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Influence of Notch Geometry and Temperature on the Mechanical Properties of Al-Mg Alloy Using Molecular Dynamics Simulations

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ABSTRACT

At the near-threshold regime, small irregularities on the surface can interact with the microstructure and affect the nucleation and propagation of cracks. Molecular dynamics is an effective methodology to investigate the damage evolution at this scale, and three types of defects, namely, triangular, rectangular, and crack, are examined. The effects at different temperatures (10, 300, and 450 K) and depths (2, 4, and 8 nm) are investigated in an aluminum alloy containing 5% magnesium. Cracks propagate via amorphization of the crack tip and, at low temperatures, also through the formation of voids. Elevated temperatures and deeper pits reduce the mechanical strength of the materials, increasing the radius of amorphization, while the effect of the shape on the mechanical properties is negligible. The observed behavior follows a trend observed experimentally and through finite element modelling in the literature, extending the results from the macroscale to the microscale.

1 | Introduction

Aluminum is widely used across various industries, including machining, transportation, and electronics, for its light weight, ease of workability, and excellent corrosion resistance. However, as a pure element, aluminum lacks the necessary strength for many applications, which has driven the development of a wide range of alloys. These alloys incorporate elements such as copper (Cu), silicon (Si), magnesium (Mg), and zinc (Zn) to significantly enhance aluminum's mechanical properties. Among the commercially available alloys, the 5xxx and 6xxx series, both of which use magnesium as an alloying element, are extensively used in marine, automotive, construction, and storage applications. Magnesium not only contributes through solid solution strengthening but also enhances corrosion resistance and toughness.

While the bulk properties of these aluminum alloys are critical, the performance of a component is also highly dependent on its shape, manufacturing process, and environmental conditions. These factors can introduce defects that may compromise the material's performance, especially under mechanical loading. A common defect is surface damage, which may arise from manufacturing processes, early-stage corrosion, or surface roughness, and can reduce fracture stress levels below the expected threshold [1].

Studies have shown that pit depth is the primary factor influencing mechanical properties, with slight variation in yield and tensile strength observed between different pit shapes, provided the diameter-to-depth ratio remains consistent [2]. Although pit geometries can be quite complex, particularly for corroded specimens, they are often simplified in simulation. Rectangular,

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Summary

- A molecular dynamics model is developed to capture the crack nucleation in Al alloy.
- Effect of temperature and notch geometry on the shape and extension of the amorphous zone.
- J-integral evaluated for different notch shapes to quantify the effects on fracture strength.
- Effects of temperature and notch shape on ductility and Young's modulus.

cylindrical, semiellipsoidal, or conical shapes with constant depth and diameter are usually used for pitting. Typically, these pits fall within the micron range, as smaller dimensions are not practical for finite element analysis (FEA).

Wang et al. [3] compared the mechanical effects of conical, cylindrical, and semiellipsoidal pits and concluded that pit depth is the key parameter reducing mechanical performance. For pits with the same diameter-to-depth ratio, they found only a 1% variation in yield and tensile strength. It has also been observed that tensile stress increases the susceptibility to pitting corrosion in both steel [4] and aluminum [5]. To study materials at scales smaller than what finite element modelling (FEM) can handle, there has been increasing interest in atomistic modelling, commonly known as molecular dynamics (MD).

Li et al. [6] examined how temperature and strain rate affect aluminum single crystals. Their findings indicated that while strain rate had a limited impact on mechanical properties, temperature caused a significant reduction in maximum strength, decreasing from approximately 10 GPa at 10 K to about 6 GPa at 500 K. Yuan et al. [7] investigated the tensile deformation of aluminum single crystals under different temperatures and reported that the yield stress decreased from 2.7 GPa at 10 K to 2.39 GPa at 800 K. Kong et al. [8] explored the effects of silicon and copper on aluminum under shear stress, revealing that copper atoms provided a superior strengthening effect. Jang et al. [9] evaluated the role of zinc in an alloy system containing magnesium, copper, and silicon, resembling Al7075, by employing a modified embedded-atom method (MEAM) potential. Their study found that the presence of zinc reduced the formation of partial dislocations, resulting in higher yield stress and ultimate tensile strength (UTS).

Luo et al. [10] used MD to investigate the Portevin–Le Chatelier (PLC) effect in aluminum alloys with varying magnesium concentrations using the Liu interatomic potential. Their results indicated that the PLC effect, linked to magnesium's influence on dislocation motion, was more pronounced at lower strain rates (e.g., 10^8 s^{-1} exhibited higher instability than 10^{10} s^{-1}), lower temperatures (more pronounced at 100 K than at 500 K), and higher magnesium concentrations (higher at 5% than at 3%).

Similarly, Cui et al. [11] explored surface cracks in aluminum and copper single crystals under quasi-static conditions near 0 K, using Mishin's potential [12]. They observed crack propagation in a zigzag pattern, with nanovoid coalescence leading to stress undulation.

Stepanova et al. [13] studied the evolution of a central crack in aluminum and copper under mixed stress at near 0-K conditions, focusing on the maximum tangential stress (MTS) criterion and strain energy density (SED) criterion. They demonstrated that fractures propagated through rapid vacancy coalescence near crack tips and void formation.

In their research on aluminum single crystals with different orientations, Ma et al. [14] examined the influence of crystal orientation on crack propagation at room temperature. By studying cracks aligned along the (010), (110), and (111) directions, they calculated Young's modulus and yield stress values ranging from 120 GPa (111 orientation) to 78 GPa (110 orientation).

Since real-world materials are polycrystalline and contain multiple grains and phases, which can influence the mechanical behavior at various temperatures [15], authors have also tried to investigate the effects of grain boundaries or additional phases. Kazemi et al. [16] studied the effect of 5% Mg on the tensile properties of a polycrystalline Aluminum cube at 300 K using a Finnis–Sinclair type of interatomic potential [17]. Their findings showed increased dopant concentration at grain boundaries and an enhancement in tensile strength compared to pure aluminum, particularly at various strain rates. Rajput et al. [18] instead investigated the effect of Mg and Ti inclusion in Al single crystal, observing a strain-softening effect in the presence of a soft Mg inclusion and a strain hardening effect in the presence of a hard Ti inclusion. Although polycrystalline simulations are a closer representation of materials, simulations on single crystals are an important starting point as they allow isolation of deformation and fracture mechanisms without the complexity of grain boundaries. In addition, a few other limitations should be acknowledged when comparing MD simulation and experiments. The volume investigated is usually limited (from several nanometers to several hundreds of nanometers) and very high strain rates (usually between 10^{-7} s^{-1} to 10^{-10} s^{-1}) are applied, an order of magnitude above typical experimental values. This can lead to unrealistic quantitative results but can provide reliable qualitative insight into deformation mechanisms and fracture modes [6, 19]. For example, Ruaz et al. [20] simulated metal hardening at high strain rates, and while the magnitude of the results was higher than experimental data, it captured the behavior of different crystal orientations in agreement with the experiment from Takeuchi [21] on single crystals. A direct comparison is also hindered by the difficulty of experimentally replicating MD conditions and dimensions, but a few authors have been able to investigate the behavior of thin plate samples of a few micrometers with high resolution microscopy and microtensile testing, providing a valuable partial validation.

For example, Okamoto et al. [22] observed a stress-induced amorphization of a NiTi alloy at temperatures below 600 K. Li et al. [23] investigated the formation of an Al amorphous zone when straining a sheet of near pure Aluminum. Wang et al. [24] observed the evolution of a crack through nanovoid and amorphization in a Cantor Alloy with the formation also of lamellar areas in the surrounding region. Feng et al. [25] studied the crack propagation in an Al-Cu-Mg alloy, discussing the formation of the dislocation free zone, formation of nanovoids, and movement of dislocations. Han et al. [26] observed a similar behavior in a 3 mm by 4-mm nanowire of Ni subjected to

a compression test at 10^{-5} s^{-1} strain rate at room temperature. This amorphization was predicted using MD [27], despite the strain rate used in simulation being significantly larger than the one used in the experiments, and its formation has been linked by Idrissi et al. [28] to several factors including very high strain rates, very low temperatures, very high lattice friction, and very small sample sizes.

Nanopillar compression is another technique for obtaining mechanical data at small scales; for example, Ha et al. [15] identified a different behavior for the (19 1 23) and (5 2 9) orientation in Mn-steel.

MD simulations have also been applied to calculate J-integral and energy release rate (ERR) for various materials, including metals, ceramics, and polymers. Various methodologies have been developed to derive these parameters from atomistic simulations, including potential energy-based methods, kernel-based approaches, and atomic stress-based calculations.

Dewapriya et al. [29] and Le et al. [30] calculated the J-integral from the potential energy required to form a unit surface area in graphene. Xu et al. [31] used the difference between the potential energy of a perfect and a cracked nickel crystal to calculate the J-integral, normalizing the energy difference by the crack area. Jones et al. [32] applied a kernel-based method based on Hardy's formulation, while Roy et al. [33, 34] and Jia et al. [35] employed Gaussian quadrature to evaluate the J-integral in graphene.

Chowdhury et al. [36] used an atomic stress-based approach to calculate the J-integral for silica by summing discrete regions near the crack tip. Velilla-Diaz [37, 38] applied a similar methodology to aluminum single and bicrystals, comparing results with the crack-tip opening displacement (CTOD) and ERR methods. Their findings showed similar J-integral values to ERR for single crystals, while CTOD values were slightly higher for bicrystals. Ji et al. [38] used this method to study Cantor alloys near 0 K, and Sohail et al. [39] applied it to polymers, comparing their results with linear elastic fracture mechanics (LEFM) principles.

To overcome the complexity associated with modelling corrosion and crack growth and the limitations with FEA in terms of possible crack geometry, we have implemented MD simulations

to investigate the stress-strain behavior and J-integral of Al-5%Mg single crystals with atomically sharp surface crack, rectangular crack, and triangular crack at 10, 300, and 450 K with different lengths.

Using MD simulations with the embedded-atom method, we seek to elucidate the nanoscale mechanisms of crack propagation and quantify the associated changes in mechanical properties to complement the observations made at the macroscale.

2 | MD

The MD simulations in this study use the embedded-atom method (EAM) potential developed by Liu et al. [40], which has been previously employed for simulating Al-Mg alloys [41]. To construct models with three different crack geometries (sharp, rectangular, and triangular), we first generated a simulation box measuring $198.45 \text{ Å} \times 198.45 \text{ Å} \times 12.15 \text{ Å}$ for the smallest crack, with slightly larger dimensions for longer cracks, as detailed in Table 1. The x-axis is aligned along the [1,0,0] direction, the y-axis along [0,1,0], and the z-axis along [0,0,1]. Due to its high symmetry, we choose this orientation as a reference system to compare the effect of temperature and crack geometry, as it has been investigated also on pure aluminum [19, 42, 43].

Periodic boundary conditions were applied along the z-axis, while a fixed layer of atoms on EDGE 2 (Figure 1a) is restricting the displacement along the x-axis to minimize boundary effects and mimic an edge surface crack [40]. To simulate an atomically sharp crack, we removed the interactions between two groups of atoms. For the rectangular crack, we deleted a set of atoms from the edge, and for the triangular crack, we excluded atoms in a region between two intersecting lines. The sharp notch is referred to without a specific label, while the rectangular and triangular notches are labeled as "N" and "T," respectively. The model initially consists of aluminum atoms, and 5% of these are randomly substituted with magnesium atoms to achieve the final composition.

The side view of the model is shown in Figure 1a, with the aluminum atoms in blue and the magnesium one represented in red. The edges have been labeled from EDGE1 to EDGE4, and d

TABLE 1 | Parameters of the various configurations.

Sample ID	Dimension EDGE1 $\times$ EDGE2 $\times$ thickness (Å)	h/d	Temperature
5a	198.45 $\times$ 198.45 $\times$ 12.15	0	10 K, 300 K, 450 K
5a-N	198.45 $\times$ 198.45 $\times$ 12.15	5	10 K, 300 K, 450 K
5a-T	198.45 $\times$ 198.45 $\times$ 12.15	5	10 K, 300 K, 450 K
10a	283.5 $\times$ 283.45 $\times$ 12.15	0	10 K, 300 K, 450 K
10a-N	283.5 $\times$ 283.45 $\times$ 12.15	10	10 K, 300 K, 450 K
10a-T	283.5 $\times$ 283.45 $\times$ 12.15	10	10 K, 300 K, 450 K
20a	486 $\times$ 486 $\times$ 12.15	0	10 K, 300 K, 450 K
20a-N	486 $\times$ 486 $\times$ 12.15	20	10 K, 300 K, 450 K
20a-T	486 $\times$ 486 $\times$ 12.15	20	10 K, 300 K, 450 K

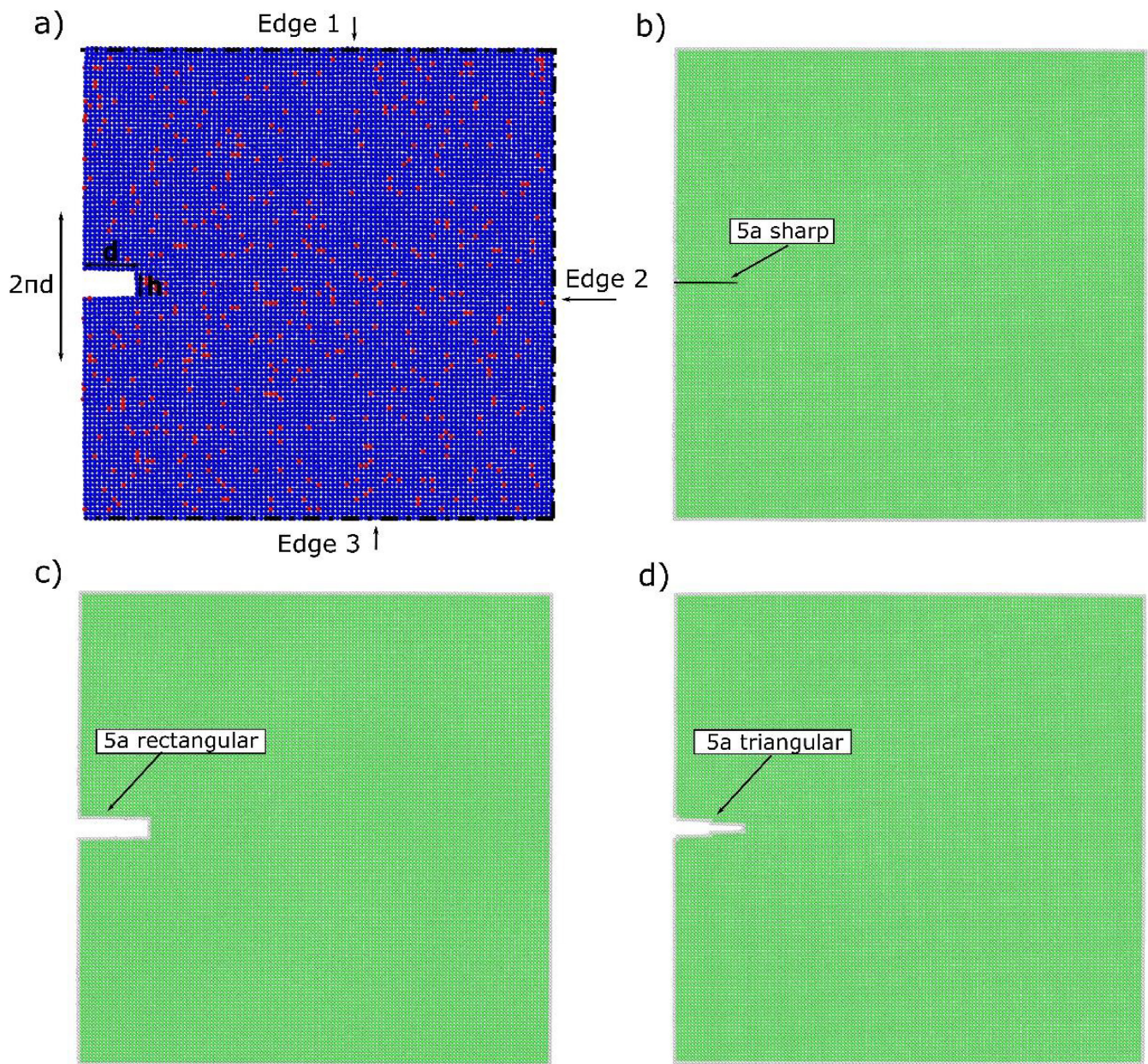


FIGURE 1 | (a) Model illustrating the distribution of Mg atoms (red) and Al atoms (blue) with representation of samples with a 10a pit depth for different shapes: (b) sharp, (c) rectangular, and (d) triangular. [Colour figure can be viewed at wileyonlinelibrary.com]

represents the crack depth, h the crack height (or opening), and $2\pi a$ the length of the ineffective zone.

The depth (d) is scaled by the lattice parameter ($a = 4.05 \text{ \AA}$), with values of $5a$, $10a$, and $20a$. All cracks share the same height (h), except for the sharp crack; an example of the different crack shapes is shown in Figure 1b–d. Due to the free surface, the regions adjacent to the crack do not carry load, and the height of this ineffective zone is approximately $2\pi d$ [36]. To balance the need to limit finite geometry effects with computational efficiency, the model dimensions were chosen based on the crack depth, as listed in Table 1, while maintaining a ligament-to-depth ratio of at least 5.

Three temperatures were selected for the study: 10 K to evaluate the effect of crack shape and length without thermal

contributions; 300 K to represent the behavior at room temperature; and 450 K to evaluate the behavior of the aluminum alloy subjected to service temperature characteristic of automotive applications.

The model was initially relaxed to equilibrium using the isothermal-isobaric ensemble (NPT). A strain rate of $\approx 10^9 \text{ s}^{-1}$ was then applied by moving EDGE 1 and EDGE 3 (Figure 1a) rigidly and in opposite directions along the y-axis to subject the notch to Mode I loading conditions. Temperature control was maintained with a Nose–Hoover thermostat, using a time step of 1 fs. All simulations were performed using the LAMMPS open-source code [44] and using OVITO to postprocess the results [45]. The dislocation and amorphous zones were analyzed using the Dislocation Extraction Algorithm (DXA) and Common Neighbor Analysis (CNA) implemented in OVITO

[46]. The atoms are classified into structural types, namely, face-centered cubic (FCC) and hexagonal close-packed (HCP). If they are not in either of these two, they typically represent an amorphous structure resulting from crack-tip plastic deformation [19, 42, 43]. Table 1 shows the dimensions of the 27 configurations investigated with the numerical model, with d the depth of the crack and h the opening (Figure 1a).

The global stress is calculated using the virial theorem and the virial stress, σ_{ij} is defined as [29, 47];

$$\sigma_{ij} = \frac{1}{V} \sum_{\alpha} \left(\frac{1}{2} \sum_{\beta=1}^N (R_i^{\alpha} + R_i^{\beta}) F_j^{\alpha\beta} - m^{\alpha} v_i^{\alpha} v_j^{\alpha} \right) \quad (1)$$

where i and j are the directional indices (x, y, and z); β is a number assigned to neighboring atoms which varies from 1 to N ; R_i^{β} is the position of atom β along direction i ; $F_j^{\alpha\beta}$ is the force along direction j on atom α due to atom β ; m^{α} is the mass of atom α ; v^{α} is the velocity; and V is the total volume.

The strain is calculated using the equation:

$$\varepsilon = \frac{L - L_0}{L_0} \quad (2)$$

where L_0 is the initial model height and L is the instantaneous height. A derivation of the virial stress [24, 36] is used to calculate the J-integral.

3 | J-Integral Calculation

J-integral is a continuum-based concept used to characterize the fracture properties of materials. The expression proposed by Rice [48] is

$$J = \int_{\Gamma} \left(W dy - T_i \frac{\partial u_i}{\partial x} d\Gamma \right) \quad (3)$$

where W is the strain energy density, T_i ($i=x,y,x$) are the component of the traction vector, $\frac{\partial u_i}{\partial x}$ are the component of the displacement gradient, and Γ is the counterclockwise path around the crack tip (Figure 2).

It is, however, challenging to apply a line integral at the atomic level due to fluctuations in stress and strain, as well as the difficulty in defining them atom by atom [49]. Instead, we can calculate the J-integral by summing the contributions from different discrete regions, selected to simplify the formulation of the J-integral.

The integration contour is placed at least 2 nm away from the right boundary, ensuring it remains outside both the plastic zone and the material surface [36–38].

Based on Equation (1), the J-integral can be expressed as

$$J = \int_{\Gamma_1} \left(W dy - T_i \frac{\partial u_i}{\partial x} d\Gamma \right) + \int_{\Gamma_2} \left(W dy - T_i \frac{\partial u_i}{\partial x} d\Gamma \right) + \int_{\Gamma_3} \left(W dy - T_i \frac{\partial u_i}{\partial x} d\Gamma \right) + \int_{\Gamma_4} \left(W dy - T_i \frac{\partial u_i}{\partial x} d\Gamma \right) + \int_{\Gamma_5} \left(W dy - T_i \frac{\partial u_i}{\partial x} d\Gamma \right) \quad (4)$$

According to previous findings [36–38], the displacement gradient $\partial u_y / \partial x$ is zero for path $\Gamma_2 - \Gamma_4$ (Figure 2) due to the uniform deformation along y and stress-free conditions along the x -axis [38], while for $\Gamma_1, \Gamma_3, \Gamma_5$, the traction T_i is zero because of the free surface, simplifying Equation (4) as follows:

$$J = \int_{\Gamma_1} (W dy) + \int_{\Gamma_2} (W dy) + \int_{\Gamma_3} (W dy) + \int_{\Gamma_4} (W dy) + \int_{\Gamma_5} (W dy) \quad (5)$$

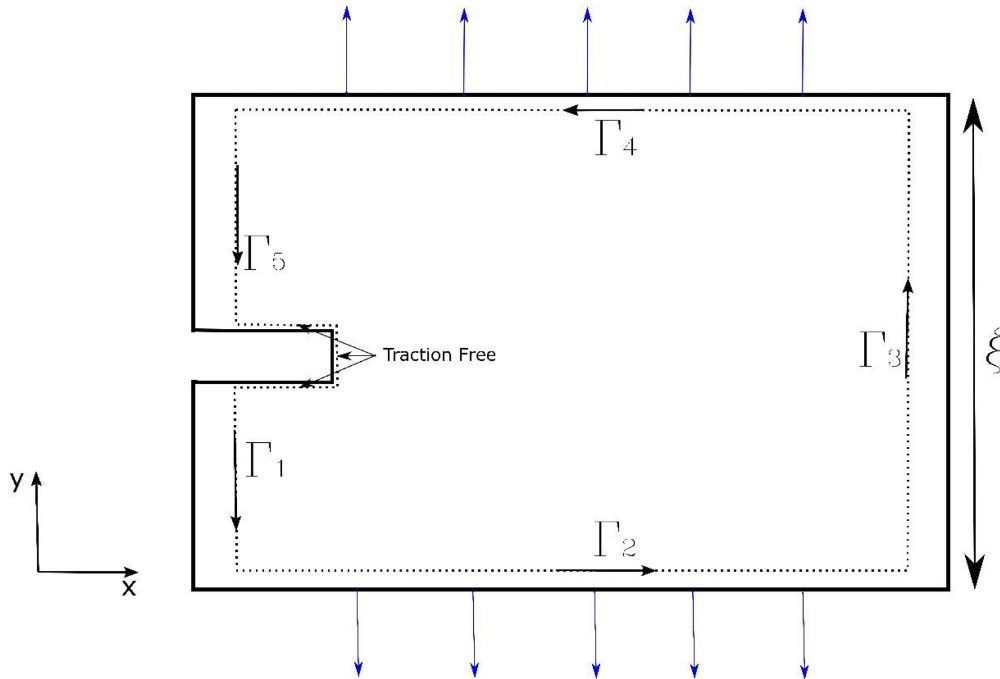


FIGURE 2 | The J-integral path; blue arrows indicate the displacement direction. [Colour figure can be viewed at [wileyonlinelibrary.com](https://onlinelibrary.wiley.com)]

Further simplification occurs for paths Γ_2 and Γ_4 , where $dy \approx 0$ due to the localized strain field near the crack tip [30].

This leads to

$$J = \int_{\Gamma_1} (Wdy) + \int_{\Gamma_3} (Wdy) + \int_{\Gamma_5} (Wdy) \quad (6)$$

where ξ the height of the system.

Since the strain energy density W is approximately zero for all paths but Γ_3 [36], the J-integral can be reduced to

$$J = \int_{\Gamma_3} w dy = \int_0^{\xi} w^{\Gamma_3} dy = w^{\Gamma_3} \xi = \left(\int_0^{\epsilon_{ij}} \sigma_{YY}^{\Gamma_3} d\epsilon_{ij} \right) \xi \quad (7)$$

Thus, the evaluation of the J-integral mainly depends on the stress in the y -direction, σ_{YY} . Following previous studies [36, 37] the atomic stress is averaged over several atoms within the potential cutoff distance, using the Hardy stress method. This averaged atomic stress is then summed for all atoms along path Γ_3 and normalized by the volume to compute the J-integral.

The Hardy stress for a given atom is expressed as [36, 38, 50]

$$\sigma_{avg}(i) = \frac{1}{N} \sum_{j=1}^N \sigma(j) \quad (8)$$

where $\sigma(j)$ is the atomic stress in the y -direction at the atom j within the cutoff distance at atom i . This method, introduced by Zimmerman [51], has been used in other studies [37, 50] and is considered a reliable approach for calculating atomic-level stresses.

4 | Results and Discussion

Table 2 summarizes all the data obtained from the 27 configurations analyzed. The samples are named using the notch length (5a, 10a, and 20a) and the temperature value at which the simulation has been performed. The results reported include the maximum stress, averaged over the entire volume and taken as the maximum value attained during the simulation. The elastic and plastic components of the J-integral are calculated and the dimension of the plastic region (D), expressed as the diameter of the circle containing the amorphous region, is reported at 6% strain.

The data reveal a small but notable variation in Young's modulus influenced by crack length, shape, and temperature. At 10 K, the modulus measures 90.5 ± 1.5 GPa for a 5a crack, 91.5 ± 0.5 GPa for 10a, and 85.5 ± 0.5 GPa for 20a, with an average value of 89 GPa and a reduction of 5.5% as the size of the defect increases. When the temperature increases to 300 K, these values decrease to 84 ± 1 GPa for 5a, 82 ± 1 GPa for 10a, and 81 ± 1 GPa for 20a, averaging 82 GPa with a 3.6% reduction as the size of the defect increases. At 450 K, the modulus further drops to 74.5 ± 0.5 GPa for 5a, 75.5 ± 0.5 GPa for 10a, and 77 ± 1 GPa for 20a, with an

average of 75 GPa and an increase of 3.2% as the size increases, in contrast with what observed at the other two temperature values.

Interestingly, while the variations due to crack shape are generally small ($< 5.5\%$), they are most pronounced at lower temperatures. At room temperature, the variation stabilizes; but at higher temperatures, an inversion is observed where the longest crack (20a) exhibits the highest modulus. The influence of crack length is more prominent at low temperatures, with the modulus for the 20a crack being approximately 6% lower compared to the shorter cracks.

As reported by Li et al. [6], temperature can influence Young's modulus. The average modulus decreases from 89 GPa at 10 K to 82 GPa (a reduction of 8%) at 300 K, and further to 75 GPa (a further reduction of 8.5%) at 450 K (Figure 3a).

In Figure 3b the maximum stress values are grouped for notch dimensions against the temperature value. The shape does not affect significantly the stress value; however, the dimension produces an offset with a decrease as the dimension increases. For every dimension of the notch, the stress linearly decreases with the increase in temperature.

Figure 3c shows the diameter values of the plastic region as a function of temperature. The results for different notch shape are grouped together and parametrised with the dimension. Increasing the size of the notch, the extent of the plastic zone increases and for a given length the plastic region increases with the temperature. For small notch (5a) it is observed that there is a significant scatter at 300 K due to the difference in the stress field between the configuration with the crack and those with rectangular and triangular notch.

It is also possible to identify that the plastic region for 5a at 300 K, when comparing the rectangular notch with the sharp and the triangular notch, is very different because it is characterized by a zigzag path with a larger amorphous region. The comparison of the shear strain for the crack (Figure 4a), rectangular (Figure 4b), and triangular (Figure 4c) notch highlights that the strain is localized at the crack tip for the sharp and triangular notches, while in the rectangular notch, it extends into the amorphous region.

4.1 | Effect of Notch Length for Different Shapes

The results are presented first comparing the effects of different shapes to evaluate their effects on the strength, the extent of the plastic region, and the J-integral. The stress is calculated with volumetric averaging of the values over the volume, while the strain values are calculated by dividing the variational dimension along the y -axis (Figure 1a).

4.1.1 | Sharp Shape

Figure 5 presents the effects of sharp notch lengths on the mechanical response of Al-5%Mg at 10 K. The analysis focuses on the stress-strain response across different crack lengths,

TABLE 2 | —Elastic properties with maximum stress and J-integral at fracture for every configuration investigated.

Sample	Young's modulus GPa	Maximum stress GPa	J-integral elastic J/m2	J-integral plastic J/m2	D (Å)
5a 10 K	89	5.79	1.52	2.25	26
10a 10 K	91	4.98	1.24	2.28	36
20a 10 K	85	4.05	0.8	2.6	68
5a 10 K N	89	5.69	1.56	2.11	29
10a 10 K N	92	5.0	1.37	2.21	48
20a 10 K N	86	4.12	0.76	2.69	70
5a 10 K T	92	5.20	1.49	2.25	28
10a 10 K T	91	4.78	1.2	2.3	41
20a 10 K T	85	4.05	0.73	2.57	80
5a 300 K N	85	4.08	1.13	2.42	46
5a 450 K N	74	3.66	0.9	2.17	51
10a 300 K N	83	3.89	0.87	2.46	56
10a 450 K N	75	3.28	0.85	2.16	70
20a 300 K N	82	3.41	0.81	2.46	78
20a 450 K N	77	3.04	0.3	2.7	91
5a 300 K	83	4.61	1.1	2.26	32
5a 300 K T	84	4.25	1.06	2.39	33
10a 300 K	83	3.85	1.02	2.28	56
10a 300 K T	81	3.90	0.92	2.39	61
20a 300 K	80	3.39	0.7	2.52	85
20a 300 K T	80	3.45	0.63	2.6	86
5a 450 K	75	3.84	0.86	2.24	50
5a 450 K T	74	3.78	0.83	2.28	54
10a 450 K	76	3.33	0.83	2.17	65
10a 450 K T	76	3.29	0.85	2.1	68
20a 450 K	78	3.04	0.47	2.55	100
20a 450 K T	76	2.9	0.3	2.63	101

isolating the effects of crack geometry by eliminating thermal contributions.

Doubling the crack length from 5a to 10a leads to a reduction in maximum stress by approximately 13%, while further extending the length from 10a to 20a results in a 19% reduction. This decrease in stress demonstrates that longer cracks significantly diminish the material's load-bearing capacity. Additionally, fracture initiates earlier in longer cracks, as the stress begins to decline at a lower strain, indicating that the presence of a longer crack accelerates failure. Elastic deformation is initially observed in all samples, followed by plastic deformation, which eventually leads to fracture.

At the end of the elastic phase, stress localizes behind the crack tip, reaching a significantly higher value compared to other areas

of the material, as shown in Figure 6a–c; it remains confined to a small region at increasing crack length. The asymmetry in the stress field is largely attributed to the presence of Mg atoms that produce the stress in the vicinity of Mg clusters. Due to the orientation, dislocation formation is limited; instead, an amorphous zone develops at higher stress levels, as shown in Figure 6d–f.

For pure Al the orientation adopted in this work produces a cleavage fracture [43, 52, 53] with some exceptions as the one reported by Ma et al. [14]. Other directions can present a combination of amorphous regions depending on the strain rate [19]. Another parameter that strongly affects the fracture mechanisms is temperature, as shown in Ni alloy by Wu et al. [53], where for the same orientation as this work a pure cleavage fracture near 0 K was observed; it became more ductile when the temperature increased.

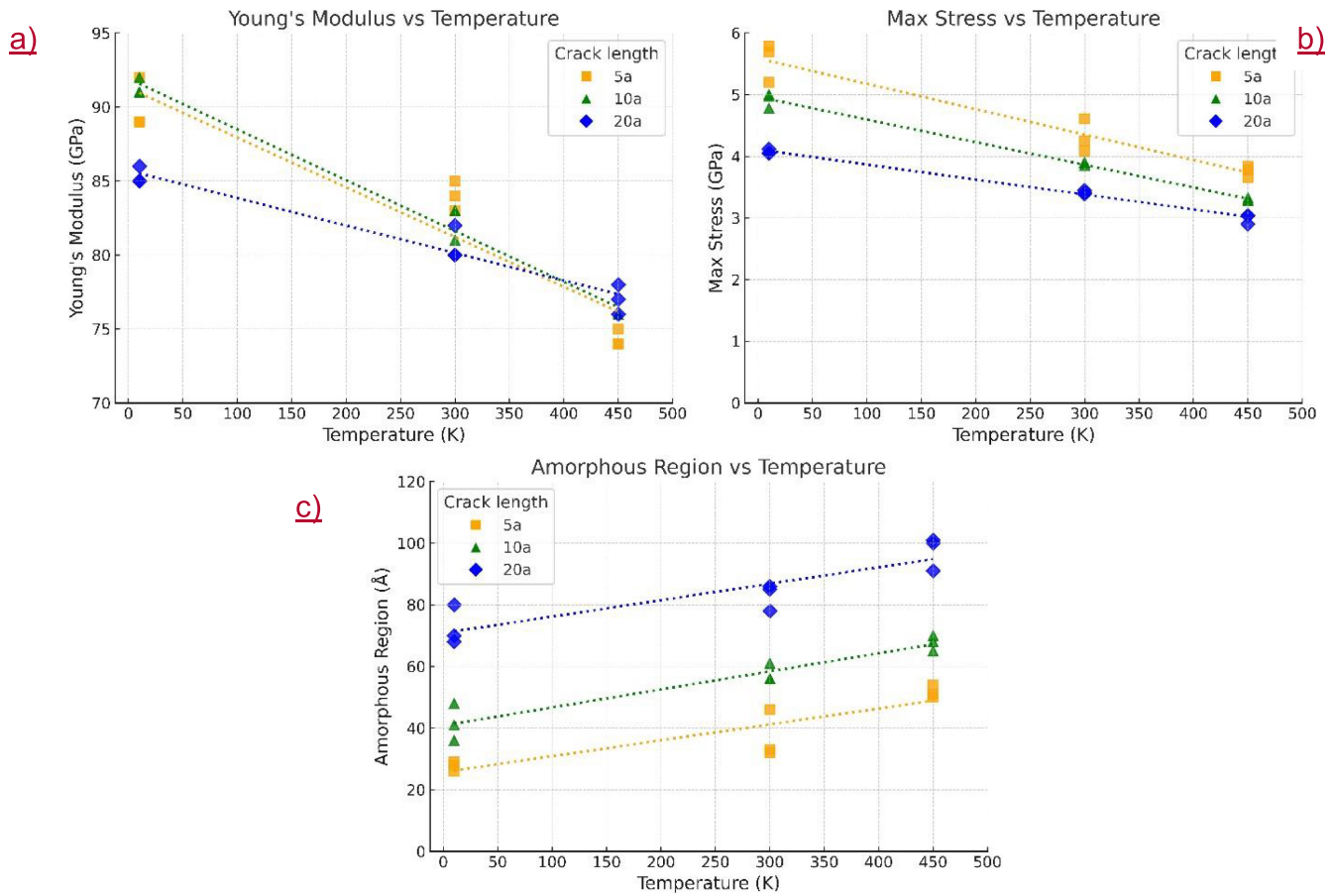


FIGURE 3 | (a) Young's modulus as a function of temperature, (b) maximum stress as a function of temperature and (c) diameter of the amorphous region as a function of temperature for different depth of the pit. [Colour figure can be viewed at wileyonlinelibrary.com]

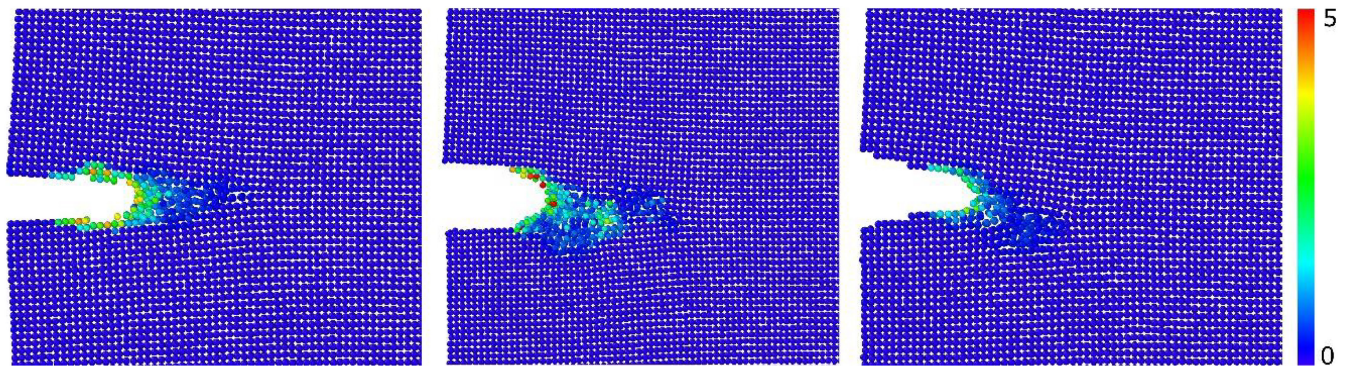


FIGURE 4 | Shear strain for different configurations highlighting the different response of the rectangular notch (b), compared to sharp (a) and triangular (c) notch. [Colour figure can be viewed at wileyonlinelibrary.com]

A similar amorphization in the same direction has been reported by Zhuo et al. [54]; although the Molecular Static (MS) approach at 0 K was used, it was not pure tensile displacement. Moreover, the formation of the amorphous zone was related to a decrease in stress load.

Amorphization has also been observed through MD for other metals such as Cu [55, 56], Ni [57], and Ag [58]. Li et al. [23] investigated with MD and TEM high strain rate amorphization, showing that it is the preferred deformation mechanism, at least

for the chosen orientation. Similar behavior has been observed in nanocrystalline Ni [59] and other materials [60].

It has been reported in literature that the presence of another element in the alloy can contribute to the amorphization. Barik et al. [61] studied pure Fe and Fe-Ni alloy, and from low temperature up to about 300 K, the pure iron fracture evolves through cleavage and then becomes mostly ductile at 800 K; however, when Ni is added, the fracture always shows some degree of ductility. Zhang et al. [62] investigated the effect

of crack and surface pit on the behavior of Al with Cu doping. Despite the crystal orientation not being declared by the authors, this system also experiences the formation of an amorphous zone behind the crack tip at a stress level below the maximum and grows without dislocation formation until stress starts to decrease.

Wang et al. [24] investigated high entropy alloys (HEA) and showed the amorphization behind the crack tip using TEM; they also performed MD simulation using a Cu-Al potential with a high lattice resistance to dislocation glide. The deformation happened mostly through the formation of amorphous zones, with the formation of stacking faults and twinning with a limited number of dislocations depending on the orientation. Ji et al. [63] investigated a HEA using a different potential and concluded that the amorphization was purely a

deformation-induced phenomenon related to high lattice resistance to dislocation glide.

Fracture occurring alongside the formation of voids and bridges between crack faces was observed at 10K, as also reported by others including Cui et al. [11], Krull et al. [50], and Stepanova et al. [13]. Moreover, the amorphous zone dissipated substantial energy until void formation (Figure 6f) as also reported by Hu et al. [64].

4.1.2 | Rectangular Shape

The mechanical response of rectangular cracks at 10K is shown in Figure 7. As with the sharp crack, increasing the pit length from 5a to 10a results in a 14% reduction in peak stress, with a further 19% reduction observed when extending the length to 20a. Following the initial elastic phase, the material becomes amorphous behind the crack tip, and crack propagation begins shortly afterward, followed by the formation of voids and bridges.

As observed for the sharp notch, the increase in length does not have any impact on the stress distribution, with the stress rise localized to a small area ahead of the crack.

For rectangular notch, the crack tends to initiate at the center of the notch for lengths of 5a and 20a. However, in the case of the 10a sample, crack formation starts at the edge, which can be attributed to the localized distribution of Mg atoms near the notch surface. Initially, the amorphous zone forms between the two (1 0 0) surfaces exposed by the notch, and as the stress increases, it follows a zigpath, a phenomenon also observed in previous studies [11]. At high deformation, when the amorphous zone has grown significantly, despite the constraint of the thickness, there are short dislocations forming and quickly disappearing as in Figure 8a where there is a star-rod dislocation $1/6\langle 110 \rangle$ and a Shockley dislocation $1/6\langle 112 \rangle$. However, the zigzag mechanism is particularly evident in shorter cracks but

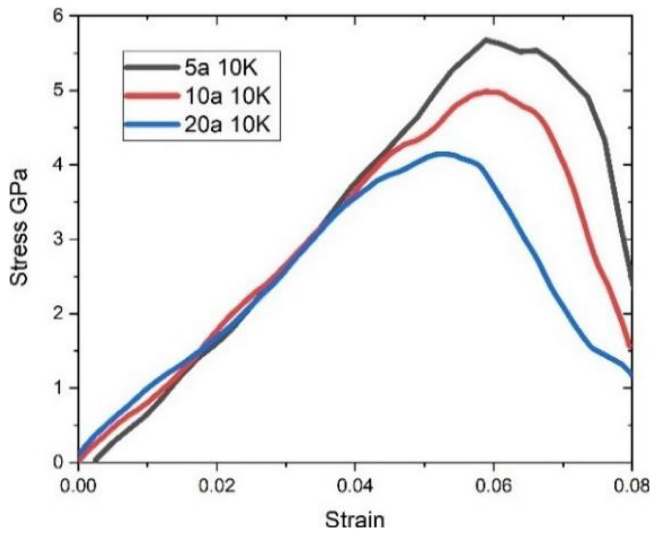


FIGURE 5 | Stress-strain curve at different length of a sharp crack. [Colour figure can be viewed at [wileyonlinelibrary.com](https://onlinelibrary.wiley.com)]

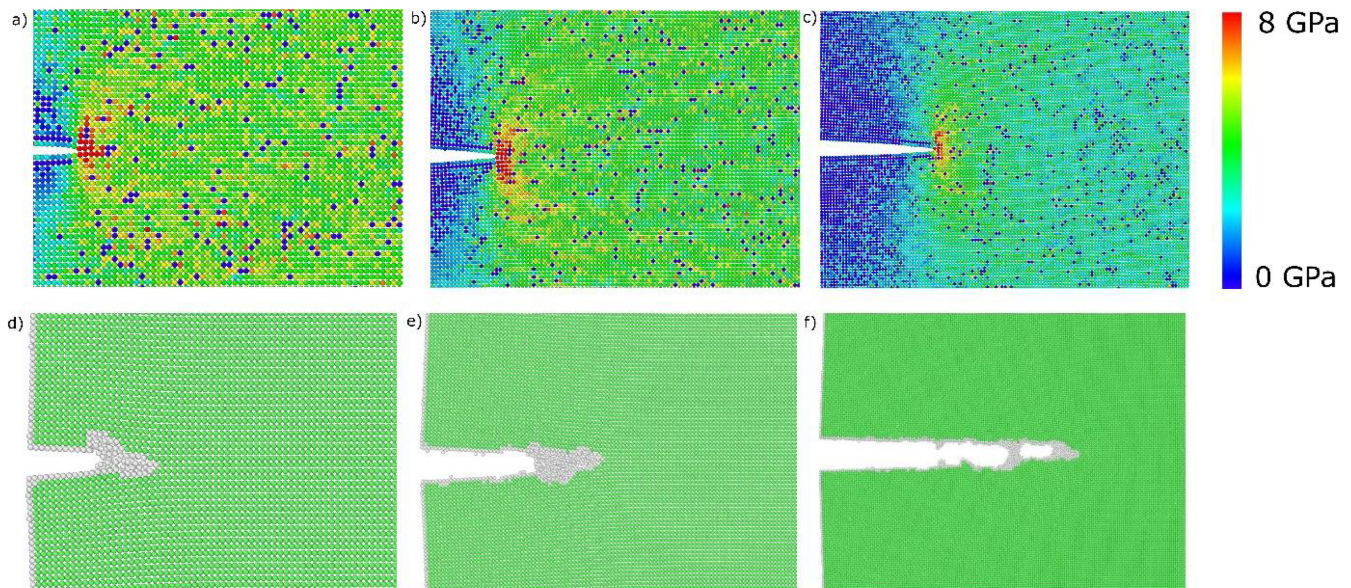


FIGURE 6 | —Stress at the end of the elastic region for 5a (a), 10a (b) and 20a (c). Extent of the amorphous regions for 5a (d) 10a (e) 20a (f) at 10K and 6% elongation. [Colour figure can be viewed at [wileyonlinelibrary.com](https://onlinelibrary.wiley.com)]

is less pronounced in 20a cracks due to earlier void formation (Figure 8b).

4.1.3 | Triangular Shape

The triangular notches are modelled with a constant opening width, leading to a decreasing tip angle as the depth increases. Figure 9 displays the stress–strain response for triangular cracks. Unlike the sharp and rectangular cracks, the reduction in maximum stress from 5a to 10a is only 10%, while a further extension to 20a results in a 16% reduction. This can be attributed to the fact that the maximum stress at 5a is lower for triangular notches compared to the other geometries, whereas the stress for 10a and 20a notches is similar across all shapes.

Stress distribution for this notch geometry is comparable to the other two configurations here investigated, characterized by a localized stress rise at the tip of the notch. Also, for this notched configuration, the damage propagates with the formation of voids and bridges, although a zigzag path is not observed, despite varying surface planes exposed by the pit. This lack of

zigzag growth behavior distinguishes the triangular pits from the rectangular and sharp pits.

4.2 | Effect of Temperature

The influence of temperature on the mechanical properties of Al-5%Mg was studied for the notched configuration. Figure 10 presents the stress–strain curves for different crack lengths at 10, 300, and 450 K.

Increasing the temperature has a pronounced effect on the material's mechanical strength. For instance, the peak stress for a 5a crack decreases by approximately 25% from 10 K (cryogenic conditions) to 300 K (room temperature). This reduction is less severe for longer cracks, with a 21% decrease for 10a and 14% for 20a cracks. Further increasing the temperature from 300 to 450 K reduces the stress by an additional 14% for all crack lengths.

Increasing the temperature has a detrimental effect on the mechanical strength of the material, but the reduction is higher

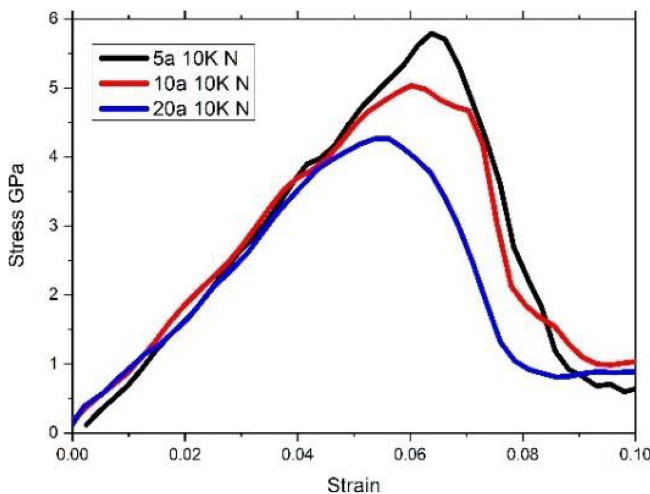


FIGURE 7 | Stress–strain curve at different length of the notched configuration. [Colour figure can be viewed at wileyonlinelibrary.com]

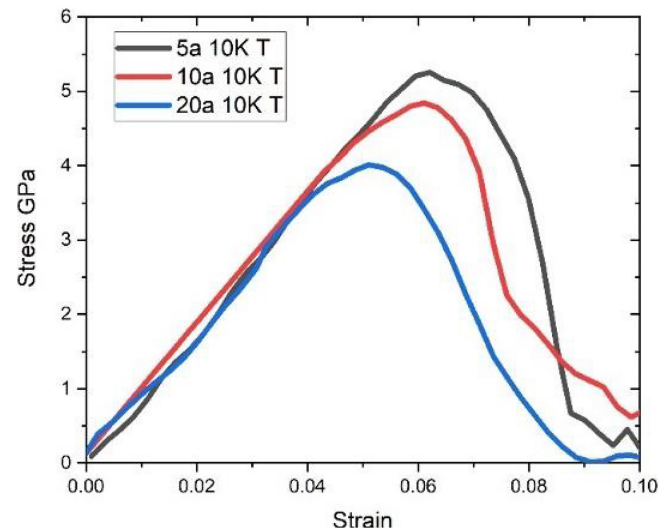


FIGURE 9 | Stress–strain curve at different length of the notched configuration. [Colour figure can be viewed at wileyonlinelibrary.com]

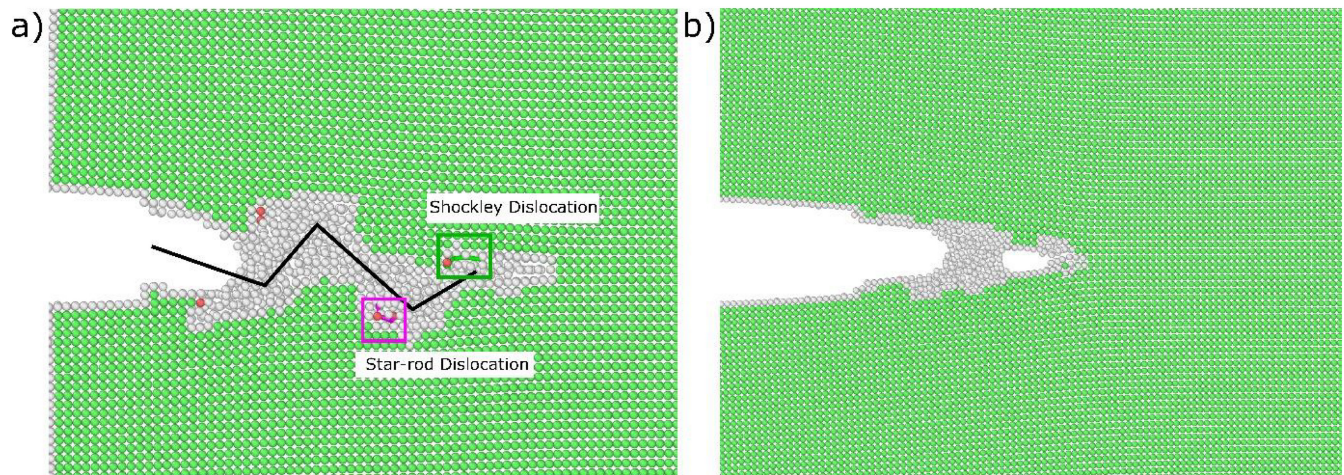


FIGURE 8 | (a) 5a-N at 7.43% of strain (b) 20a-N at 5% strain. [Colour figure can be viewed at wileyonlinelibrary.com]

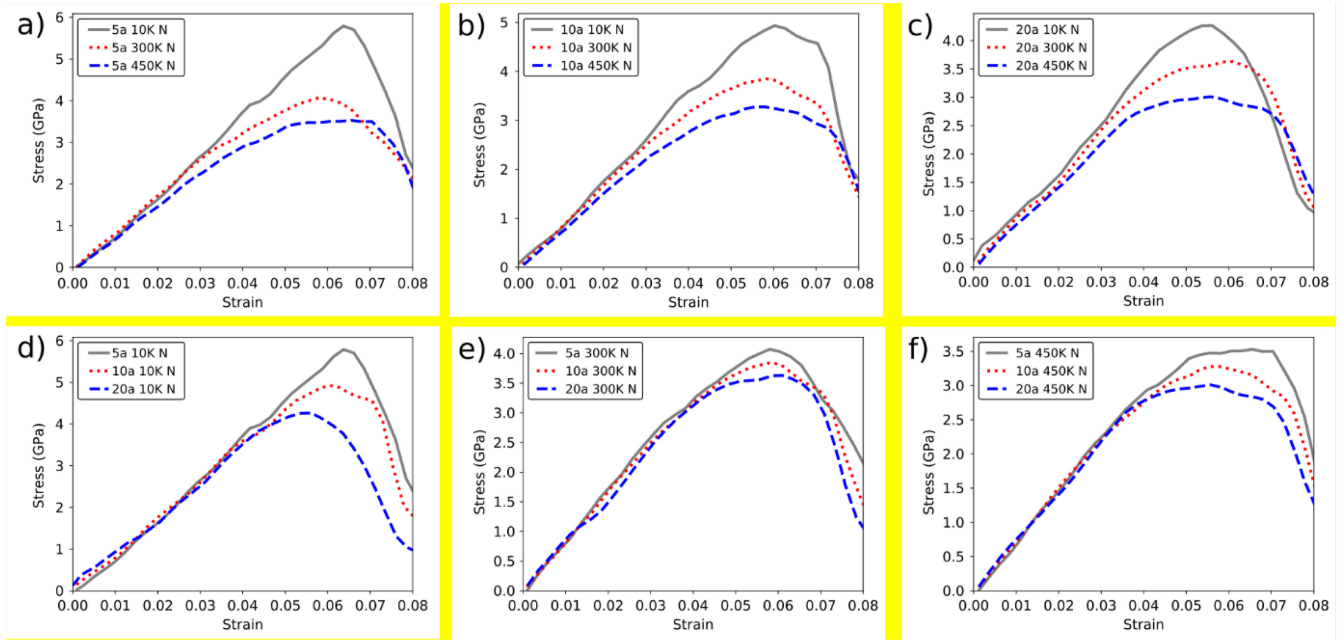


FIGURE 10 | Stress–strain curves of (a) 5a-N (b) 10a-N and (c) 20a-N at 10,300 and 450K and stress–strain curves at different length at (d) 10 (e) 300, and (f) 450 K. [Colour figure can be viewed at [wileyonlinelibrary.com](https://onlinelibrary.wiley.com)]

for lower crack length. The reduction in peak stress from cryogenic temperature to room temperature is about 25% for 5a, while it is about 21% for 10a and just 14% for 20a. Increasing the temperature from 300 to 450 K produces a reduction in the peak stress of $\approx 14\%$ for all lengths. Increasing length has a lower effect at different temperatures; as previously discussed, it is quite significant at 10 K but reduces at higher temperatures. At 300 K, the reduction from sharp crack to N shape is $\approx 10\%$ and further reduces by 8% at 20a. At 450 K, instead, the maximum stress at a depth of 5a and 10a is very close but reduces by 11%.

At both 300 and 450 K, the stress–strain curves exhibit a plateau (Figure 10e,f), which can be attributed to the plasticization of the amorphous zone. While it might be expected that at 450 K, that plasticization would allow for greater deformation at constant force, this is not observed. Instead, the increase in kinetic energy promotes the formation of vacancies and distortions [13] enlarging the amorphous region and causing the crack to propagate at a similar rate.

At all temperatures the onset of amorphization occurs at a lower average stress as the temperature increases, as shown in Figure 11a–c. As strain increases, the diameter of the amorphous zone also grows with rising temperature.

The amorphous zones, as highlighted in Figure 11d–f, measure $48\text{ \AA}$ at 10 K, $56\text{ \AA}$ at 300 K, and $70\text{ \AA}$ at 450 K. The increase in the dimension of the amorphous region is attributed to the fact that higher thermal energy facilitates defect formation, evidenced by the presence of extended plasticity further from the crack tip at 300 and 450 K and represented by the gray island in Figure 11e,f. However, at elevated temperatures, void formation is absent. Consequently, the amorphous zone can continue sustaining stress, which results in the appearance of a plateau in the stress–strain curve (Figure 10f). This indicates that while

defect formation becomes more pronounced at higher temperatures, the absence of voids allows the material to maintain its structural integrity over a wider range of deformation.

4.3 | Effect of Notch Shape

The influence of notch shape on the mechanical properties of the alloy is consistent across various temperatures. For reference, the results at 300 K are illustrated in Figure 12, which displays the stress–strain curves for different crack lengths. A similar trend has been observed at the other temperature values.

No significant differences are observed at 10a in the mechanical response among the various geometries (Figure 12b). Comparing the stress vs. strain at 5a, the maximum stress is attained by the sharp crack, while the triangular configuration shows approximately 5% lower stress, and the notched configuration demonstrates a 10% lower maximum value. The notched configuration achieves the highest peak stress at 20a, with the sharp crack yielding about 5% lower and the triangular crack exhibiting a 10% lower stress level.

For all the shapes investigated in this work, the amorphous region, characterized by its diameter reported in Table 2, varies slightly, measuring approximately $56\text{ \AA}$ for both the sharp and notched configurations, while the triangular configuration has a diameter of $61\text{ \AA}$.

4.4 | Comparison of J-Integral Values for Different Configurations

The J-integral values calculated for all the combinations are reported in Table 2 for different temperature values. The end of the elastic region, determined through OVITO DXA analysis,

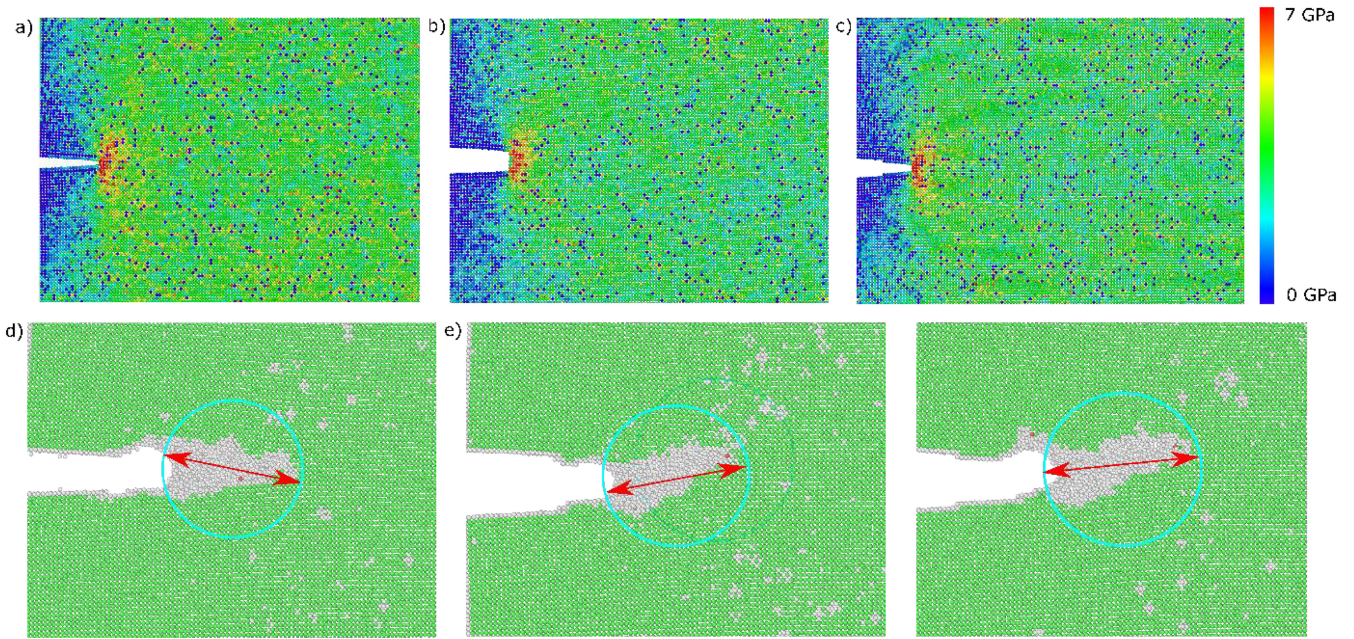


FIGURE 11 | 10a at 10, 300, and 450 K at the end of elastic region (a), (b), (c) and at strain of 6% (d), (e), (f). [Colour figure can be viewed at [wileyonlinelibrary.com](#)]

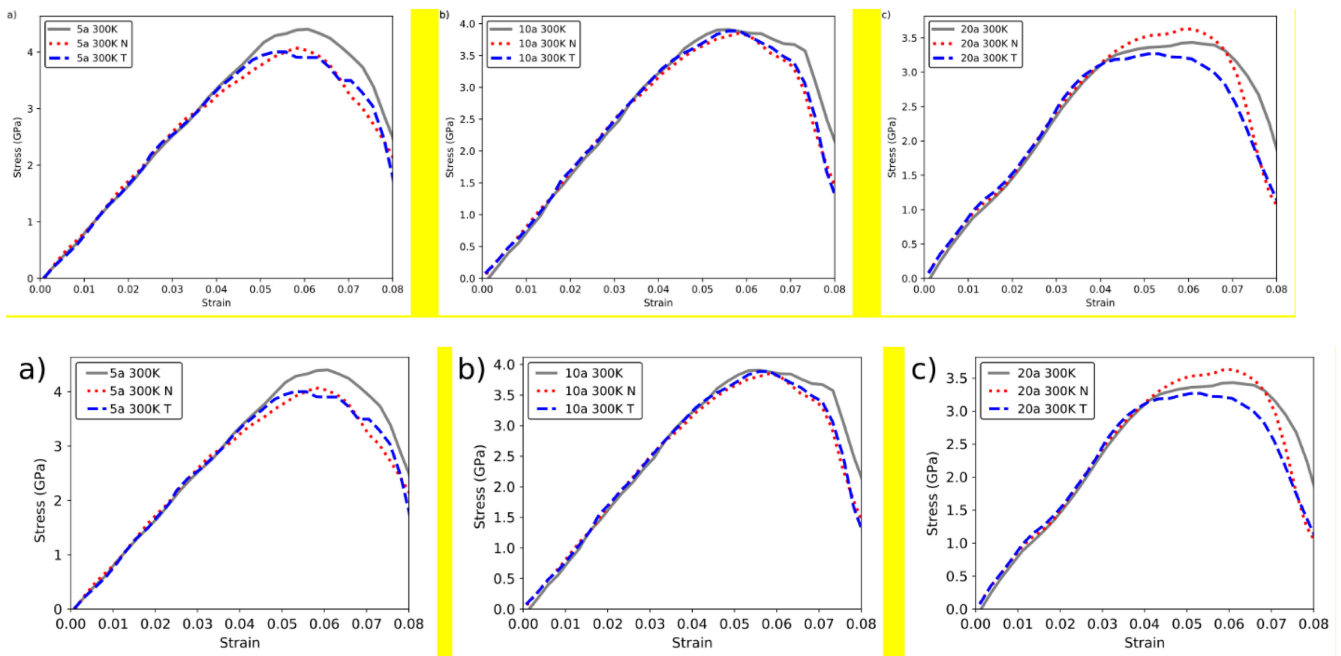


FIGURE 12 | Stress-strain curve at 300 K for various pit shape (a) 5a (b) 10a, and (c) 20a. [Colour figure can be viewed at [wileyonlinelibrary.com](#)]

corresponds to the last configuration before amorphization occurs behind the crack tip. The J-integral is calculated in correspondence with a 6% strain to ensure the calculation volume remained unaffected by plasticization [39].

The data indicate that notch shape has a negligible influence on the J-integral, with variations of less than 5% observed up to 300 K. However, at 450 K, the sharp pit demonstrates a J-integral value that is 25% higher compared to other shapes.

Increasing the crack length reduces the energy absorbed prior to the onset of plasticization, with a critical stress being achieved at

lower deformation levels [30]. When notch depth increases from 5a to 10a, the energy absorbed decreases by approximately 13%; a further reduction of about 40% occurs at 20a. This trend persists with rising temperatures, where increased thermal energy enhances defect formation.

The overall plastic energy remains relatively constant across different temperatures and lengths. Although maximum stress decreases with increasing crack length, the diameter of the plastic deformation area expands ranging from 46 Å for 5a-N to 78 Å for 20a-N at 300 K. Similar patterns are observed at various temperatures for a depth of 10a-N, with diameters measuring 46 Å

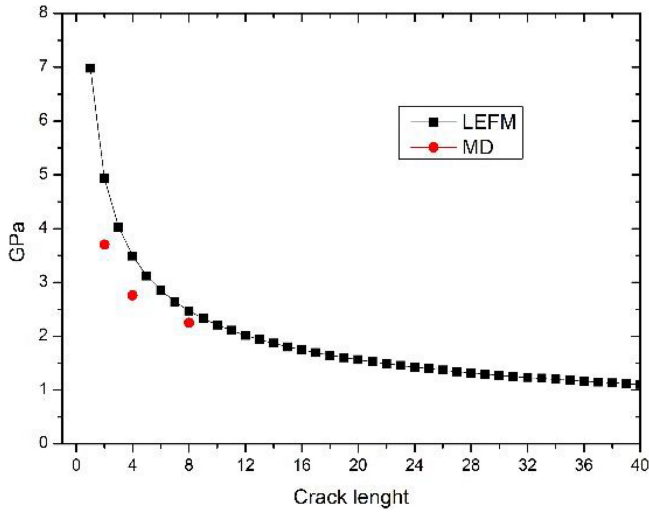


FIGURE 13 | Comparison of LEFM values and average MD values at 10 K. [Colour figure can be viewed at wileyonlinelibrary.com]

at 10 K, 56 Å at 300 K, and 70 Å at 450 K, compensating for the reduction in maximum stress.

According to fracture mechanics, the yield stress can be expressed as

$$\sigma = \sqrt{2E/\pi a} \quad (9)$$

where E is the Young's modulus, γ is the surface energy and a is the crack length, by using the values obtained at 10 K, and the γ is obtained from the potential for a (1,0,0) surface [40]. The comparison with LEFM was performed at 10 K to minimize thermal vibrations and highlight deviations arising purely from lattice discreteness (Figure 13).

The σ average values of the MD simulations are extracted at the end of the elastic region, their values approach the LEFM predicted values for higher crack length (8 nm) but diverge slightly at lower crack length due to lattice discreteness and atomic-scale effects [65, 66].

5 | Conclusion

This study used MD simulations to investigate the mechanical behavior of Al-5%Mg alloy, focusing on the effect of notch geometry, crack length, and temperature.

Results showed a temperature-dependent decrease in Young's modulus, from ~89 GPa at 10 K to ~75 GPa at 450 K, with more pronounced differences at lower temperatures and shorter cracks. Maximum stress varied with both crack length and temperature. At 10 K, longer cracks (20a) exhibited a significant decrease in stress compared to shorter cracks (5 a), which was less marked at higher temperatures.

The diameter of the plastic zone, representing the amorphous region, increased with crack length and temperature; it has similar trends for all shapes, while the fracture evolves differently with temperature. Void and bridges are formed at low temperature,

but they are suppressed at higher temperature, likely because of the larger amorphous zone.

J-integral analysis indicates increased plastic deformation with temperature. For 5a cracks, elastic J-integral values dropped from 1.52 J/m² (10 K) to 0.86 J/m² (450 K), while the plastic component remained relatively stable. Similar trends are observed for longer cracks, with plasticity dominating energy dissipation.

Overall, the results highlight increased ductility and plastic zone formation with temperature and crack length. Notch geometry had a limited effect; in agreement with FEM predictions, indicating the diameter-to-depth ratio as a key factor in mechanical performance.

Nomenclature

$\frac{\partial u_i}{\partial x}$	component of the displacement gradient
$F_j^{\alpha\beta}$	force along direction j on atom α due to atom β
L_0	initial length
m^α	mass of atom α
R_i^β	position of atom β along direction i
σ_{ij}	global stress
$\sigma_{avg}(i)$	average stress on atom i
v_i^α	velocity of atom α in the i direction
v_j^α	velocity of atom α in the j direction
a	lattice parameter
CNA	common neighbor analysis
CTOD	crack tip opening displacement
D	diameter of amorphous zone
d	notch depth
DXA	dislocation extraction algorithm
EAM	embedded atom method
FCC	face-centered cubic
FEA	finite element analysis
FEM	finite element modelling
h	notch opening
HCP	hexagonal close-packed
HEA	high entropy alloy
i, j	directional indices
L	final length
LAMMPS	large-scale atomic/molecular massively parallel simulator
LEFM	linear elastic fracture mechanics
MD	molecular dynamics
MEAM	modified embedded atom method
MS	molecular static
MTS	maximum tangential stress
N	rectangular notch
NPT	isothermal-isobaric ensemble
OVITO	open visualization tool
PLC	Portevin–Le Chatelier
SED	strain energy density
T	triangular notch
TEM	transmission electron microscopy
T_i	component of the traction vector
V	is volume
W	strain energy density
x, y, z	axis direction
α	number assigned to an atom
β	number assigned to neighboring atoms
$\Gamma_1, \Gamma_2, \dots, \Gamma_5$	component of the J-integral path
ϵ	strain
$\sigma(j)$	atomic stress in the y -direction

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Conflicts of Interest

The authors declare no known conflicts of interest.

Data Availability Statement

Data supporting this study are included within the article and/or Supporting information.

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