Molecular dynamic simulation of edge dislocation-void interaction in pure Al and Al-Mg alloy

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Abstract

In this study, the interaction of edge dislocations with nano-scale voids was investigated for the face centered cubic (FCC) structure of pure aluminum and Al-Mg alloy. The effect of Mg solute atoms on the Peierls stress (required for dislocation motion) at different temperatures, and the critical resolved shear stress (CRSS) for dislocation-void interaction was investigated in this study. In addition, the influences of void diameter(1, 2 and 3 nm), inter-void distance (7.5 and 15 nm) in a void array, and of temperature (300°K) on resolved shear stress were determined. It was found that substitutional Mg atoms was highly effective on improving the mechanical behavior of the Al lattice and on the type of dislocation-void interaction (simultaneous or separate passing of partial dislocations). In addition, it was obtained that no void-induced climbing occurred during the interactions for these systems. Higher void diameter and in particular lower inter-void spacing led to a considerable increase in the CRSS, while the latter changed the type of dislocation-void interaction. Finally, it was shown that Peierls stress was decreased for pure aluminum from $0°K$ to $10°K$, while different results were obtained for Al-Mg alloy that were discussed in detail.

Keywords: Aluminum-Magnesium alloy, Atomistic simulation, Dislocation

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interactions, Voids

1. Introduction

Interaction of dislocations with defects such as nano-voids affects the mechanical properties of metals and their alloys. Therefore, improving the mechanical behavior requires a fundamental understanding of the deformation mechanisms at different length scales, from the atomic structure to the continuum level. There have been many studies [1–7] on mechanical behavior of materials at the atomistic level using molecular dynamics simulations. Studies at the atomistic level can help to elucidate important aspects of dislocation motion and dislocation-defect interaction. Atomistic simulations can describe the dislocation core structure and its interaction with solute atoms and structural defects [8].

Molecular static (MS) simulation can be performed at zero temperature (0°K) where the system is relaxed by potential energy minimization to analyze the unpinning of the dislocation. On the other hand, molecular dynamics (MD) simulation can be carried out at finite temperature to understand the thermal escape of dislocation from the energy barriers due to solutes [9]. There have been some atomistic studies [8–43] on dislocation motion and its interaction with defects for various metallic materials and alloys. For face centered cubic crystals, the interaction of dislocation with void was investigated by MD calculations for Aluminum [10, 11], Nickel [12, 13] and Copper[14–16]. For body centered cubic crystals, this interaction was investigated by MD calculations for iron [17–24], for molybdenum [25] and for binary alloys such as Fe/Cu, Fe/Ni, Ni/Al and Al/Mg [38, 39, 41, 43–45].

It is well known that dislocations are pinned by the solute atoms and by comparing with the pure crystal, higher stresses for movement through solute fields are required [9]. There have been some atomistic studies on dislocation motion and its interaction with solute atoms in Al/Mg alloys [38, 39, 41, 43] Olmsted et al.[39] studied dislocation velocities and mobilities for edge and

screw dislocations in Al-2.5 at% Mg and Al-5.0 at% Mg random substitutional alloys. Curtin et al. [38] studied on mechanisms of dynamic strain ageing in aluminum-magnesium alloys. In an important study, solute strengthening in Al/Mg alloys was investigated by Olmsted et al.[41]. Depending on the stress and temperature, a range of behaviors were observed for steady motion, pinning, and unpinning of edge and screw dislocations. The effect of magnesium configuration on the stress required for dislocation de-pin was precisely studied, and also the effect of applied stress on the energy barrier for motion of dislocations was investigated. More recently, Ma et al.[55] have reported computationally efficient and quantitatively accurate multiscale simulation of solid-solution strengthening by ab initio calculation for Al-Mg and Al-Li alloys. The volumetric misfit interaction energy and slip misfit interaction energy values were explained and calculated based on the ab initio method for both the alloys. More importantly, the relationship between required stress for dislocation motion values with temperature was shown in their study for Al-1.1 at.% Mg and Al-3.3 at.% Mg alloys.

To the best knowledge of authors, no detailed atomistic simulation of the dislocation-void interaction in the Al-Mg alloys has been completed. In this work, MS/MD simulations were used to elucidate the effect of random Mg solute additions on dislocation motion and its interaction with nanometer scales voids in Al-0.5 % wt. Mg alloy. In addition, the effect of void diameter and distance between void arrays on CRSS in pure Al was discussed. Edge dislocation structure in the slip plane (111) of pure Al and Al-Mg alloy was investigated using MS at zero temperature and MD at finite temperature.

2. Numerical Methods

The edge dislocation motion and its interaction with voids were studied using MS and MD simulations based on the work of Osetsky and Bacon [17]that set up their simulation model to allow the analysis of edge dislocation in an infinite period glide plane. MD code LAMMPS [46] was used in either static or dynamic

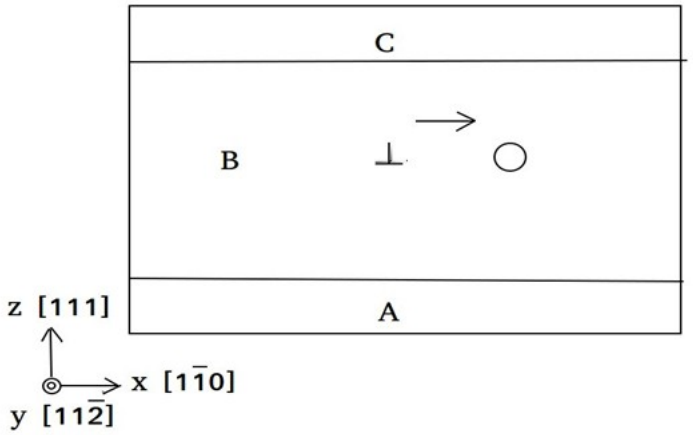

Figure 1: Sketch of the simulation cell containing edge dislocation and cavity.

loading conditions with Finnis and Sinclair type of Embedded Atom Method (EAM) to describe Al-Al, Mg-Mg and Al-Mg inter-atomic interaction with the potential model parameter provided from the work of Mendelev et al. [47].

The material examined was pure Al with FCC atomic structure and randomly inserted Mg atoms in its crystal structure. The study was focused on (i) analyzing the core structure of edge dislocation on its slip system, (ii) calculating the Peierls stress on its slip system, (iii) investigation of the effect of void diameter and void array distance on the CRSS of the slip plane, and (iv) determining the effect of temperature on the CRSS of the slip plane, at finite temperature in both Al and the Al-Mg alloy.

The computational simulation cell is a three-dimensional box with x, y, and z coordinates as shown in Fig. 1. In region B, the atoms were set to follow Newtonian behaviour and were mobile. The atoms in regions A and C were set as boundary zones, while atoms in region C were constrained to remain static and incrementally displaced in the x direction to simulate a shear loading. The atoms in region A were static to anchor the sample to avoid drift. The periodic boundary condition was applied along the x and y directions and free surfaces were set along the z direction. In this case, the system can be represented

as an infinite dislocation, infinite periodic glide, and as an array of voids that periodically repeating in space.

2.1. Creation of edge dislocation

To create an edge dislocation, an ideal crystal (simulation cell) divided into the upper and lower-half regions in z direction and in the lower half region two adjacent atomic half-planes $[1\bar{1}0]$ were then removed from the ideal crystal. After that, atoms in the upper half region were compressed, while the atoms in the lower region were elongated so the distance between the two adjacent half-planes would be the same while their y and z coordinates were kept identical. Finally, by freezing atoms in the regions A and C, and relaxing the atoms in region B to the minimum potential energy of the entire simulation system, the pure edge dislocation dissociated into two Shockley partial with stacking fault between them according to Eq. 1 [48].

$$\frac{a}{2}[1\bar{1}0] \rightarrow \frac{a}{6}[\bar{2}11] + \frac{a}{6}[\bar{1}2\bar{1}] \tag{1}$$

The centro-symmetry deviation (CSD) method [49] was used to visualize the dislocation core atoms and cavity. The atoms with CSD parameters falling in the range of $0.5A^{\circ 2} < CSD < 20A^{\circ 2}$, corresponded to the core of partial dislocations, stacking fault region, and cavity. The dissociation of an edge dislocation into two Shockley partials with a stacking fault region between them, cavity location, and free surfaces in Al-Mg alloy are shown in Fig 2.

2.2. Molecular static simulation

MS calculation was used to extract the value of Peierls stress at 0°K for edge dislocation lying on the slip plane. In this calculation, a strain increment was applied on the atoms in region C for each step, and the system was then allowed to take minimum potential energy. For this purpose, the conjugate gradient relaxation algorithm was used by assuming that the minimum potential energy is reached when the change in total energy is lower than 10^{-14} or the maximum force of x, y and z components of any atoms is $10^{-14}\frac{ev}{A^{\circ}}$.

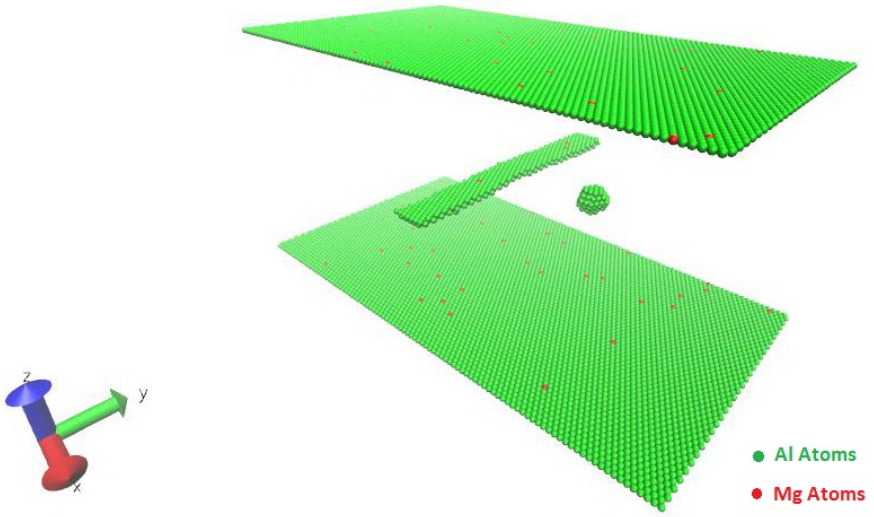

Figure 2: Dissociation of edge dislocation into two Shockley partials with stacking fault region between them, cavity location, and free surfaces in Al-Mg alloy.

Some studies have shown that the shear modulus and the value of the Peierls stress were not affected by the change in strain increment, and also these values were not significantly affected by the simulation cell size [8, 17]. These studies used one unit cell in the y direction due to the applied periodic boundary condition. This is useful for pure Al crystal since it is reasonable to assume that this unit cell will repeat in the y direction, but for Al-Mg alloy to make sure that the Mg atoms are randomly distributed in each direction, it is important to have several unit cells in the y direction. To extract the values of Peierls stress, static simulation were performed with simulation cell dimensions of $100b \times 3b \times 40b$ for pure Al and $100b \times 30b \times 40b$ for Al-Mg alloy, where the magnitude of b is $\frac{\sqrt{2}}{2}a$, $\frac{\sqrt{6}}{2}a$ and $\frac{\sqrt{3}}{2}a$ in the x, y, and z direction, respectively, under strain increment of 2×10^{-5}.

2.3. Molecular dynamics simulation

To simulate edge dislocation motion at finite temperature and its interaction with voids, MD was utilized. After dissociating of edge dislocation into two

Shockley partial and cavity creation, atoms in boundary zone were fixed and the system was equilibrated in Canonical ensemble (NVT) for 4ps ($4 \times 10^{-12}s$) for temperature stabilization. As temperature maintained constant, a Nose/hoover temperature thermostat was used [50]. MD simulations were performed using simulation cell with dimensions of $100b \times 30b \times 40b$ given by $29 \times 15 \times 14nm^3$ that contains 360000 atoms. The time step was 2 fs ($2 \times 10^{-15}s$). To apply shear strain ($3 \times 10^{-8}fs^{-1}$), a constant velocity in the x-direction was then applied on region C while the atoms in region A were being fixed. During this process, the temperature of the system was kept constant using Nose/Hoover thermostat after excluding the x-component of the atom velocity. To study the dislocation-void interaction for both the Al and Al-Mg alloy, the box size in y direction was changed to keep constant the inter-void spacing in the direction of the dislocation line due to the periodic boundary condition. In addition, to investigate the effect of inter-void spacing, the box length in y-dimension was halved.

3. Results and discussion

3.1. Effect of used potential and simulation cell size on Peierls stress

The Mendelev et al. potential [51] was used for pure Al and its modification was utilized for Al/Mg alloy [47]. For these potentials lattice parameter $a = 4.04527A^\circ$, burgers vector $b = 2.8673A^\circ$ and the zero temperature elastic modulus C_{11}= 110 GPa, C_{12}=61 GPa and C_{44}= 33 GPa. To evaluate the differences of dislocation core structure obtained by these potentials with other potentials, dislocation core structure was extracted using Liu et al. potential [52] which was corrected by Liu et al. [53] for Al/Mg alloys. For Liu et al. potential, lattice parameter $a = 4.032A^\circ$, burgers vector $b = 2.851A^\circ$ and the zero temperature elastic modulus C_{11}= 118 GPa, C_{12}=62 GPa and C_{44}= 32 GPa. To extract the effect of used potentials, image forces and boundary conditions on measured Peierls stress, simulations were performed with different cell dimentions, $100b \times 40b$, $100b \times 100b$, $120b \times 120b$, $140b \times 140b$ along the displace-

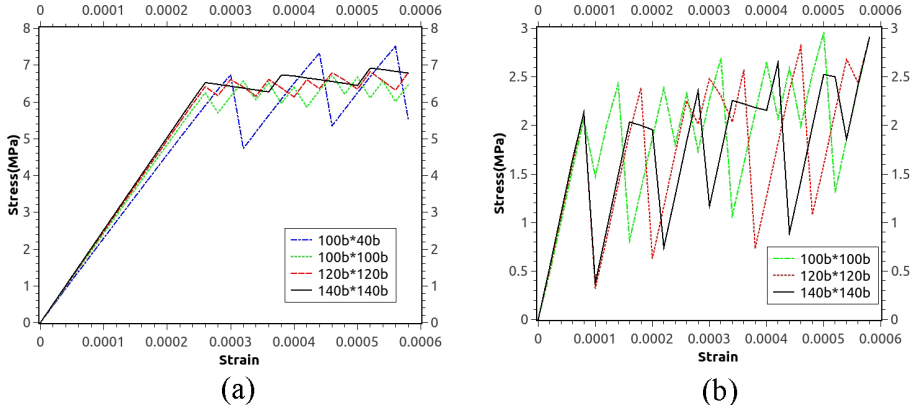

Figure 3: Stress-strain curve obtained by MS simulation of dislocation motion in Al using (a) Mendelev et al. potential and (b) Liu et al. potential in different simulation cell size along the displacement and normal direction of dislocation.

ment and normal direction using Mendelev et al. and Liu et al. potentials. As can be seen in the Fig. 3, the value of Peierls stress in pure Al was not significantly affected by simulation cell size. However, Olmsted et al.[40] reported that, image forces and boundary conditions can affect Peierls stress values, and the size of $100b \times 40b$ is big enough to evaluate the Peierls stress (as shown in the Fig. 3 (a)). Also, dissociated distance of Al edge dislocation between Shockley partials was evaluated. Table 1 shows the results of this study and previous studies for comparison. As can be seen, the results are in good agreement with the previous studies. Finally, the simulation cell size of $100b \times 40b$ along the displacement and normal direction and Mendelev et al. potential were used for subsequent simulations.

3.2. Effect of Mg solute atoms on Peierls stress

Fig. 4 (a) shows a stress-strain behavior of pure Al crystal and Al/Mg at different Mg concentration. As can be seen, a linearly increasing trend for stress was initially obtained for the pure Al crystal by increasing the strain with a shear modulus similar to that obtained for a perfect crystal. When the stress reached a critical value, the dislocation moved continuously, leading to

Table 1: comparing the values of dissociated distance and Peierls stress obtained in this study with previous studies for Al.

	Dissociated Distance($A°$)	Peierls Stress(MPa)
This study(Mendelev et al.)	10.1	7
This study(Liu et al.)	15.68	2.13
Srinivasan et al.[54]	16 , 5-15	
Kuksin et al.[48]	15	
Wang and Fang[42]		2.65
Olmsted et al.[40]		2
Dong[43]	14.4	2.4

an increase in the strain. The maximum stress where corresponds to the Peierls stress ($\sigma_{xz} \sim 7MPa$) occurred at a strain equal to $\varepsilon_{xz} \sim 0.32 \times 10^{-3}$. As can be seen from Fig. 4 (b), the values of Peierls stress were increased (from 7 MPa to 55 MPa) with an increase in Mg solute concentration (from 0.0 %wt to 2.0 %wt). Also, this figure shows that the dependence of the Peierls stress on the Mg concentration is linear. Such linear dependency was reported in the study of Ma et al.[55] for Al/Mg binary system, while in other studies [41, 43], $c^{\frac{2}{3}}$ (c is solute concentration) dependence were reported.

Mg solute atoms are oversized and cause dilatation field that interact with dislocation. This interaction energy is approximated by the interaction energy due to volume misfit of the Mg atoms against the pressure field of dislocation and the interaction energy due to the slip misfit (these misfit parameters are obtained by ab-intio calculation). Such dislocation-solute interaction energy is used to evaluate energy barrier against the dislocation motion in randomly distributed Mg solute atoms, and finally the shear stress to overcome this energy barrier. Mg solutes introduce large and positive extra volume that causes higher energy barrier and higher stress required for dislocation motion. (for more details see

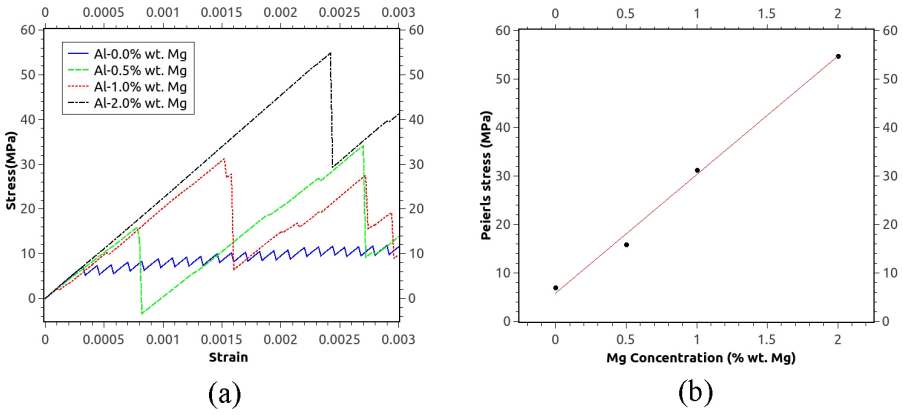

Figure 4: (a) Stress-strain curve obtained by MS simulation of dislocation motion in Al and Al-Mg at different concentration of Mg solute atoms. (b) linear dependence of Peierls stress on the Mg concentration.

[55, 56])

3.3. Effect of Mg solute atoms on edge dislocation-void interaction

In order to study the effect of Mg concentration on CRSS of slip plane, edge dislocation and its interaction with nanometer voids at finite temperature, the pure Al and Al-Mg systems were subjected to a shear loading in the MD simulation. Fig. 6 shows the stress-strain curve of edge dislocation interaction with 1 nm void in Al crystal and Al-0.5% wt. Mg alloy at 10°K. As can be seen in stage A, the stress required to move edge dislocation at 10°K in Al-Mg system was larger than Al crystal due to the pinning effect of solute atoms, and the Peierls stress at 10°K obtained by MD simulations in both systems were closed to the corresponding Peierls stress at 0°K obtained by MS simulations (see Table 2). As can be seen in Table 2, the value of Peierls stress in Pure Al was decreased with increasing temperature to 10°K, but in the Al-0.5% wt. Mg alloy, this value showed a little increase. For better understanding of this effect, stress required for dislocation motion at 100°K and 300°K were also extracted. The results were shown in the Fig. 5. As can be seen in this figure, the value of critical stress for dislocation motion in Al-0.5% wt. Mg at 10°K and 100°K are

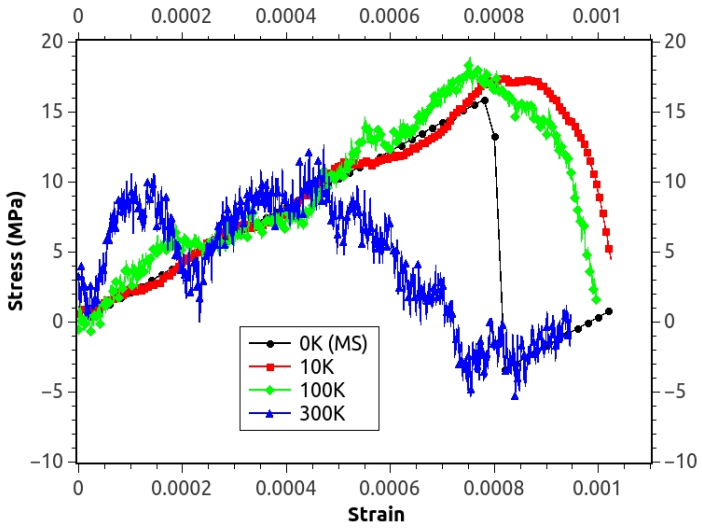

Figure 5: Stress-strain curve obtained by MS and MD simulation for extracting the stress required to dislocation motion in Al-0.5% wt. Mg at different temperature.

closed to the value for 0°K, however, with a slight increase, whereas the value at 300°K shows a significant reduction. Phonon friction and solute atmosphere can justify these results. At a very low temperature, phonon friction is not as much as higher temperatures, and dislocation can pass through an array of solute atoms with the help of inertia, however, dislocation motion is controlled by the solute atmosphere. At a higher temperature, phonon friction becomes higher, and dislocations can pass the solutes with the aid of thermal activation, leading to a decrease in the stress. Therefore, it can be seen that due to consideralbe thermal activation dislocation motion at 300°K, a lower stress was obtained, while before 100°K, the solute atoms act a stronger obstacle as they have a higher mobility in respect to zero temperature. Although, the mobility of solute atoms becomes considerble at 300°K, however, thermal activation dislocation motion seems to be dominent at 300°K. [55]

In Fig. 6, four stages of an edge dislocation interaction with 1nm void can be observed. A, the glide of dislocation towards the void before interaction.

Table 2: values of Peierls stress at T=0°K and T=10°K in Al and Al-0.5% wt. Mg obtained by MS and MD calculation.

	Al	Al-0.5% wt. Mg
T=0°K (obtained by MS)	7 MPa	15 MPa
T=10°K(obtained by MD)	3 MPa	16.5 MPa

B, its attraction with the void. C, bowing out just before the release, and D, releasing from the void and continuing to the glide. Figs. 7 and 8 show the corresponding atomic configurations from different directions, indicating dislocation-void interaction in Al and Al-Mg systems with stages A to D as marked on the stress-strain curve, see Fig. 6. As can be seen in these figures, the dislocation in bowing pulls into two dislocation segments pinned by cross cut of the void, since passage of edge dislocation sheared the void (see Fig. 9). Literature [15] reported that void-induced climb occurs for BCC metal. However, in the case of FCC metals, it has not been well understood if this type of climbing occurs during dislocation-void interaction. Some authors [57, 58] suggested that it might occur for FCC metals with a high value of SFE. The simulation results presented in Fig. 10 show that this type of climbing for edge dislocation did not occurred for both Al and Al-Mg systems at 10°K.

3.4. Effect of void dimension on the CRSS

Stress-strain curve corresponded to edge dislocation interaction with 1, 2 and, 3nm void diameters at 300°K is shown in Fig. 8. As can be seen, the CRSS was decreased by decreasing of the void size. In fact, an increase in the void size has a strengthening influence on Al crystal by increasing the interaction area between the dislocation core and voids. Therefore, more atoms will be pinned, leading to a request of a higher stress (see Fig. 11). However, it should be noted that the increase rate of CRSS was decreased by the increasing the void diameter from 2 to 3 nm with respect to that of 1 to 2 nm, indicating that there might be an optimum value (see Fig. 12) of void diameter for strengthening [21].

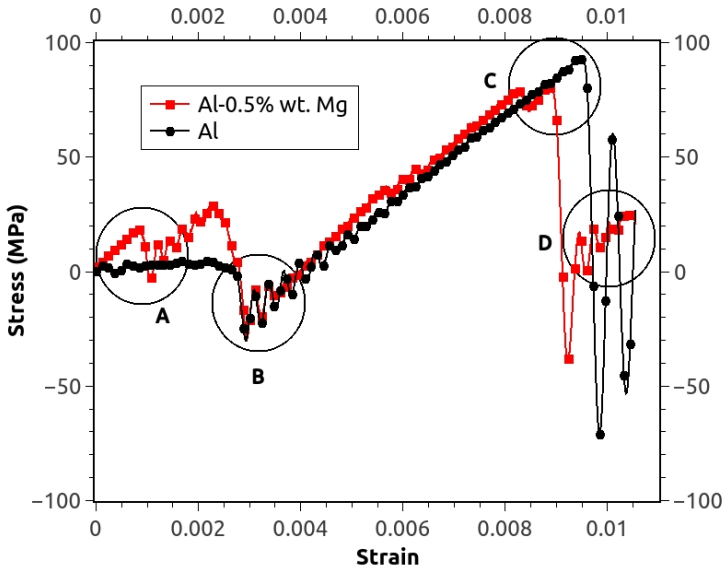

Figure 6: Stress-strain curve obtained by MD simulation of an edge dislocation interaction with 1nm void in Al and Al-Mg at 10°K [A, the glide of dislocation towards the void, before interaction. B, its attraction to the void. C, bowing out just before the release, and D, releasing from the void and continuing to the glide].

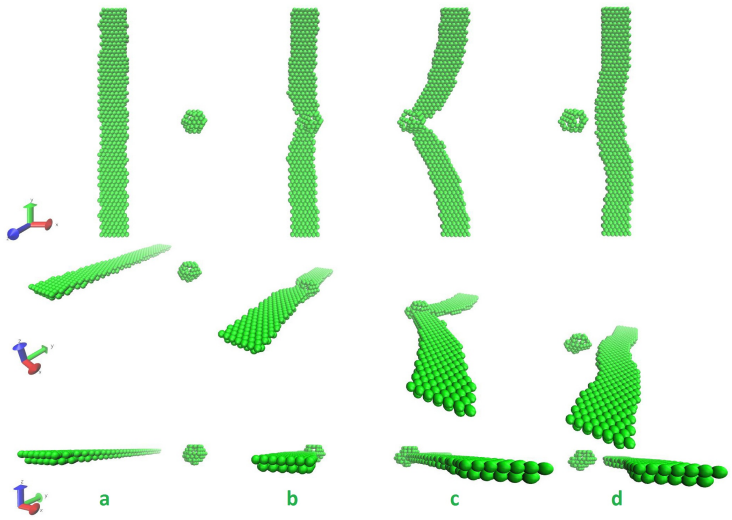

Figure 7: Atomic configuration associated with stages A to D, as marked on the stress strain curve of Fig. 6 for Al crystal, (a) A, (b) B, (c) C, and (d) D.

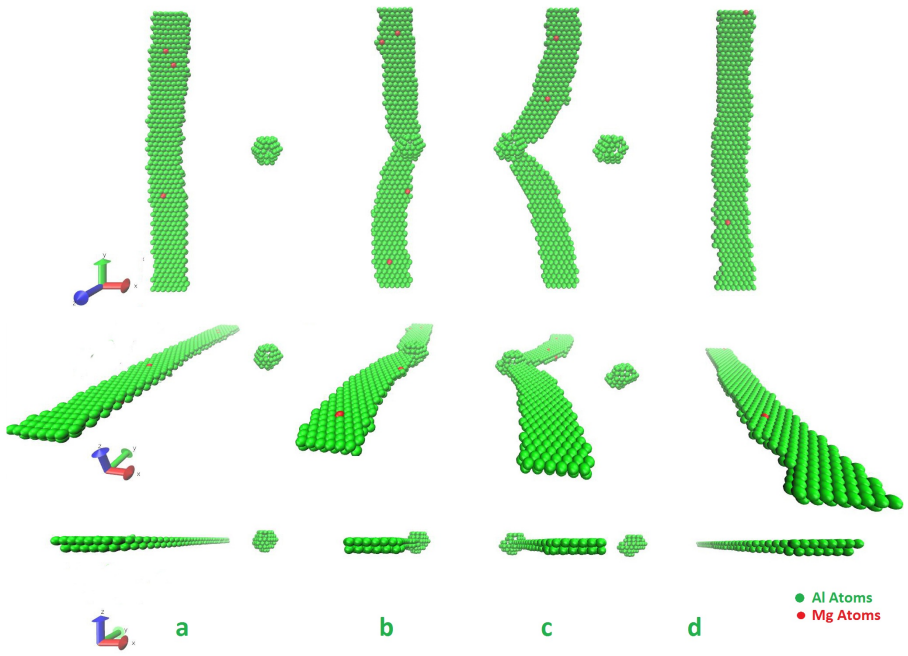

Figure 8: Atomic configuration associated with stages a through d, as marked on the stress strain curve of Fig. 6 in Al-Mg alloy, (a) A, (b) B, (c) C, and (d) D.

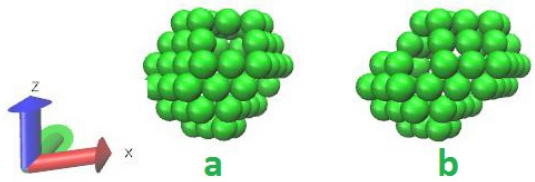

Figure 9: Shape of the void a) before and b) after the passage of the dislocation.

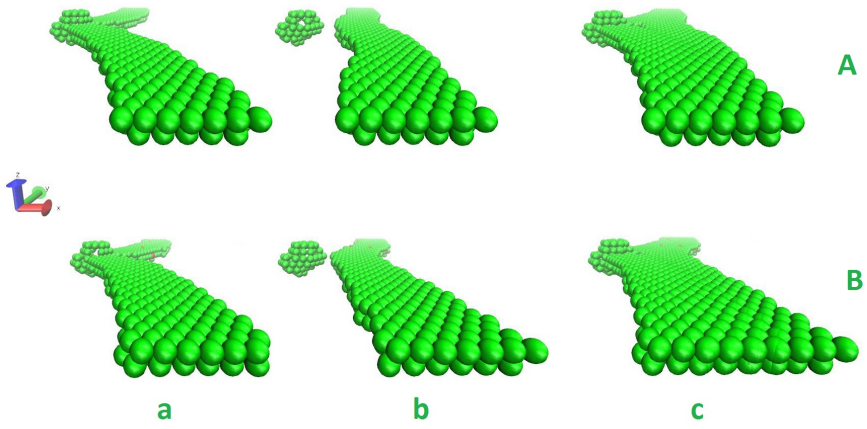

Figure 10: a: bowing out just before the release, b: releasing from the void, and c: this two stages together in A for Al and B for Al-Mg alloy.

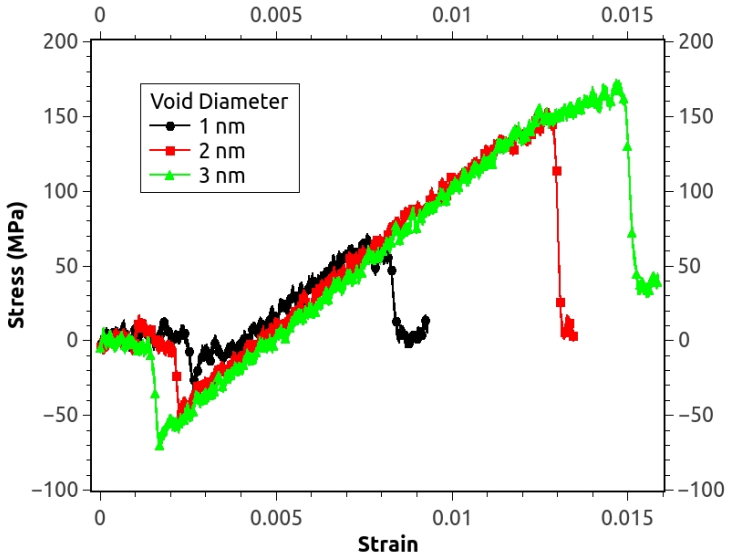

Figure 11: Stress-strain curve of edge dislocation interaction with different void diameter in Al lattice at 300°K with 15nm inter-void spacing.

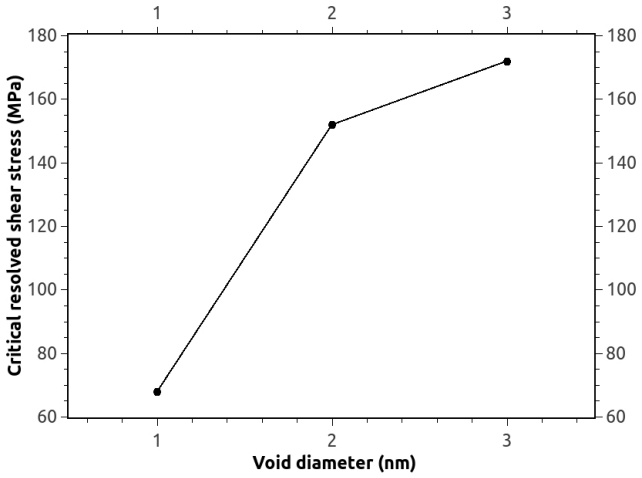

Figure 12: Critical resolved shear stress vs. void diameter in Al lattice at 300°K with 15nm inter-void spacing.

Another parameter that was investigated in this study was inter-void spacing. To obtain the influence of the parameter on the CRSS, the simulation box in the y dimension was halved and stress-strain curve was obtained as shown in Fig.13. It can be seen that by decreasing the inter-void distance the CRSS increased.

To compare these results with the suggested strengthening equations in the frame of the elasticity of the continuum, the following relation was used that reported by Bacon and Scattergood [59, 60], for copper and iron [15, 16, 18, 19], based on the dislocation self interaction stress:

$$\tau_c = \frac{Gb}{2\pi L}[Ln\frac{(D^{-1}+L^{-1})^{-1}}{b}+\Delta] \quad (2)$$

where G is the Aluminum shear modulus for the $< 1\bar{1}0 > 111$ system, which is 24.4 GPa according to our calculations using Mendelev potential, b is Burgers vector, L is the distance between void centers, D is the void diameter and Δ is a constant, which is 1.52 for a void [16]. Fig. 14 confirms that this equation could not be used for aluminum. The reason that the result does not fit to the above equation might be related to the curvature and release angle of the dislocation

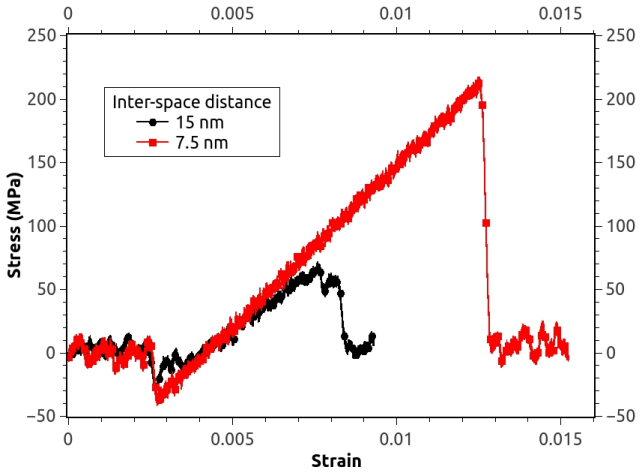

Figure 13: Stress-strain curve of edge dislocation interaction with different inter-void spacing at 300°K obtained by MD calculation in Al.

from void, which depend on temperature and inter-void spacing. While the elastic calculation does not take into account temperature dependence, it is interesting to consider the dislocation morphology temperature dependence, as observed in the MD simulations, and its possible impact on the CRSS. [21]

3.5. Effect of temperature on CRSS

Figs. 15 and 16 show the stress-strain curve of interaction of edge dislocation with 1nm void at 10°K and 300°K in Al crystal and Al-Mg alloy, respectively. Some important points could be understood from these figures. First, from Fig. 15, it can be seen that for pure Al, both the partial dislocations simultaneously passed through the void at 10K, while this occurrence did not happen at 300K. It can be observed that no simultaneous passing of partial dislocations occurred for the Al-Mg alloy (see Fig. 16) which is line with previously reported findings [57] that a higher CRSS is required during simultaneous passing of partial dislocations. Fig. 15 shows that higher than 92 MPa CRSS was required for dislocation-void interaction in pure Al at 10°K. Therefore, irrespective of temperature increment that reduced the required CRSS, this behavior of partial

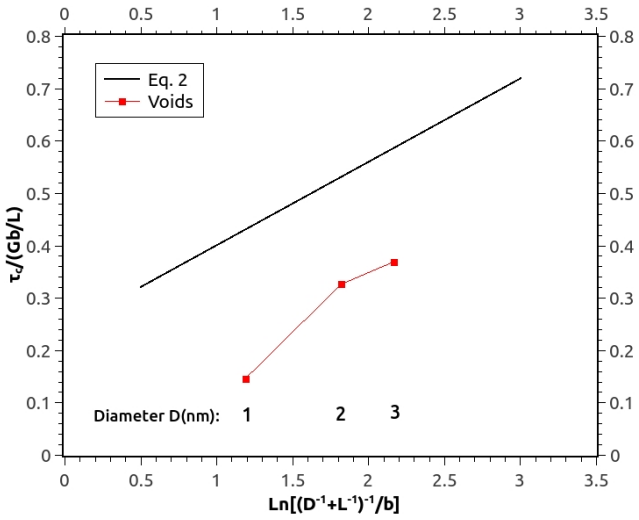

Figure 14: CRSS, scaled by Gb/L vs. harmonic mean of obstacle spacing and void diameter at 300°K in Al. In this figure a solid line plots the Eq. 2

dislocations during interaction with the voids seems to be very important. Second, by comparing both the Figs. 15 and 16 at 300°K (see Fig. 17), it can be observed that Mg solute atoms showed their pinning effects when edge dislocation was passing through the voids. It was mentioned that leading and trailing partial dislocations were separately passed through the void for both the systems at 300K. Third, in contrast with pure aluminum, the temperature effect on CRSS could be clearly seen for Al-Mg alloy. It was reported in literature [15, 16, 18, 19, 21, 22] that around 300K increment in temperature led to a need for a lower CRSS for dislocation-void interaction, due to the higher mobility of dislocation segments.

4. Conclusions

In this study, the interaction of an edge dislocation with nano-scale voids was investigated for pure Al and Al-Mg alloy. From the MD/MS simulation results, the following conclusions can be drawn:

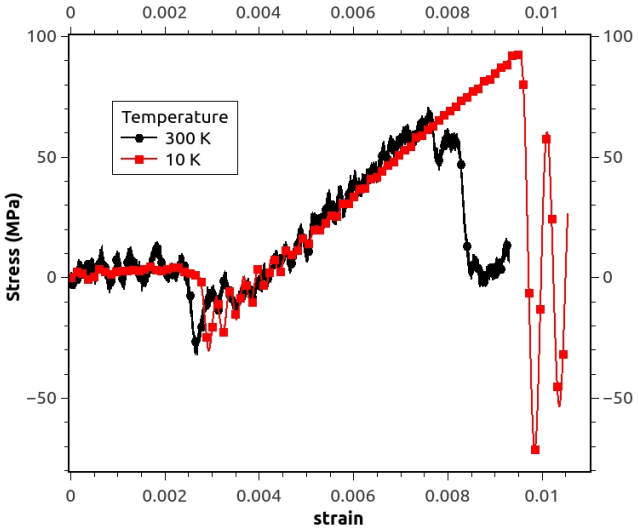

Figure 15: Stress strain curve of edge dislocation interaction with 1nm void at different temperature in Al crystal.

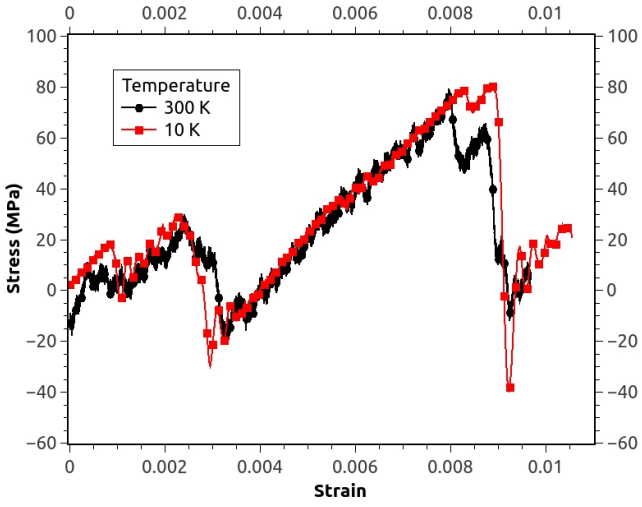

Figure 16: Stress strain curve of edge dislocation interaction with 1nm void at different temperature in Al-Mg alloy.

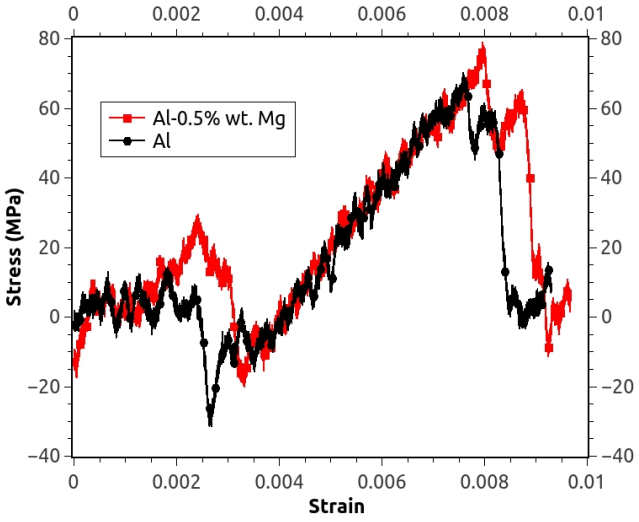

Figure 17: Stress-strain curve obtained by MD simulation of an edge dislocation interaction with 1nm void in Al and Al-Mg at 300°K.

1. It was found that just 0.5% wt. Mg was highly effective on increasing the Peierls stress and CRSS.
2. The type of dislocation-void interaction was changed by replacing of the Mg solute atoms at 10°K, in which separate passing of partial dislocations occurred in contrast with pure Al. This occurrence considerably reduced the CRSS for Al-Mg alloy.
3. It was found that no void-induced climbing occurred at $10°K$ during loading for the systems investigated.
4. Higher void diameter and in particular lower inter-void spacing led to a considerable increase in the CRSS for the pure Al lattice, while the latter changed the type of dislocation-void interaction, in which simultaneous passing of partial dislocations occurred when the inter-void spacing was 7.5nm instead of 15nm.
5. An increase in the temperature from $10°K$ to $300°K$, led to a lower required CRSS for the pure Al and Al-Mg alloy, due to the higher mobility

of dislocation segments.

6. It was shown that the stress required for dislocation motion was decreased for pure aluminum from $0°K$ to $10°K$, while, due to the presence of Mg atoms, different results were obtained for Al-Mg alloy. Mobility of Mg solute atoms that increases by temperature can control the motion of edge dislocation, and thermal activation at elevated temperature can cause easier motion of dislocation. These two factors led to the difference between the results of pure Al and Al-Mg alloy.
7. The Peierls stress increased linearly with increasing Mg solute concentration.

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