding a particle at distance, r , from a reference particle is plotted. Typically, the first peak denotes the first nearest neighbor with respect to a reference particle and can be interpreted as the bond length (Fig. S.5). In this work, the evolution of bond length was tracked as a function of strain. All present atomic bond pairs were investigated in the Mg-Al-Zn alloy systems, including: Mg-Mg, Mg-Al, Mg-Zn, Al-Al, Al-Zn and Zn-Zn. The r -value of the first peak was obtained at 3% intervals of strain for each bond pair.

2.7. Crystal structure analyses

The Common Neighbor Analysis (CNA) [51] modifier was used to track the crystal structure evolution and quantify their corresponding %-proportions (fractions) present at 3% strain intervals during tensile loading (example, Fig. 4A). The alloy base is Mg which adopts a HCP crystal structure, and therefore a recommended cut-off distance is mid-way between the 1st and 2nd peaks [51]. The cut-off radius was determined to be approximately $3.9 \text{ \AA}$ (Fig. S.6). The available structural types are: face-centered cubic (FCC), HCP, body-centered cubic (BCC), icosahedral (ICO) and "other" (unknown co-ordination structure). As "other" denotes unknown structures, this may be considered as defected structural regions or of amorphous character, emerging to relieve strain through local structural-disordering and atomic hinging at key points, aluminum centres in particular, known to act as atomic, nanoscopic fulcrums influencing mesoscale structure and properties [52,53]. Since BCC and ICO are not present at any points during loading, the analyses conducted only considered FCC, HCP and "other" crystal structures and/or amorphous regions.

2.8. Dislocation analyses

Dislocation analyses were performed using the Dislocation eXtraction Algorithm (DXA) [54]. The algorithm takes an initial, perfect atomic crystal arrangement (in this case, HCP for the alloy base metal Mg) and identifies dislocations *via* a Burgers vector—representing the magnitude and direction associated with a lattice distortion. These dislocations were then converted from an atomistic representation to a line representation (Fig. 4B). The quantity of dislocations was recorded for all alloys and porosity models at 3% strain intervals.

2.9. Grain analyses

The evolution of grain density, size and geometry were tracked as a function of strain for pure Mg-metal, and the two commercial alloys AZ31 and AZ91, at $p = 0\%$ and 1% porosity. The grain segmentation modifier in OVITO was employed, which identifies the individual grains in a polycrystalline microstructure. The crystal structure environments are initially determined, followed by grain assignment by grouping atoms in crystal regions with similar local lattice orientations (Fig. 4C).

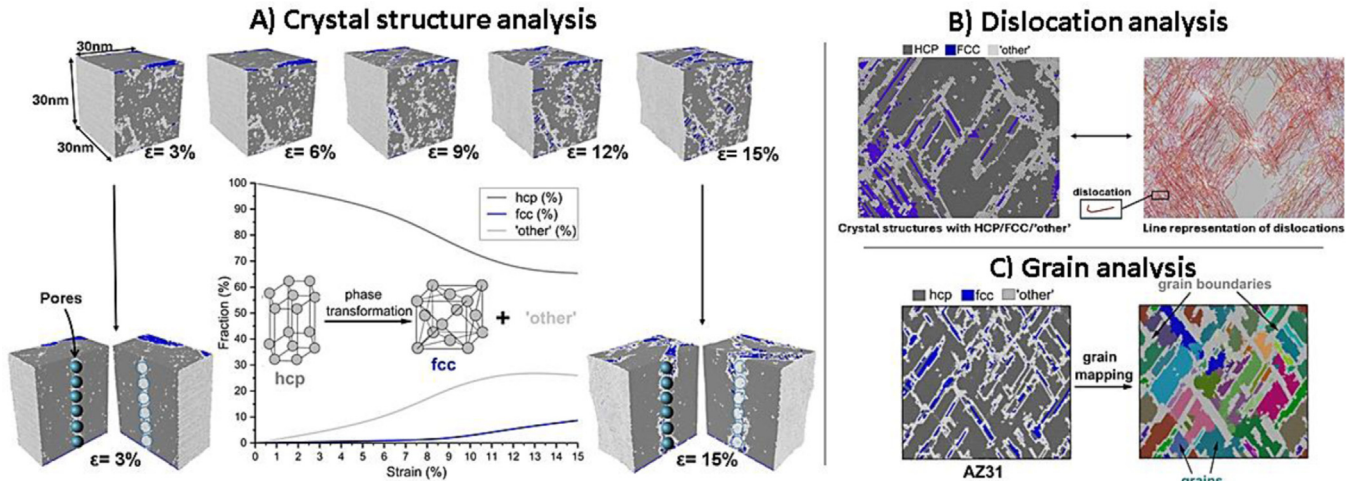


Fig. 4. A) Evolution of crystal structure (example: AZ31) is tracked during the loading process, with visual models of HCP/FCC/“other” showing structure distribution. B) Dislocations are identified *via* regions with a Burgers vector to characterize regions of lattice distortion, which are then visualized as crystal structure types or line representations. C) The grain segmentation modifier first performs a crystal structure identification and subsequently groups atoms of similar local lattice environments, into a defined grain.

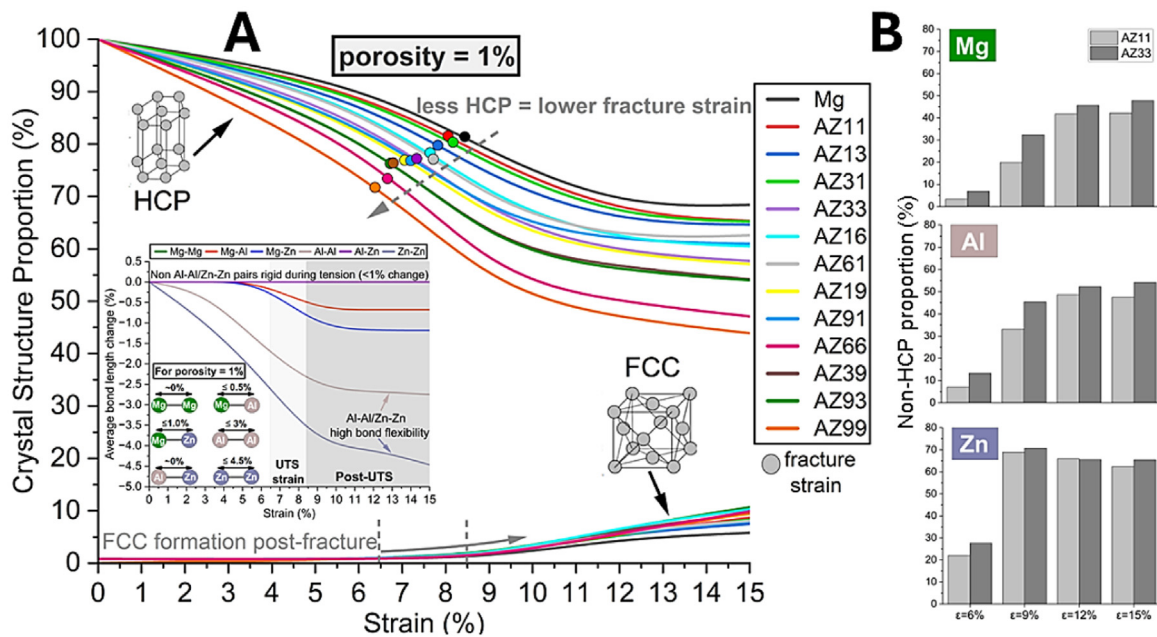


Fig. 5. A) The evolution of HCP:FCC ratioing (%) as a function of strain (%) were explored for all alloys at 1% porosity. This is supplemented with the average bond length changes of all bond pairs to support the observation that higher alloying is linked with increased bond variability from Al-Al and Zn-Zn atoms pairs. B) Proportion of non-HCP (FCC and “other”) was compared for a lower (AZ11) and higher (AZ33) alloyed system at different strains. In all cases, Al and Zn typically adopt higher proportions of non-HCP than Mg. Higher alloying is also generally associated with more %non-HCP.

3. Results and discussion

3.1. Influence of alloying on structure and mechanics

The evolution of HCP and FCC phases during uniaxial tensile loading was systematically tracked for all investigated alloys, with those at $p = 1\%$ porosity graphically presented (Fig. 5A). Fracture strains for each alloy are provided, with values ranging from approximately 6–9%, consistent with previously reported stress–strain behavior of Mg–Al–Zn alloys

[55–60]. A progressive decrease in the HCP phase proportion (i.e., phase fractions or ratioing) was observed with increasing strain, with the extent of this reduction intensifying as alloying content increased. Concurrently, the fracture strain of each alloy generally decreased with higher concentrations of Al and Zn, indicating a reduction in ductility. The same trends are observed across all porosities (Fig. S.7). These trends suggest a correlation between the mechanical toughness of Mg–Al–Zn alloys and the retention of the HCP phase. In particular, pronounced declines in HCP content immedi-

ately preceded fracture, followed by post-fracture stabilization, with intermediary amorphous phases observed. Although the “other” phase has not been characterized structurally or compositionally, its higher fraction in alloys with increased fracture strains may suggest that these phases improve deformation tolerance. Previous studies have shown that intermediate or equilibrium phases, as well as solute cluster formation, can contribute to strengthening and hardening mechanisms in Mg alloys [61]; a type of functional-disorder, mechanically beneficial in this case. However, in the present work the identity of the “other” phase remains non-fully resolved, hence characterization may uncover the presence of solute clusters and intermetallic phases which would improve understanding of the relationship between nano-through mesoscale structure and mechanical behavior. In contrast, the emergence of the FCC phase is only observed after failure onset, suggesting that FCC formation is not a precursor to failure, rather is a result of post-failure structural reconfiguration. The strain-induced HCP→FCC transition has also been observed in prior investigations of an Mg-Al-Zn alloy [62]. Herein, we evidence an evolved HCP→[amorphous]’→FCC mechanism, where []’ denotes a transitory phase, akin to a transition state in chemical transformations.

The transformation away from the HCP structure may act as a driving mechanism for mechanical failure. This behavior can be attributed to the limited number of active slip systems in HCP structures, which albeit actively assisting to constrain dislocation motion and reduces ductility, HCP-fractions simultaneously enhance strength; hence, strength falls with reduction of HCP-content (HCP-fraction). Such HCP-strengthening has previously been observed in metals such as Mg and HCP-Titanium (Ti-HCP) compared to Al and FCC-Copper (Cu-FCC) [63]. Trends uncovered herein indicate that transformation into more ductile crystal structures is instead associated with a lower failure-onset strain. This suggests that a higher retention of the strength-enhancing HCP phase delays the initiation of failure, resulting in higher failure strains. Such behavior implies that the observed increase in failure strain arises not from enhanced ductility, rather from the prolonged structural stability of HCP regions under applied load.

To elucidate the atomic-scale mechanisms behind these phase changes, radial distribution functions (RDFs) were evaluated for all relevant bond pairs (Fig. 5, inset). Analyses revealed that Al–Al and Zn–Zn pairs undergo the most pronounced bond length fluctuations approaching and near-to the fracture point, whereas Mg–Mg and Mg–Al pairs remained comparatively stable. Given that higher Al and Zn content corresponds to increased HCP→non-HCP phase transformation, it can be hypothesized that these alloying elements play an active role in destabilizing the HCP structure. Additionally, the pronounced bond length variations observed in Al–Al and Zn–Zn pairs during tensile loading suggest that these bonds may function as active load-bearing links within the alloy. This behavior aligns with the observed promotion of HCP to non-HCP phase transformation by Al and Zn atoms, implying that the alloying elements play a key role in restructuring during mechanical deformation. To further investigate this hy-

pothesis, the crystal structure preferences of Mg, Al, and Zn atoms were compared during tensile loading (Fig. 5B). The following two representative systems were analyzed: AZ11 (lower alloying content) and AZ33 (moderately higher alloying content). In both cases, Al and Zn atoms consistently exhibited a higher tendency to occupy non-HCP environments than Mg-atoms during deformation.

This confirms that Al and Zn are not only structurally disruptive but actively promote the transition away from HCP, thereby facilitating phase transformation and ultimately contributing to mechanical degradation. While Al and Zn additions are intended to enhance the mechanical performance of Mg-alloys, excessive alloying, typically beyond 4%, leads to mechanical degradation. Analysis of UTS across the alloy series reveals a non-linear trend: moderate alloying levels, particularly in AZ11, AZ13, and AZ31 compositions, result in improved strength relative to pure Mg-metal. However, increasing the alloying content beyond these proportions (e.g., AZ33 and higher) results in a progressive decline in UTS (Fig. 6A), due to the promotion of non-HCP structuring, and driven by alloying elements, Al and Zn in particular in the Mg-Al-Zn systems characterized. This effect has been experimentally observed with addition of up to 3% Al in Mg-Zn alloys improving strength and elongation, followed by deterioration of mechanical properties beyond 3% Al [64]. The optimal regions with alloying content corresponding to the highest fracture strains and UTS values are presented in a heat map (Fig. 6B), with these regions comprising <4–5% at alloying and <1% volume porosity. This suggests that while limited alloying can be beneficial, excessive Al and Zn content may trigger microstructural instability, such as increased phase transformation, initiating at local sites (involving a relatively small number of “player” atoms, progressively influencing adjacent “spectators”, and in large numbers, affecting mesoscale structuring), and ultimately compromising mechanical integrity. Additionally, there is a distinct compromise in strength when porosity is introduced at >0%, suggesting that even diminutive porosity levels reduce the mechanical performance of Mg-Al-Zn alloys.

3.2. Mg-Al and Mg-Zn binary alloys

As previous results have shown that higher levels of Al/Zn alloying (>~4 at.%) lead to reduced tensile strength, earlier fracture, and a progressive loss of the HCP crystal structure (and/or due to this HCP-loss), binary Mg–Al and Mg–Zn systems were investigated to isolate the individual effects of each alloying element. Simulations were performed at 1%, 3%, and 9%at. and incorporating $p = 1\%$ porosity to reflect typical pore-volumes observed in real-world systems. Stress–strain behavior was evaluated alongside crystal structure analyses and comparison of RDFs. The stress-strain curves for each binary system are presented in Fig. 7A, with accompanying values for UTS and Young’s modulus (E). In general, all mechanical properties (UTS, Young’s modulus (E), fracture strain, etc.), decline with increasing alloying content. However, this degradation is more pronounced in the Mg–Zn al-

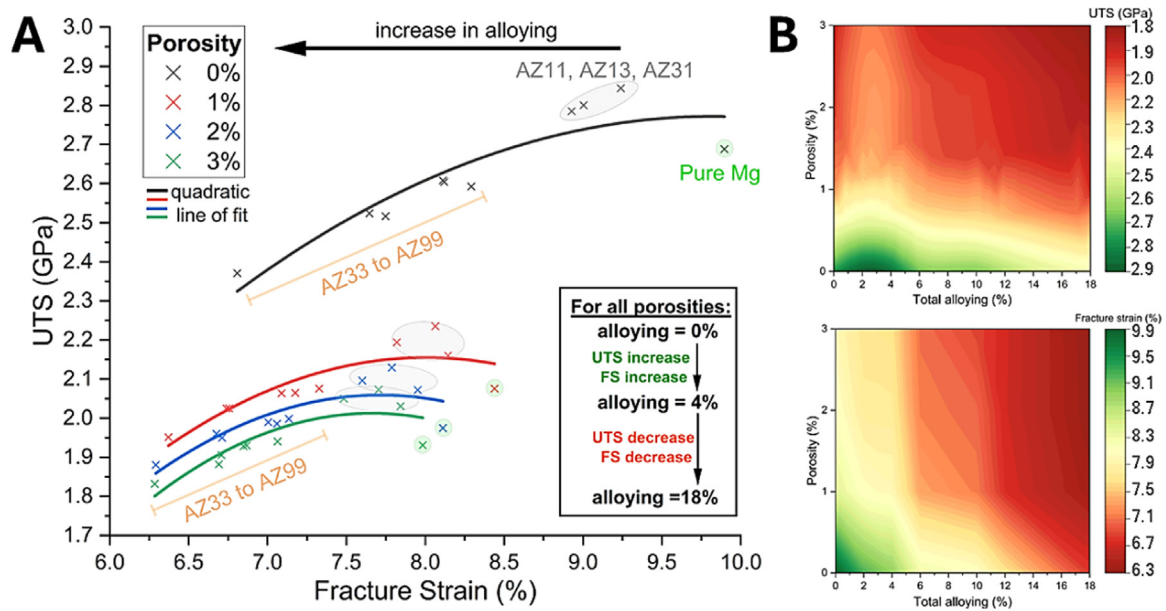


Fig. 6. A) UTS peaks at alloying levels <4 at.%, followed by a decline across all porosities. Distinct reductions in UTS are observed at each porosity volume. B) Expressed as heat maps to identify the optimal regions, towards guiding rational alloy mix-design.

loys than in Mg–Al. This supports the concept of a “Zn limit,” as tensile strength drops sharply above 1 at.% Zn — helping resolve the bases for the amount of Zn used in the most common Mg–Al–Zn alloys, including AZ31, AZ61, AZ80 and AZ91 [65]. Similar trends have been observed experimentally, where Mg–9 Zn shows reduced tensile strength and elongation compared to Mg–1.5 Zn [66]. The same increase in Al content however leads to a more moderate reduction. Notably, 3 at.% Al results in mechanical properties similar to those of 1 at.% Zn, whilst increasing Zn content from 1% to 3 at.% leads to a pronounced ~21% decrease in UTS. A similar trend is observed in Young’s modulus (E), where increasing Al content from 1% to 3% reduces E by approximately 1.0 GPa, whereas the same Zn increase results in a 2.4 GPa reduction. These findings further reinforce the idea that Zn-content in Mg and Mg–Al alloys, should be limited to ~1 at.% or less, consistent with typical industrial Mg–Zn alloy compositions, in order to maintain mechanical integrity.

The bonding behavior of the binary systems was analyzed as a function of strain (Fig. S.8). RDFs were considered up to 5 Å to resolve the structure of the first full coordination shell, which corresponds to nearest neighboring atoms, encompassing a range around double their interatomic bond lengths. As in the ternary systems, the dominant bond variations in the binary ones occur in the Al–Al and Zn–Zn pairs. For all binary alloys, the Mg–Mg and Mg–X (X = Al or Zn) bond lengths shift slightly toward shorter distances under increasing tensile strain, while the X–X bond lengths (Al–Al and Zn–Zn) tend to increase. This divergence in bond behavior suggests that Al–Al and Zn–Zn pairs play a key role in accommodating applied strain, acting as the primary load-bearing components within the alloy; again, as “atomic hinges and fulcrums,” as previously observed for Al in other material systems [52,53].

In contrast, the Mg-rich matrix remains relatively stable. This supports the observed trend of decreasing Young’s modulus (E) with increasing alloying content: as more alloying atoms are introduced, there is a greater number of bonds with higher flexibility, reducing overall stiffness.

Notably, as the concentration of Al or Zn increases, the flexibility of the X–X bonds (Al–Al, Zn–Zn) diminish, as indicated by reduced variation in the RDF profiles (narrower peaks). This reduced bond adaptability may explain why alloy strength declines at higher alloying levels despite the strain-bearing role of the alloying elements. Therein, the declining flexibility of interatomic bonding and rigidification of their local coordination-geometry limits stress redistribution, making the system more susceptible to failure. These results support the hypothesis that the mechanical performance of Mg alloys is closely linked to the ability of the alloyed phases to deform and redistribute stress; and the need to ‘avoid too much of a good thing’. This translates to an interplay between bond flexibility and stability, and the rigidity of atomic coordination geometry determining how effectively the alloy accommodates strain.

As previously established for the ternary systems, the mechanical properties of Mg alloys are strongly influenced by the proportion/fraction of the HCP crystal structure. This relationship was further investigated for the binary Mg–Al and Mg–Zn alloys (Fig. 7B) alongside their respective UTS values. A clear correlation is observed: increasing alloying content accelerates the transformation from HCP to non-HCP structures under strain. Not only is the rate of HCP decline steeper with higher alloying levels, but the onset of this structural breakdown also occurs at lower strains. Notably, Zn has a significantly greater destabilizing effect on the HCP structure than Al. For example, at 9 at.% alloying, the initial HCP

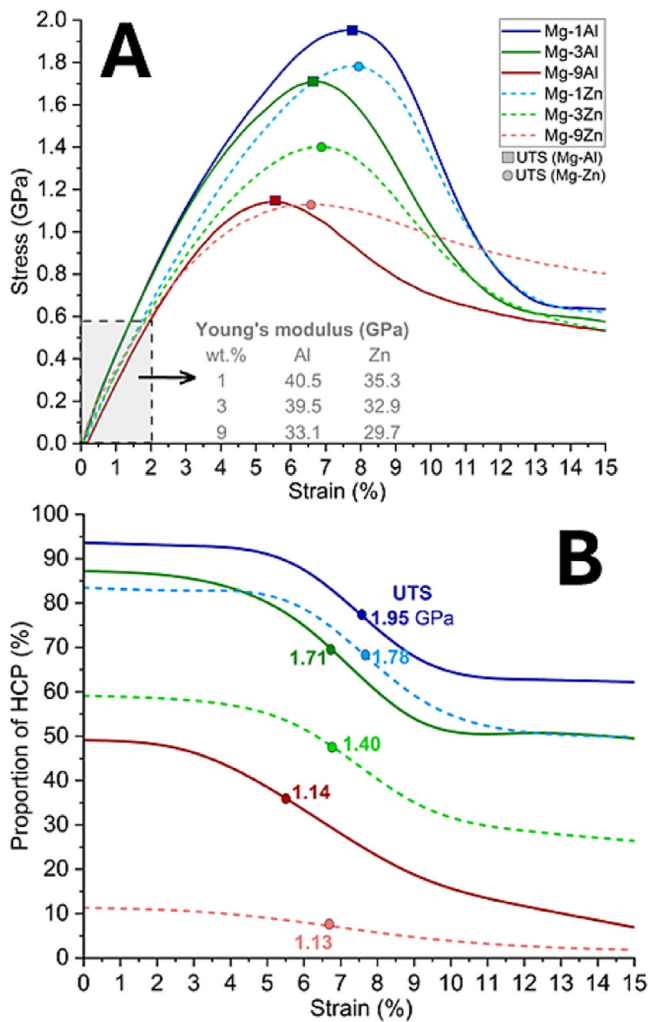


Fig. 7. A) Stress-strain plots for binary Mg-Al and Mg-Zn alloy systems, with accompanied values of Young's modulus (E) and UTS markers. Both UTS and E fall with rising %at. alloying, with this being more prominent in the Mg-Zn alloys. B) Proportion of HCP decreases as a function of strain across all binary alloys. Concurrently, lower levels of HCP equate to lower UTS and fracture strain values. For a given at. % alloying, the Mg-Zn alloys exhibit significantly lower HCP-retention than Mg-Al.

fraction is approximately 50% in Mg-9Al, while it drops sharply to just ~10% in Mg-9 Zn. This highlights Zn's magnified role in driving HCP-to-non-HCP transformation. Since higher HCP retention correlates to both higher UTS values and increased fracture strains, these atomistic findings reinforce the importance of limiting Zn content in Mg-alloys, typically below 1-2 at.%, to preserve structural integrity and mechanical performance.

The observed deterioration of mechanical properties with increasing Al and Zn can be attributed to the influence of alloying atoms on the stacking fault energy (SFE). Stacking faults act as precursors for the HCP $\rightarrow$ FCC (or other non-HCP) structural transitions, as observed in prior studies of an Mg-Al-Zn alloy [62]. Increasing both Zn and Al concentrations is known to reduce SFE in Mg-based alloys [67], thereby increasing the formation of stacking faults during de-

formation. However, this effect is more pronounced in Zn-containing systems. Prior calculations of binary Mg-X alloys show that Mg-Zn possesses a lower SFE than Mg-Al [66] hence lower barriers to fault-formation and translating to a higher likelihood for stacking fault formation than in Mg-Al alloy systems. This explains the sharper decline in the HCP fraction and earlier onset of fracture observed in Mg-Zn alloys. The enhanced faulting tendency in Mg-Zn systems may stem in-part from the greater atomic size mismatch between Mg (160 pm) and Zn (134 pm) relative to that of Mg and Al (143 pm); $\Delta = 26$ pm (-16.25%) and 17 pm (-10.63%), respectively. This mismatch introduces higher local strain energy and promotes local lattice distortions, therefore facilitating nucleation of non-HCP phases under stress. These findings suggest that optimal alloy design must balance alloying content to preserve bond adaptability and HCP structural integrity. Zn in particular accelerates HCP destabilization in Mg-alloys, reinforcing the "Zn limit" to avoid compromising strength. This provides a rationale for compositional limits and supports tailoring Mg-alloy design by linking underlying atomistic structuring and behavior with mechanical performance.

3.3. Grain refinement in Mg-alloys

Strain-induced grain refinement is a common phenomenon observed in metals [68–70], a process in which the grain size in a material decreases due to deformation. In this study, we investigate the evolution of grain structure in pure Mg, AZ31, and AZ91 alloys subjected to uniaxial tensile strain, considering both non-porous ($p = 0\%$ porosity) and porous ($p \geq 1\%$ porosity) models. Grain evolution is characterized using the following three key metrics: (i) the number of grains (grain density) as an indicator of dynamic recrystallization and grain fragmentation, (ii) grain size to assess degree of refinement, and (iii) the evolution of grain aspect ratios to capture morphological changes. By correlating these parameters with applied strain herein, we evaluated the influence of alloy composition and porosity on grain refinement mechanisms.

3.3.1. Grain density evolution in Mg-alloys

With applied tensile strain, the number of grains remains relatively stable until a critical strain is reached, beyond which a sharp rise in grain count is observed, indicating the onset of dynamic recrystallization (Fig. 8A). For both the $p = 0\%$ and 1% porous models, this critical strain corresponds closely to the onset of the failure point associated with the UTS observed in the stress-strain curves. This suggests that grain refinement here is strain-driven and occurs in the final stages of deformation, triggered by a buildup of internal stresses. Notably, beyond the critical strain, the non-porous alloys develop a significantly higher number of grains compared to their porous counterparts. Given that the dislocation density is higher in alloys of lower porosity (Fig. 10C), the association between dislocation density and grain multiplication indicates that the formation of new grains is strongly linked

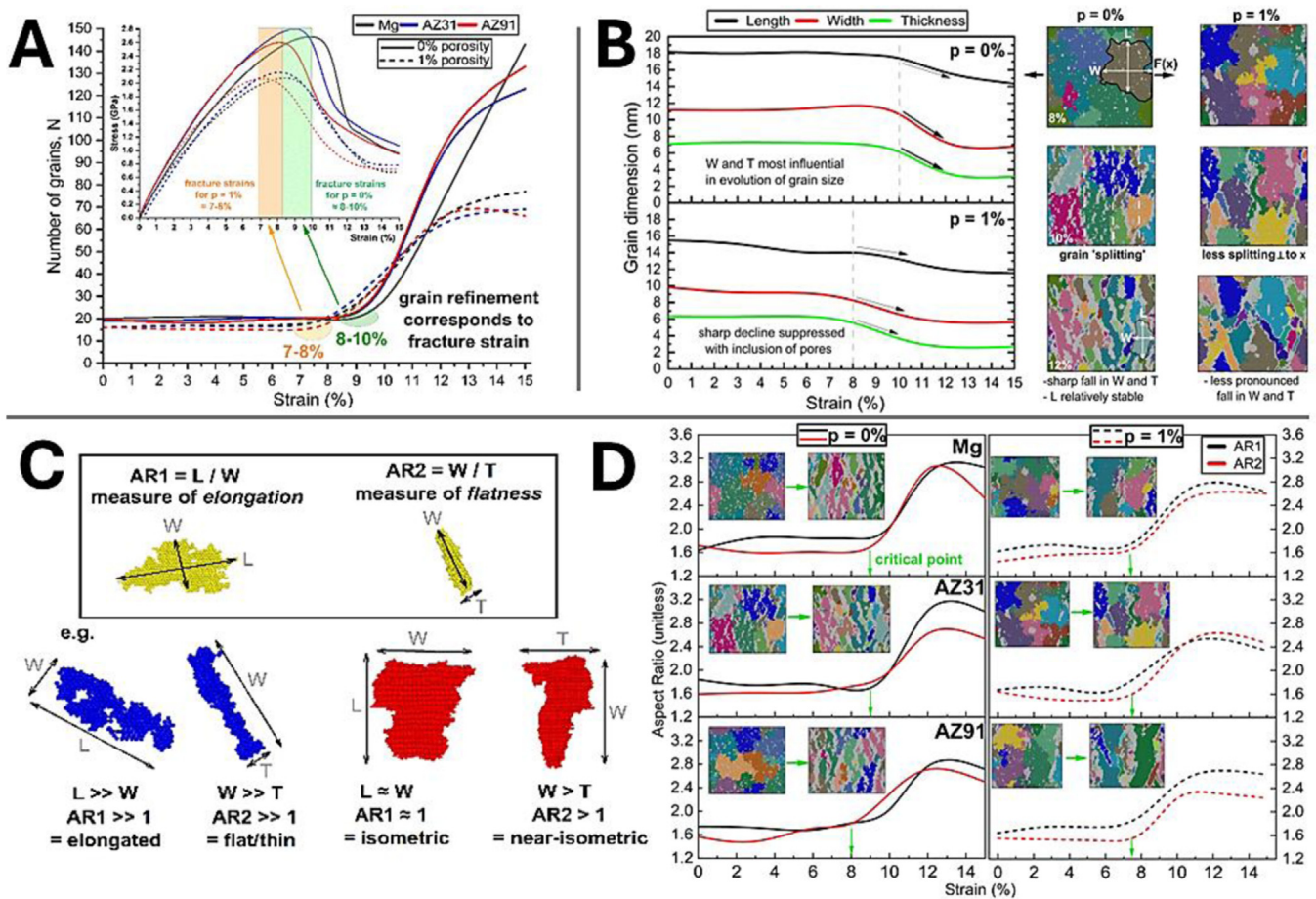


Fig. 8. A) Evolution of grain density was tracked as a function of strain. Strong association between the critical strain for rapid grain nucleation and the fracture strain extracted from stress-strain profiles was found. B) The change in three orthogonal dimensions of the AZ31 alloy was tracked as a function of strain for $p = 0\%$ and 1% porosity. Both the porous and non-porous model exhibit a steep decline beyond the critical strain, yet this is sharper in the $p = 0\%$ model. Microstructural snapshots reveal that grain splitting occurs for $p = 0\%$ in a homogenous manner. The nature of grain splitting for both models support rationale of the sharp fall in width and thickness observed for the non-porous system. C) Aspect ratios (AR1: elongation, AR2: flattening) used to quantify strain-induced grain morphology changes. D) AR1 and AR2 trends for Mg, AZ31, and AZ91 at 0% and 1% porosity. Alloys exhibit a critical strain beyond which grains become significantly elongated or flattened. Microstructures before and after this point are shown for each model.

to dislocation activity, potentially due to the role of dislocations in providing nucleation sites for dynamic recrystallization. In porous systems, the reduced ability to accumulate dislocations may therefore limit the extent of recrystallization, leading to strength implications associated with smaller quantities of grains in the alloy.

3.3.2. Grain size evolution

Grain refinement with increasing strain is inevitably linked to a reduction in the size of pre-existing grains. While initial observations may suggest elongation and flattening during deformation, relying on a single grain dimension is insufficient to fully characterize the refinement process. Instead, three orthogonal dimensions—length, width, and thickness—are tracked independently to describe the evolution of grain size (Fig. 8B). At low to moderate strain levels, all three dimensions remain relatively stable. However, a pronounced decrease occurs beyond the fracture strain, consistent with the strain for onset of grain fragmentation. In the AZ31 non-

porous model, the most significant reductions are observed in grain width and thickness, suggesting that refinement may occur primarily through splitting perpendicular to the loading axis. The absence of pores—and therefore of localized stress concentrations—facilitates a more uniform distribution of stress, enabling symmetrical grain subdivision. In contrast, the $p = 1\%$ porous model exhibits more gradual reductions in grain dimensions. In this case, stress concentrates around pore sites, disrupting the uniform deformation seen in the non-porous alloy. Consequently, grain fragmentation proceeds in a more anisotropic and heterogeneous manner, with fewer abrupt transitions in grain dimensions at the fracture point. These interpretations are supported by microstructural snapshots (Fig. 9B) where at 8%, 10%, and 12% strain, the non-porous $p = 0\%$ model exhibits clear evidence of grain subdivision aligned perpendicular to the loading axis—consistent with strain-driven grain splitting behavior. In the porous model, this perpendicular splitting is much less evident, and the grain structure appears more irregular and spa-

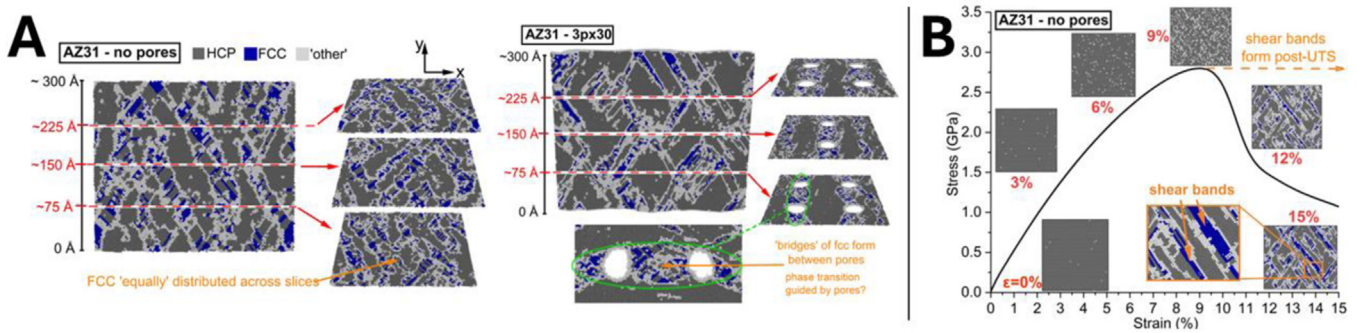


Fig. 9. A) Graphical 'slices' of the AZ31 non-porous (left) and 3px30 (right) porous models showing the distribution of FCC. Non-porous tends to form evenly distributed of FCC steaks in XY direction whilst 3% porous model forms localized FCC regions around and bridging pores in the (X)loading direction. B) Stress-strain curve for the non-porous AZ31 model with snapshots showing crystal structure distribution at 3% strain intervals. Shear bands typically form as the last stage of deformation before failure, as observed here post-UTS at 12% strain as FCC (blue) and "other" (light grey) streaks.

tially heterogeneous, reflecting the localized nature of deformation around pores.

3.3.3. Grain morphology evolution

Although reductions in grain length, width, and thickness provide evidence of manifold grain-structuring, they do not quantify morphological changes in grain shape. To complement these dimensional analyses, the evolution of grain morphology is examined with focus on aspect ratio transformations that reveal elongation and thinning mechanisms under increasing strain. Morphological evolution is characterized using two distinct measures as follows: Aspect Ratios 1 and 2 (AR1 and AR2, respectively), where AR1 quantifies grain elongation as the ratio of length to width, while AR2 captures grain thinning or flattening as the ratio of width to thickness (Fig. 8C).

Similar to the trend observed in grain density evolution, both AR1 and AR2 remain relatively stable at low to moderate strain levels. However, at the critical strain, again corresponding to the fracture strain seen in the stress-strain data, a sharp increase is observed in both measures (Fig. 8D). This indicates that in the late stages of deformation, when the alloy is under maximum stress, there is a distinct transition not only to a higher number of grains but also to more distorted grain shapes. Specifically, grains become significantly thinner and more elongated, forming morphologies that resemble bands or filaments. This behavior is consistent with previous experimental studies on Mg-alloys, where dynamic grain refinement has been associated with the transformation of coarse grains into more anisotropic structures such as bands [71] and plates [72]. Consistent with prior observations of porous systems exhibiting more stable grain dimensions (Fig. 8B), the increase in aspect ratios for porous systems is also generally less pronounced. This suggests that pores, known to act as stress concentrators, reduce the effective transmission of stress across and/or between grains. Consequently, they limit the extent of deformation and delay the morphological transitions typically associated with grain refinement. This interpretation is supported by the structural snapshots taken before and after the critical strain points, which show a relatively

homogeneous grain distribution in non-porous models compared to the more heterogeneous structure in porous models (Fig. 8B and D) thereby rationalizing the differences in stress distribution.

3.4. Role of porosity in structural evolution

To investigate the influence of porosity on phase transformation, cross-sectional slices from both non-porous ($p = 0\%$) and $p = 3\%$ porosity models were analyzed (Fig. 9A). This analysis focused on the manifestation of the FCC phase, due to its contribution toward mechanical properties when formed *via* strain-induced phase transition, in both the presence and absence of pores. In non-porous systems, the distribution of the FCC phase was found to be notably more uniform (Fig. 9A, left), despite having comparable amounts of FCC present. This uniform distribution further reinforces that, in the absence of pores, the applied tensile stress is more evenly distributed across the system, facilitating a homogeneous formation of the FCC phase. Although the load was applied in the x-direction, FCC phases appeared as "streaks" in the XY-plane, indicating the formation of shear bands. These are thin, localized regions where strain is concentrated to accommodate deformation and typically emerge after significant material deformation [72,73], as observed in our models post-UTS (Fig. 9B).

In contrast to the non-porous system, the FCC phase in the porous models localizes around the pores (Fig. 9A, right). Pores act as stress concentrators, leading to higher stress in the regions surrounding them with respect to the wider structural networks of the alloy during loading. This elevated stress seems to facilitate phase transitions from HCP to FCC, particularly in areas where atomic rearrangement is more readily achieved due to the localized stress, such as around the pores and in regions bridging them; amorphous, manifold structuring serving as intermediaries, providing lower free-energy (spontaneous) pathways to such changes to and along the potential energy hypersurfaces of these systems. Atomistically, the increased ductility of the FCC phase enhances atomic mobility, which is expected to be more pronounced near the

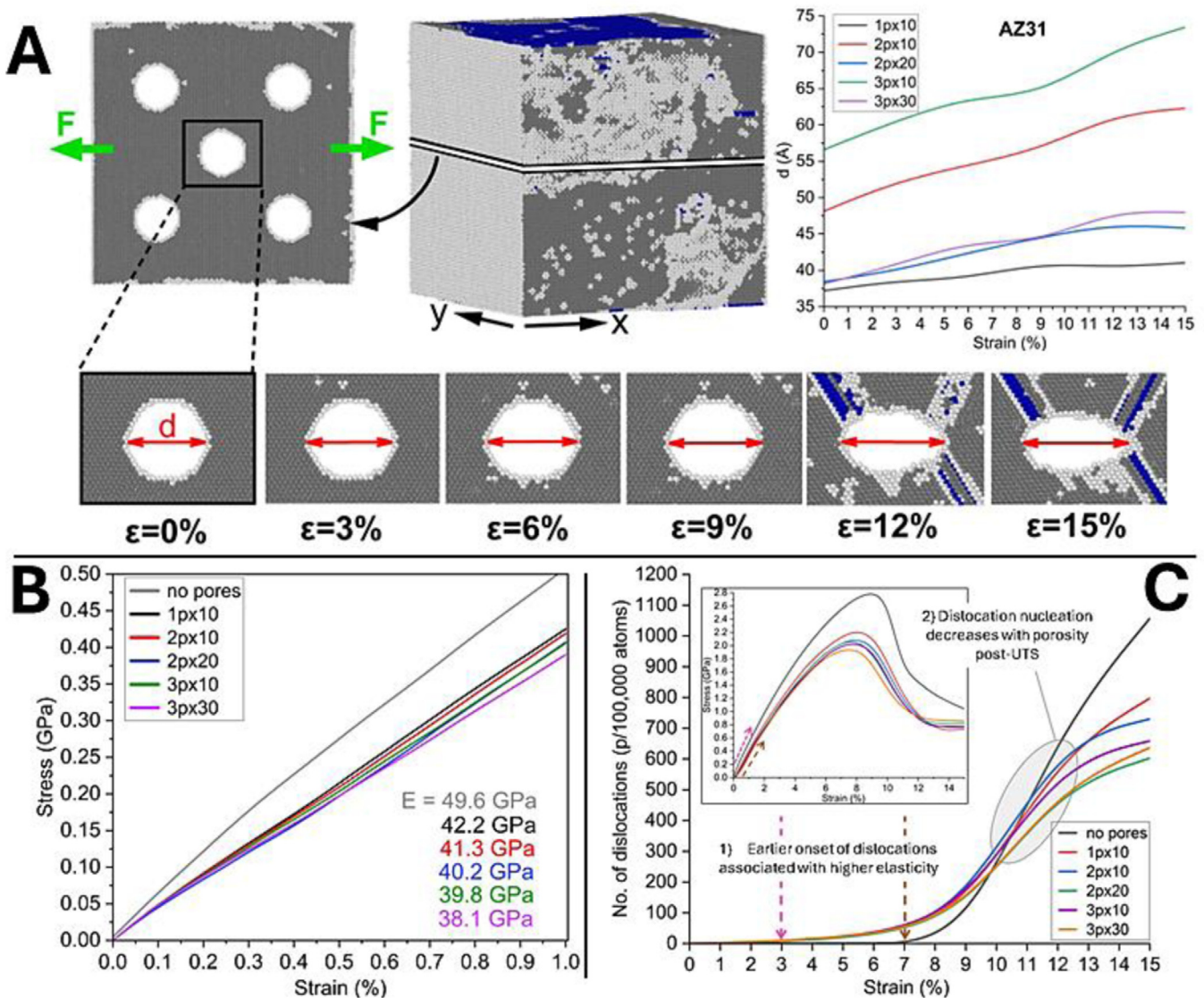


Fig. 10. A) Graphical 'slices' from the AZ31 porous model depicted evolution of pore morphology as a function of strain. Pore shape develops from circular to oval with formation of non-HCP phases (blue, light grey) around pores. Plot of pore diameter vs strain reveals that pore diameter (parallel to x-loading direction) increases for all porous systems, with the steepest increases in systems with large pores (2px10, 3px10). B) Young's modulus (E) associated with the porous and non-porous AZ31 models. A decrease in E is observed as porosity increases, hence reflecting the increased elasticity of alloys with increasing porosity. C) Evolution of dislocation density with progressive loading for the AZ31 alloy at all porosity levels. The non-porous alloy exhibits a later onset of dislocations that is correlated with lower elasticity and earlier onset of UTS (and *vice versa* for porous models). There is also an observed correlation between higher UTS and lower dislocation density.

pores. To explore the magnitude of this effect, the morphology of the pores was monitored throughout the loading process, and the pore diameter (d), was quantified (Fig. 10A). It was observed that the pore diameter (d), measured parallel to the x-loading direction, increases during loading, with the pore shape transitioning from circular to oval. This observation confirms that there is relatively high atomic mobility around pores, with this effect becoming more pronounced in systems containing larger pores (2px10 and 3px10 models) with respect to their smaller-pore counterparts (2px20 and 3px30 models). The concentration of FCC, non-HCP and amorphous phases around the pores, coupled with the enhanced atomic

diffusion, suggests that pores act as energetic "sinks" for both stress and FCC phase formation. As a result, the presence of pores is expected to increase the ductility of alloys with higher porosity, as characterized by increased atomic motion around pores. This is supported by the Young's modulus (E) data from the AZ31 models (Fig. 10B), which demonstrate a decrease in elastic modulus with increasing porosity, effectively characterizing lower stiffness alloys. Notably, models with larger pores exhibit a lower Young's modulus with respect to those with smaller pores (2px10 vs 2px20, and 3px10 vs 3px30), reinforcing the link between pore size, atomic mobility, and ductility.

3.5. Dislocation-driven stress-strain response

Dislocation density is directly correlated with key mechanical properties, including ultimate tensile strength (UTS). For the AZ31 alloy, dislocation density was tracked as a function of strain across all porosity models (Fig. 10C). The porous models ($p = 1\text{--}3\%$) exhibited an earlier dislocation nucleation, initiating around 3% strain compared to 6% strain in the non-porous model ($p = 0\%$). This pronounced difference in dislocation onset can be attributed to two factors: 1) the alloy's elasticity and 2) the strain at which UTS occurs. The increasingly porous models exhibit a lower modulus of elasticity, indicating lowered stiffness. As dislocation propagation is associated with ductility, this suggests that the porous alloys form dislocations earlier due to their ability to elastically deform and facilitate dislocation mobility. Additionally, the porous alloys reach their UTS at a lower strain than the non-porous model, indicating that earlier dislocation formation may lead to earlier deformation and a shorter plastic range; with consequent lowered strain-tolerance and raised "fracture-immediacy", (eg. sharpness of fracture-onset trends). Furthermore, Mg–Al–Zn alloys with lower porosities exhibit higher rates of dislocation nucleation post-UTS, supporting the presence of a more homogeneous stress distribution in non-porous alloys. While dislocation formation in porous alloys is likely localized around pores, the uniform stress in non-porous alloys enables rapid and widespread dislocation activity beyond the fracture point, highlighting porosity as a key facilitator in directing alloy deformation and failure mechanisms. Future work is planned to characterize additional mechanical properties for alloys explored in this work, including bulk and shear moduli, as well as Poisson's ratio and inroads to melt mechanisms, glassy transition (if any) and prediction of molten state properties [74,75].

4. Conclusions

This work employed molecular dynamics (MD) simulations to investigate the effects of alloying and porosity on the atomistic and mesoscopic structuring, and mechanical behavior of Mg–Al–Zn alloys under uniaxial tensile loading. A range of compositions (0–18% alloying content) with varying Al and Zn ratios were investigated, and the mechanical responses were analyzed using stress–strain behavior, dislocation evolution, RDFs, and multi-dimensional grain structure metrics.

The results highlight the critical influence of phase stability and alloying concentration on mechanical performance. A progressive reduction in HCP phase fraction with increasing strain, more pronounced in alloys with higher Al and Zn content, was correlated with reduced fracture strain and tensile strength, highlighting the importance of HCP phase retention for maintaining mechanical toughness, in Mg–Al–Zn alloys. The emergence of FCC phases solely post-fracture suggests that HCP destabilization is a driving factor for failure, while FCC formation, *via* amorphous structural-transitioning, is a post-fracture structural response; the system mitigating in-

stability through adoption of a structure with consequently lowered mechanical utility (FCC). Radial distribution function (RDF) atom-pair structural analyses further revealed that during loading, Al–Al and Zn–Zn bonds experience significant inter-atomic bond-length fluctuations particularly near fracture, confirming their active role in structural rearrangement and stress accommodation. These alloying elements also tended to preferentially occupy non-HCP environments, localizing transitory amorphization, effectively promoting HCP-to-non-HCP, to FCC, phase transition, including possible transitory amorphous phases, which could be potentially validated experimentally, for example, with operando *in-situ* neutron scattering in real-time. Although moderate alloying enhances strength, excessive Al and Zn additions ($>3\text{--}4\text{ at.}\%$) leads to reduced UTS due to phase instability. Overall, Al contributes primarily to solid-solution strengthening and moderate HCP destabilization through converting HCP to non-HCP phases (e.g., FCC), with Zn exhibiting this destabilizing effect to a greater extent. The "Zn limit" ($\sim 1\%$) is rationalized in terms of the lower stacking fault energy of Mg–Zn relative to Mg–Al, which itself is a result of the greater atomic radius mismatch between Mg and Zn ($\Delta r_{\text{Mg-Zn}} = +16.25\%$) relative to Mg and Al ($\Delta r_{\text{Mg-Al}} = +10.63\%$; $\Delta \Delta r = +5.62\%$). The interplay between these two elements in ternary systems is discussed and rationalized in terms of their combined influence on bond flexibility (eg. Al–Al and Zn–Zn pair fluctuations), local coordination geometry including coordinative-rigidity, HCP phase retention, and UTS.

Grain structure analyses revealed a critical strain valuation, coinciding with fracture onset, where grain density sharply increases, grain size decreases, and grains become elongated and flattened. Grain refinement was found to manifest differently in porous and non-porous systems ($p = 0\%$), as follows: non-porous alloys exhibited uniform grain splitting perpendicular to the loading axis, while porous systems ($p \geq 0\%$) display more heterogeneous, anisotropic grain fragmentation due to uneven stress distributions.

The influence of porosity on structural evolution was further demonstrated by the localized formation of (transitory) amorphous networks in the vicinity of pores, with subsequent stabilization and accumulation of FCC phases at those sites. These act as stress concentrators, promoting stress-induced phase transformations and enhancing ductility in their immediate vicinities; yet to a point, beyond which they become detrimental to material toughness and durability. This behavior is supported by observed reductions in Young's modulus (E) and morphological transitions of pores from circular to elliptical shapes, indicating elevated atomic mobility in porous regions. In contrast, non-porous alloys exhibit delocalized FCC formation in the form of shear bands, consistent with a more uniform stress distribution.

Dislocation analyses revealed that porous alloys initiate dislocation activity at lower strains ($\sim 3\%$) than their non-porous counterparts ($\sim 6\%$), aligning with their earlier onset of failure and lower elastic modulus. Higher dislocation densities were associated with increased strength, suggesting a dislocation hardening mechanism where greater resis-

tance to dislocation motion enhances the alloy's load-bearing capacity.

In summary, herein we provide a comprehensive atomic-scale insight into how alloying content and porosity interact to influence phase transformations, dislocation dynamics, and grain refinement in Mg-Al-Zn alloys. These findings offer valuable guidance for the optimization of alloy composition and microstructural design in applications where mechanical integrity under strain is critical, in addition to the design and inroads to tracking metrics for advanced operando, *in-situ* measurements in real-time including neutron scattering and positron spectroscopy [76]. Further understanding of the microstructure-mechanical property relationship may be achieved *via* elucidation of the composition and structure of the "other" phase, which may encompass clusters and intermetallic features associated with enhanced mechanical behavior, including localized rigidity/flexibility and atomic hinge-points (eg. Al fulcrums). In addition, to target more accurate predictions of mechanical behavior, consideration of thermomechanical history is planned *via* simulated heating, cooling and annealing to introduce realistic defect structures and capture thermomechanical history dependent deformation and failure mechanisms.

Data availability statement

The data and simulation scripts used in this study are available at DOI [10.5281/zenodo.18510426](https://doi.org/10.5281/zenodo.18510426). Additional data are available from the corresponding author upon request.

Declaration of competing interest

None.

CRediT authorship contribution statement

Alina Zakrjevsky: Writing – original draft, Visualization, Methodology, Investigation, Formal analysis, Data curation. **Mohammed S. Salha:** Writing – review & editing. **Henry Adenusi:** Writing – review & editing. **Rickey Y. Yada:** Writing – review & editing. **Gin-Gee Khat:** Conceptualization. **David F. Farrar:** Writing – review & editing. **Devis Di Tommaso:** Writing – review & editing, Supervision, Funding acquisition. **Kun Viviana Tian:** Writing – review & editing, Supervision, Project administration. **Gregory A. Chass:** Writing – review & editing, Validation, Supervision, Funding acquisition, Conceptualization.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at [doi:10.1016/j.jma.2026.102192](https://doi.org/10.1016/j.jma.2026.102192).

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