Numerical Investigation of Mechanical Properties of Aluminum Alloys at Nanoscale
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Abstract

Nanoindentation is a powerful tool capable of providing fundamental insights of material elastic and plastic response at the nanoscale. Alloys at nanoscale are particularly interesting as the local heterogeneity and deformation mechanism revealed by atomistic study offers a better way to understand hardening mechanism to build a stronger material. In this work, nanoindentation in Al-Mg alloys are studied using atomistic simulations to investigate the effects of loading direction, alloying percentages of Mg via dislocation-driven mechanisms. Also, finite element (FE) nanoindentation simulations are performed using MD tensile test results as input parameters for the FE simulations. Material properties, such as hardness and reduced modulus, are computed from both the FE and MD simulations and then compared. Considering the fundamental difference between these two numerical approaches, the FE results obtained from the present study conform fairly with those from MD simulations. This paves a way into finding material properties of alloys with reduced simulation time and cost by using FE instead of MD. The results have been presented as load-displacement analysis, dislocation density, dislocation loops nucleation and propagation, von-Mises stress distribution and surface imprints. The techniques adopted in this paper to incorporate atomistic data into FE simulations can be further extended for finding other mechanical and fracture properties for complex alloy materials.

Keywords: Al-Mg alloy, Nanoindentation, Molecular dynamics, Finite element, Dislocation

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1. Introduction

Aluminum is one of the major engineering materials and has wide varieties of application in modern technology.\textsuperscript{1–3} Although pure Al is a good conductor for electricity and heat, it is a very soft material which restricts its application in engineering fields that demand high mechanical strength. On the other hand, alloying the Al with different solute atoms such as Mg, Cu, Zn, Si, Mn can improve the properties significantly and makes it possible to apply in different applications. \textit{Al–Mg} and \textit{Al–Cu} alloys are two of the major alloys of Al. Researchers have implemented molecular dynamics simulations to study \textit{Al–Mg} and \textit{Al–Cu} alloys in recent years.\textsuperscript{4–6} The addition of Mg enhances the material properties by the solid solution strengthening\textsuperscript{6} and strain hardening.\textsuperscript{7} Again, Ma \textit{et al.}\textsuperscript{8} studied lattice misfit due to the Cu solute atom in Al metal and concluded that strengthening capability is highly dependent upon the solubility. The inclusion of Cu and Mg in Al structure is found to show improved corrosion resistance and high strength.\textsuperscript{9} These alloys are generally used for construction purposes such as vehicle bodies,\textsuperscript{10} ships,\textsuperscript{11} pressure vessels, cylindrical tanks etc. Application of these alloys have found its way to nano and macro-electronics, which provides further motivation for detailed study of these alloys in nanoscale.\textsuperscript{12}

Nanoindentation has emerged as a powerful tool for the measurement of localized mechanical properties of materials at micro and nanoscale. Nanoindentation also provides useful insights about the shear instability, dislocation source activation, dislocation propagation, phase transformation along with the fundamental material properties such as elastic modulus and hardness.\textsuperscript{13,14} In recent years, nanoindentations are performed on bone, tissue etc. to measure their stiffness and other mechanical properties for application in biomedical science.\textsuperscript{15} It can also be used to measure the local property of both homogeneous\textsuperscript{16} and heterogeneous materials.\textsuperscript{17,18} Furthermore, nanoindentation can provide in depth understanding of incipient plasticity and materials yielding through the dislocation nucleation and propagation in different nanomaterials. Dislocations in Al are pinned through interactions with Mg atoms and thus higher stresses is required for dislocation movement.\textsuperscript{6} Hence the dislocation propagation during nanoindentation in \textit{Al–Mg} alloy should also depend on the distribution of the Mg atom. Similar effects should also be applicable for \textit{Al–Cu} alloys. Detailed study of \textit{Al–Mg} and \textit{Al–Cu} nanoindentation is therefore critical to understand the mechanism of dislocation propagation in Al alloy.
Molecular dynamics (MD) simulation can be an effective method to implement nanoindentation in order to understand different mechanical properties of nanomaterials. The applicability of atomistic approach of nanoindentation to measure material properties and identify incipient plasticity were investigated by Landman et al. MD simulations of Si and SiC nanoindentation showed that, nanoindentation can trigger phase transformation during the loading process. This phase change due to the loading of nano-indenter has been found to have strong dependency with the temperature. With the advancement of MD simulations, researchers implement MD simulations to explain and understand experimental results of nanoindentation. Dislocation pattern in Al <111> surface for different interatomic potentials has been investigated by Lee et al. They explained the nucleation sites, dislocation locks and loops formation just underneath the indenter tip and the prismatic dislocation loops far away from the contact surface. MD study on Al nanoindentation found that, higher temperature results in pre-nucleation of dislocations. MD study of nanoindentation of pure Al revealed the effects of indenter speed, depth and size on dislocation nucleation and propagation. It is concluded from the study, that the surface roughness of the indenter can affect the nature of dislocation nucleation. In case of nanoindentation of Mg, the experimental and MD approach both reveal that, indentations on the basal plane have higher pop-in load and higher displacement than in prismatic plane. Recent works on nanoindentation of polyethylene are focused on calculating their hardness through MD simulation. So, these extensive nanoindentation studies through MD simulations point out to the fact that, atomistic approach of nanoindentation for Al alloys is expected to yield accurate and consistent material properties at nanoscale.

One of the main disadvantages of MD simulation is that it is computationally expensive compared to other numerical approaches of nanoindentation. On the other hand, Finite element method (FEM) is computationally less demanding. In recent years, there have been a wide implementation of FEM for nanoindentation simulations to characterize the mechanical properties at the bulk scale. Modeling nanoindentation for bulk material and thin film using FEM has been conducted by Bressan et al. Their modeling was conducted by using axisymmetric CAX4R element with a cylindrical substrate. FEM studies showed that, the modulus and yield strength of material significantly influence the load-displacement curve (known as P-h curve). Using the FEM technique, it is possible to model the nanoindentation for the nanoscale material. However, the major challenge for this is the availability of experimental tensile test data for the material at the
nanoscale. Though the tensile test data of the materials are more or less known for common engineering materials, their mechanical properties such as yield stress, fracture strain, etc. have different values at the nanoscale\textsuperscript{34–36} which can be attributed to the size effects. Therefore, modeling of nanoindentation using FEM, where the indentation depth is as low as few nanometers, will give erroneous results and cannot be compared with the atomistic results. To solve this problem, the mechanical properties obtained from MD tensile test can be used in FEM approach of nanoindentation.\textsuperscript{37} Using this same approach, Mojumder \textit{et al.}\textsuperscript{26} conducted a systematic study of pure Al nanoindentation for different crystallographic orientations, indentation depths, indentation speeds and indenter sizes. Their study provides a pathway to obtain the materials properties for nanoscale materials without performing large scale atomistic simulation using FEM in conjunction with MD. However, this approach has not yet been implemented on metal alloys to investigate the mechanical properties and the effects of alloying percentage on the dislocation behavior during nanoindentation.

In the present study, a systematic investigation of the atomistic nanoindentation of \textit{Al-Mg} alloy for different crystallographic orientations and alloying percentages of \textit{Mg} has been conducted. The modeling method of \textit{Al-Mg} and \textit{Al-Cu} alloys for MD study has been adopted from numerous previous works.\textsuperscript{4,5,38,39} The effects of these parameters on the dislocation nucleation, propagation mechanism and material properties such as hardness and reduced modulus have been discussed (section 3.1). Then, tensile test simulations have been performed to obtain the mechanical properties such as elastic modulus, yield strength and Poisson’s ratio of the alloy material (section 3.2). Using these material properties, FEM nanoindentation simulations have been carried out to compare the FEM results with that obtained from MD simulations (section 3.3). Similar analysis for \textit{Al-Cu} alloy have been carried out as well and the results are presented in the supplementary of the paper.

2. Methodology

In this study, we employ both MD and FE simulations to understand the effects of different crystallographic orientations and alloying percentages on the nanoindentation of \textit{Al-Mg} alloy. In order to compare the atomistic results with the FE simulations we use the material properties obtained from MD tensile tests as the input parameters of the FE simulations.
2.1 Atomistic simulation procedure

For the atomistic simulation, a box of $Al$ atoms with appropriate dimensions is created. Then the $Al$ atoms are randomly replaced by $Mg$ atoms based on their weight percentages, which is varied in the range of 0 - 10%. In a future work, this methodology has been extended further to develop a nanohub tool for building functionally graded materials. In the present study, we consider three different crystallographic orientations as for loading in $<0 \ 0 \ 1>$ direction ($<0 \ 1 \ 0>$, $<0 \ 1 \ 0>$, $<0 \ 0 \ 1>$), $<1 \ 1 \ 0>$ direction ($<1 \ 1 \ 1>$, $<1 \ 1 \ 2>$, $<\overline{1} \ 0 \ 0>$), and $<1 \ 1 \ 1>$ direction ($<\overline{1} \ 1 \ 0>$, $<1 \ 1 \ 0>$, $<1 \ 1 \ 1>$) in our present simulations. The dimensions and total number of atoms of the simulation box used for these three different crystallographic orientations are presented in Table 1.

Table 1: Simulation parameters used for the atomistic simulations

| Crystallographic orientation | $Mg$ % | Simulation box dimension | Number of atoms |
|------------------------------|--------|--------------------------|-----------------|
| $<001>$                      | 0,1,2,5,10 | 22.2 nm $\times$ 22.2 nm $\times$ 16 nm | 484000          |
| $<110>$                      | 0,1,2,5,10 | 24.55 nm $\times$ 23.14 nm $\times$ 14.31 nm | 488364          |
| $<111>$                      | 0,1,2,5,10 | 20.05 nm $\times$ 23.18 nm $\times$ 17.53 nm | 487363          |

As shown in Fig. 1, the simulation box is divided into two distinct regions. The spherical indenter penetrates the upper region. The bottom region of 2 nm thickness provides a rigid support for the substrate. Also, this region consisting of fixed atoms (also called Newtonian atoms) functions as a heat bath during the penetration of the indenter in the upper region. The rigid indenter (virtual indenter in LAMMPS) of 5 nm radius was then set up over the substrate and the indenter was pushed into the material, as shown in Fig. 1. The indenter exerts a force of magnitude, $F(r) = -K(r-R)^3$ on each atom where $K$ is the specified force constant, $r$ is the distance from the atom to the center of the indenter, and $R$ is the radius of the indenter. The force is repulsive and $F(r) = 0$ for $r > R$. In all of the simulations force constant is considered as 1 eV/Å$^3$. The loading step is followed by an unloading step adopting displacement control of the indenter. After every time step, the system has been minimized using conjugate gradient method in order to maintain the quasi-static loading process at 0 K temperature. The speed of the indentation is set to 50 ms$^{-1}$ and the indentation depth is kept as 2 nm. The same parameters are also considered for the modeling of $Al-Cu$ alloy. These parameters have also been successfully applied in a previous study of pure $Al$.26
The interactions between all the atoms within the simulation domain are described by the embedded atom method (EAM) potential \(^\text{42,43}\), which was used extensively for the \(\text{Al-Mg}\) alloy previously.\(^\text{44,45}\) In this method, the potential energy of an atom, \(i\), is given by:

\[
E_i = F_\alpha \left( \sum_{i \neq j} \rho_{\alpha\beta}(r_{ij}) \right) + \frac{1}{2} \sum_{i \neq j} \phi_{\alpha\beta}(r_{ij})
\]

where, \(r_{ij}\) is the distance between atoms \(i\) and \(j\), \(\phi_{\alpha\beta}\) is a pairwise potential function, \(\rho_{\alpha\beta}\) is a functional specific to the atomic types of both atoms \(i\) and \(j\), so that different elements can contribute differently to the total electron density at an atomic site depending on the identity of the element at that atomic site, and \(F_\alpha\) is an embedding function that represents the energy required to place atom \(i\) into the electron cloud. \(\alpha\) and \(\beta\) are the element types of atoms \(i\) and \(j\) respectively. In case of \(\text{Al-Cu}\) alloy, embedded atom method (EAM) potential\(^\text{46}\) has been used to describe interatomic interactions.

The present interatomic potential and nanoindentation procedure have been previously verified by comparing the MD load-displacement curves in case of pure \(\text{Al}\) with Hertzian contact theory for all three directions considered in the present study.\(^\text{26}\) The hardness and the indentation modulus were then calculated from the load-displacement curves using the Oliver-Pharr method.\(^\text{47}\) This method of calculating hardness and indentation modulus was implemented by Mojumder \textit{et al}.\(^\text{26}\)

As the indenter penetrates the materials, plastic deformation occurs, and dislocation loops are formed. We have calculated dislocation density using OVITO\(^\text{48}\) as a measure of plastic deformation in the indentation process using the DXA algorithm. The dislocation segments have been identified using a trial circuit of 14 x 9 and total dislocation length is then divided by the total volume of the substrate to obtain the dislocation density.

In order to simulate the nanoindentation problem in FE platform, the material properties obtained from the MD tensile test simulations have been used as input properties. The uniaxial tensile test simulations are performed for \(\text{Al-Mg}\) nanowires with the orientations mentioned above and different \(\text{Mg}\) weight percentages. The nanowires have square cross section and a dimension of 5 nm x 5 nm x 50 nm in X, Y, and Z direction, respectively. The loading direction is kept similar to the nanoindentation simulation. The aspect ratio (height: width) of all the nanowires is kept constant as 10:1 and the tensile load is applied in the \(z\)-axis of the co-ordinate system (crystal
directions of \(<0\ 0\ 1>\), \(<1\ 1\ 0>\) and \(<1\ 1\ 1>\). First, the initial geometries of the nanowires are created and the pressure of the system is equilibrated by applying the isothermal-isobaric (NPT) ensemble in \(z\)-direction at 1 bar and a temperature of 300 K for 100 ps. Finally, a uniaxial strain is applied along the \(z\)-direction of the nanowire at a constant strain rate of \(10^8\ s^{-1}\). The timestep chosen for all the simulations is 1 fs. From the tensile simulations, the stress-strain curve is obtained and the elastic modulus, yield stress and Poisson’s ratio are calculated. These results of tensile tests are then further used as the input properties in the finite element (FE) simulations. All the MD simulations are performed using LAMMPS,\(^{41}\) and visualization is done using OVITO.\(^{48}\)

### 2.2 FE simulation procedure

The purpose of the FE simulation is to get a reasonable estimation for the materials’ properties such as hardness and reduced modulus with a lower computation time than atomistic simulation. ABAQUS/Standard\(^{49}\) has been used for the FE simulations considering a deformable axisymmetric material model with a rigid indenter. The dimensions (10 nm radius, 15 nm height) of the substrate considered is the same as the atomistic simulation model and the input materials properties (elastic modulus, Poisson’s ratio, yield stress) are obtained from the molecular dynamics tensile tests of Al-Mg alloy nanowire as described in section 2.1. The material is modeled using the four-node axisymmetric element with reduced integration (CAX4R) and the indenter has been considered as analytically rigid. The indenter is pushed into the materials’ substrate using a displacement control boundary condition. The left vertical edge of the materials has been considered as the symmetric edge and the bottom of the substrate is fixed as shown in Fig. 3. The top and right vertical edges are kept free to resemble the free surface. We choose 13299 elements as an independent grid and performed all finite element simulations for that. A fine mesh is used in the contact region of the substrate and indenter and a coarse mesh is used where the contact did not occur. The mesh and numerical code used for the present study has been validated previously by Mojumder et al.\(^{26}\) From the load-displacement curve obtained from the FE simulation, the similar procedure has been used as atomistic calculation for the calculation of the materials properties such as hardness and reduced modulus.
3. Results and Discussion

3.1 Atomistic results of nanoindentation on Al-Mg alloys

3.1.1 Effects of alloying on P-h curves and dislocation density

The load–displacement curves for different alloying percentages of Mg in Al are shown for different loading directions considered in the present study in Fig. 4. In case of all considered loading directions, it is observed that the load carrying capacity is increased with the inclusion of Mg in the alloy. This is due to the fact that, as the foreign atoms of Mg replaces the host atom of Al in the alloy, it results in solid solution strengthening. The atomic misfit of Al and Mg crystals are responsible for this. At 0 K, the lattice constants of Al and Mg are 4.05 Å and 3.21 Å, respectively. Hence the lattice misfit between Al and Mg is ~21%, which significantly alters the material properties of Al-Mg alloy from pure Al. This phenomenon of material property alteration due to lattice misfit has been reported in previous studies. Furthermore, the atomic size of Mg is larger than the atomic size of the Al. When Mg atoms replace Al atoms from a crystal, these create strong localized tensile strain regions inside the crystals. Therefore, when a dislocation tries to move through this stress field, it requires higher strength to propagate further. The present result of solution strengthening due to inclusion of Mg in Al is in agreement with previous studies. Also, indentation by its nature, induces compressive stress, which gets neutralized by the localized tensile stress region in the Al-Mg alloy. As a result, the material shows some hardening effect and the load increases significantly. The results also show that, the Al-Mg alloy is capable of carrying higher load during the indentation compared to pure Al. Similar phenomenon has been observed in case of Al-Cu alloy as well. Cu inclusion in pure Al increases load carrying capacity (see Fig. S1). However, the dislocation activities are more pronounced in the Al alloys compared to that in pure Al in <111> loading direction. In Fig. 5, the dislocation density for different percentages of Mg addition is shown for different orientations of loading. For <001> and <110> loading directions, the dislocation density is higher for the 5% of Mg addition compared to other alloying percentages. On the other hand, for <111> direction, the maximum dislocation density occurs for 1% of Mg addition. It is also observed from Fig. 5 (a), (b) and (c) that, when the loading direction is <001> the dislocation densities for different Mg alloy percentages are much higher than those of the other two loading directions considered in the present study. From Fig. 5(c), it is evident that, there are no dislocations during the initial indentation period, in case of <111> loading.
direction. When the displacement of the indenter reaches from 0.5 to 0.75 nm, the dislocation density starts to increase with the displacement following almost a linear trend. On the contrary, the dislocation density changes less significantly with change in indenter displacement in case of <001> and <110> loading directions, as shown in Fig. 5(a). In case of Al-Cu alloys, the dislocation density decreases with displacement and then increases again for all loading directions (see Fig. S2). Therefore, in case of Al-Cu alloys initial displacement strengthens the alloy nanostructure.

3.1.2 Effects of alloying on formation of dislocation loops

In Fig. 6, the dislocation loops are shown for the different percentages of Mg atoms for different orientations considered in the present study. It is observed from the figure that for <001> direction, with the increment of alloying element, the dislocation loops are increased. This increase of dislocation loop with increasing Mg alloy percentage is also indicated in Fig. 5(a). At 1% Mg addition, a separated prismatic loop is visible. The dislocation networks become more dispersed throughout the material with increase in percentage of Mg. However, in <110> direction, this kind of extensive dislocation network is not visible, and in some cases, addition of Mg can blunt the dislocation loop and hinders its propagation. A comparison between Fig. 6(g) and (h) shows that, the increase in Mg weight fraction hinders the propagation of dislocation although the number of dislocations is higher for 2% Mg alloy compared to that of 1% Mg. At higher percentages of Mg, the dislocation loops move towards the bottom of the substrate. For <111> direction it is found that the dislocation loops are reduced with the higher percentage of the solute atom Mg. Overall, it can be seen from Fig. 6 that new dislocation loops seem to originate rather than lengthening of the loops near the indenter, which is a manifestation of solid solution hardening within the material.\textsuperscript{50} From Fig. 6(e), (j) and (o), it is apparent that, dislocation due to inclusion of Mg is more prominent in <001> loading direction during nanoindentation. The dislocation loops for different percentages of Cu atoms in Al show similar trend (see Fig. S3).

3.1.3 Effects of alloying on hardness and reduced modulus

Variation of hardness and reduced modulus with Mg weight percentage are shown for different loading directions, in Fig. 7(a) and (b) respectively. There are no distinct patterns in the hardness and reduced modulus values as the distribution of Mg in alloy is quite random. For <001> direction, the maximum hardness is found for 5% Mg, while for <110> the hardness is maximum for 1% Mg. Again, in <111> direction the maximum hardness is obtained for 10% of Mg. Although
there might be statistical variation in the results, for the given distribution of $Mg$ in the alloy, for $\langle 001 \rangle$ direction, $2\text{-}5\%$ $Mg$ shows better hardness, for $\langle 110 \rangle$ direction, better hardness is obtained for low $Mg$ content (1-2%) and for $\langle 111 \rangle$ direction better hardness is expected for 5-10% of $Mg$ addition. On the other hand, the reduced elastic modulus shows that the modulus is reduced for all the direction at 1% $Mg$ addition. With the higher amount of $Mg$ addition (2-10%), the reduced elastic modulus again increases for all directions of loading. The hardness and reduced modulus variation with $Cu$ percentages have been shown in Fig. S4.

3.1.4 Effects of alloying on von Mises stress distribution and surface imprint

In Figs. 8 and 9, the von Mises stress distribution are shown for the maximum loading position and after the unloading process, respectively. For pure $Al$, the stress is mostly localized where the indentation occurred for both maximum loading and unloading processed. But in $Al$-$Mg$ alloys, there are presence of a number of localized tensile stress regions that spread across the whole alloy structure. This presence is due to the difference between $Mg$ and $Al$ atomic sizes, which in turn creates localized tensile stress zones. It is observed that at the maximum loading depth, the stress distribution is non-symmetric. This is due to the fact that, different slip planes become activated and the dislocations are propagated along the different planes disregarding any symmetry. As a result, the stress distribution is different in different positions of the material which clearly indicates the anisotropy of this alloy. The $Mg$ atoms present in the alloys act as anchors for stress and alter the dislocation glide plane and somewhat increase the strength. From the unloading results, it is quite obvious that the residual stress is increasing with the percentage of $Mg$ in the alloy. Another observation from Figs. 8 and 9 is that, Von Mises stress distribution is more uniformly distributed for alloys with higher percentage of $Mg$. This indicates that the alloying makes the material better at supporting the load throughout the section and not just the plastic deformation within the imprint zone. Besides, Von Mises stress distributions for maximum loading and unloading for different $Cu$ percentages and loading directions have been included in the supplementary section (see Fig. S5 and S6).

The surface imprints for the alloys are shown in the Fig. 10. It is observed that with the higher alloying element percentage, the pile up phenomenon becomes more obvious. This is true for all three directions of $\langle 001 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$. However, with the lower $Mg$ percentages, the imprint shows more critical depths. Besides, for $Al$-$Cu$ alloys, surface imprints after maximum
loading for different Cu percentages and loading directions have been included in the supplementary section (see Fig. S7).

### 3.2 Tensile loading on Al and Al-Mg nanowire

Tensile test simulations are performed for pure Al and Al-Mg nanowires made with different percentages of the alloying element to obtain the tensile properties. From the tensile test data, the stress-strain curve is drawn which is used to determine the material properties which are further used for the finite element nanoindentation simulation. In Fig. 11, the stress-strain curves are shown for different percentages of Mg and loading in different directions considered in the present study. For all directions, there is no presence of serrations in the stress strain curves after failure, which indicates pure brittle fracture. With the increase of Mg percentage, the failure stress and strain are increased for <001> loading direction. As shown in Fig. 11(a), the maximum failure strain and strength are obtained for the 2% Mg. Therefore, alloying Mg in pure Al clearly enhances the mechanical properties of the Al structure in case of <001> loading direction. For <110> direction, the stress strain diagram shows some minor yielding phenomena before the fracture in case of different Al-Mg alloys. Here, the ultimate stress is the highest for pure Al with strength decreasing as the amount of Mg increases. The fracture strains of Al-Mg alloys are also lower than the pure Al case except that, for 1% Mg, the strain is higher than pure Al. The 5% Al-Mg alloy nanowire shows the lowest stress and fracture strain. This result shows that, along <110> direction, alloying Mg with Al does not necessarily result in improved mechanical properties. For <111> loading direction, the ultimate stress is highest for 10% Mg content and other alloying element percentages yield lower strength than the pure Al case. However, the fracture strain of pure Al is the lowest among all of the five cases. It can be summarized that among the three directions, <001> shows the highest materials strength and fracture strain.

The materials properties obtained from these stress-strain curves are presented in Table 2.

| Loading directions | Mg (%) | Elastic Modulus (GPa) | Yielding Strain (%) | Yield Stress (GPa) |
|--------------------|--------|-----------------------|---------------------|-------------------|
| <001>              | 0      | 113.6                 | 4.5                 | 3.955             |
|                    | 1      | 84.58                 | 6.6                 | 3.816             |
|                    | 2      | 86.42                 | 6.0                 | 3.598             |
3.3 FE results of nanoindentation on Al-Mg alloy

3.3.1 Effects of alloying on P-h curves, hardness and reduced modulus

The FE simulations are done considering the nanoindentation problem as a 2D axisymmetric problem for convenience and the potential to solve the problem with less computation effort. The material properties used for FE simulations are obtained from the aforementioned (section 3.2) tensile tests of pure Al and Al-Mg alloy nanowire using the MD method. Therefore, the same dimension scale has been used in the FE simulations to safeguard from the size effects.\(^{51}\) Al and Al-Mg alloy are modeled in FE considering them as isotropic homogeneous materials. From the nanoindentation simulations of the FE analysis, the load displacement curve is obtained and after analyzing the load displacement curve the material properties such as hardness and reduced modulus are calculated. In Fig. 12(a), (b) and (c), the load-displacement curves obtained from the FE simulations for Al and Al-Mg alloy are shown for indentation in different directions of \(<001>\), \(<110>\) and \(<111>\), respectively. It is observed that for \(<001>\) direction, the indentation force is maximum for 2% Al-Mg alloy which is similar to the results obtained from the MD simulations. Although the magnitudes of the forces obtained from the FE simulations are very similar to those obtained from MD simulations, the trends obtained from both the methods are different. This could be due to the difference in boundary conditions in the two approaches. Although, the boundaries are assumed to be periodic in MD, that is not the case in FEM. The discrepancies may also be for assuming the material is axisymmetric.
From the load-displacement curve obtained from the FE simulations, Oliver-Phar method is used to extract the material properties such as hardness and reduced modulus following the same method used in the MD part of the study. The variation of hardness and reduced modulus with $Mg$ percentage is shown in Fig. 13 for different loading directions. It can be observed from the figure that the values of hardness and reduced modulus, obtained from both the methods, are very similar in magnitudes for all the three loading directions and different $Mg$ percentages.

3.3.2 Comparison of FE results with MD results

The primary motivation of performing the FE analysis is to obtain the material properties with less computational time and cost. To validate the approach, results obtained by the FE simulations are compared with the previous results of MD.

The comparison of MD and FE load-displacement curves for the $Al-Mg$ alloy consisting 1% $Mg$ in $<001>$, $<110>$ and $<111>$ loading directions are presented in Fig. 14. The load-displacement curves show good agreement between MD and FE results. It is observed from these figures that there are some fluctuations in the MD indentation curves. These fluctuations are due to the plastic event such as dislocation nucleation, interactions and propagation inside the materials. However, the curves obtained from the FE simulations do not show such variation as the material is modeled considering an isotropic material. In MD, the material yielding, and plastic phenomenon can be more accurately predicted than the FE modeling. However, considering the fact that MD takes longer computation time and is limited in length scale, applying FE analysis for nanoindentation problems are useful, especially when just considering the material properties such as hardness and elastic modulus and not the dislocation mechanisms. For $<001>$ and $<111>$ directions, FE can successfully predict the load-displacement relation well up to indentation depth of 0.3nm displacement in the $P - h$ curves. In case of $<110>$ direction, FE P-h curve conforms with MD up to 1.2nm. In Fig. 12 the slopes of the unloading curves are also similar to the MD results. As a result, the obtained material properties are very close and in good agreement with each other.

The results obtained by the MD and FEM are shown for $Al-Mg$ in Table 3 showing that the obtained hardness and reduced modulus results are in good agreement.
Table 3: Comparison of hardness and reduced modulus for Al-Mg alloy at different percentage of Mg and at different direction of loading obtained by MD and FEM simulations.

| Direction | Mg Percentage | Hardness (MD) GPa | Hardness (FEM) GPa | Reduced modulus (MD) GPa | Reduced modulus (FEM) GPa |
|-----------|---------------|-------------------|-------------------|--------------------------|--------------------------|
| <001>     | 0             | 13.86             | 11.29             | 211                      | 97.68                    |
|           | 1             | 12.47             | 11.87             | 145.89                   | 118.09                   |
|           | 2             | 14.07             | 14.62             | 257.38                   | 130.72                   |
|           | 5             | 14.21             | 13.83             | 194.42                   | 126.58                   |
|           | 10            | 12.90             | 11.83             | 233.36                   | 118.88                   |
| <110>     | 0             | 12.47             | 10.88             | 204.04                   | 157.28                   |
|           | 1             | 14.26             | 10.69             | 154.32                   | 155.41                   |
|           | 2             | 14.00             | 09.59             | 231.44                   | 159.64                   |
|           | 5             | 12.61             | 09.00             | 206.22                   | 158.28                   |
|           | 10            | 13.18             | 09.05             | 209.79                   | 151.54                   |
| <111>     | 0             | 13.93             | 10.33             | 220                      | 164.41                   |
|           | 1             | 11.81             | 09.59             | 185.93                   | 116.24                   |
|           | 2             | 12.71             | 09.14             | 226.15                   | 117.24                   |
|           | 5             | 13.78             | 08.95             | 271.47                   | 105.17                   |
|           | 10            | 14.12             | 08.95             | 234.54                   | 105.17                   |

4. Conclusions

In the present study, nanoindentation simulations are performed for pure Al and Al-Mg alloys of different Mg weight percentages and in different loading directions. Both FE simulations and MD simulations are carried out to calculate the material properties such as hardness and reduced modulus. The input parameters of the FE simulations, have been obtained by performing tensile tests on pure Al and Al-Mg nanowires using MD simulations. The FE nanoindentation simulations are then performed, and their results have been compared with the MD simulation results where good agreement has been found. The technique of implementing finite element modelling at nanoscale is very advantageous because significantly less computational time is required compared to the MD simulations without sacrificing the accuracy in the results. From the results, the following conclusions can be drawn:
For $Al-Mg$ alloy, the addition of $Mg$ results in solid solution strengthening and creates local strain field inside the $Al$. This strain field creates energy barrier for the dislocations to move along its slip plane and forces the dislocations to choose energetically favorable slip plane at a higher strength than previous. The hardness and reduced modulus values vary with the different percentage of $Mg$ for different crystallographic directions.

We have observed that there are no dislocations during the initial indentation period, in case of $<111>$ loading direction for any of the $Al-Mg$ alloys.

For $<001>$ loading direction, the dislocation loops increase with increment of alloying element, and also become more dispersed throughout the material. As a result, dislocation densities and hence solid solution strengthening effects are maximum for this loading direction.

In $Al-Mg$ alloys, the stress distribution is different in different positions of the material, since the distribution of $Mg$ atoms in the structure is random, and the $Mg$ atoms act as the stress anchors which makes the alloy anisotropic.

Implementing the MD tensile test data makes it possible to obtain the hardness and reduced modulus value from FEM and compare it with the MD results. The comparison showed that the load-displacement curves obtained for all the $Al-Mg$ alloys are in fairly good agreement with the MD results considering that FE simulations is a macroscopic view into this nanoscale phenomena. In this way, both the simulation time and cost can be reduced with trivial sacrifice of the accuracy in the results obtained from the MD.

In case of $Al-Cu$ alloys, during initial indentation, the dislocation density decreases and then increases again, which points out to the strengthening mechanism during initial indentation.

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Supplementary Material

Effects of Cu percentage and loading direction on Al-Cu alloy P-h curves and dislocation density

Al-Cu alloy is one of the major alloy of Al which has wide range of applications. Typically, the percentage of Cu in Al-Cu alloy can be as high as 10% for improved properties. Here, the samples are prepared for 1, 2, 5, and 10% of Cu addition by supplanting the Al atom by weight percentage. In Fig. S1, the load-displacement curve is shown for the different Cu percentage in the Al. In the <001> direction, lower percentage of Cu addition can carry higher load compare to the higher percentage of the Cu. The yielding point is distinct for different alloying percentage. In <110> direction, alloying does not improve the materials property as it can be seen that the indentation load is maximum for the pure Al. Therefore, it is expected that pure Al in <110> direction will show higher hardness value compared to its alloys. In the <111> direction, the lower Cu percentage is able to carry the higher load which is similar to the <001> direction. Here, the yield points are very close for pure Al, and different percentage of Al-Cu alloy.

The variation of dislocation density during the indentation loading is shown in Fig. S2 for different orientations of alloying. It can be seen from the figure that there are three distinct regions in the dislocation density curve: dislocation increases with load, dislocations experience a fall, become stable and dislocation density increases again. This pattern of the curve can be explained by the solid solution strengthening mechanism. We already know that with the loading, the dislocation nucleates and multiplies. But when there are presence of Cu atoms in the Al crystals, it creates a localized stress field which anchors the dislocations movement. As a result, sudden fall in the dislocation density is experienced. With further loading, the critical shear stress is achieved and further pushes the dislocation. As a result, dislocation density increases again after a certain indentation depth for the alloy. As the Cu atoms are randomly placed, this makes the dislocation activity a complex phenomenon. Though the hardness and dislocation density can be correlated, it is more convenient to see the dislocation activity separately from material hardness.

Effects of Cu percentage and loading direction on Al-Cu alloy dislocation loops formation

The dislocation loops produced at the maximum loading position for different percentage of Cu is shown in Fig. S3. It can be seen that indentation in <001> direction have more dislocations compare to the other direction. Some of the dislocation loops are separated from the main loops under the indenter. Besides, there are some other loops in different slip planes. With the addition of Cu, it is visible that the dislocation loops are decreasing due to the fact of solid solution hardening. The maximum dislocation loops are found for the
5% $Cu$ addition in $<001>$ direction. In $<110>$ direction, the dislocation loops try to separate and form a prismatic dislocation loops along the indentation axis. When $Cu$ is added in this direction, dislocation also nucleates from the other position of the substrate. In the $<111>$ direction, $Cu$ addition shows some significant results. For 1 and 2% of $Cu$ addition, some blunting front in dislocation loops are visible but for the other $Cu$ percentages, the dislocation loops are able to propagate.

**Effects of $Cu$ percentage and loading direction on $Al$-$Cu$ alloy hardness and reduced modulus**

Figure S4 shows the variation of the hardness and reduced modulus with the variation of $Cu$ percentage. For the $<111>$ direction, the maximum hardness is found for the 5% of $Cu$ addition. However, hardness reduces significantly when the $Cu$ percentage is around 10%. For $<001>$ direction, higher hardness is observed at low $Cu$ percentage and afterwards, the hardness decreases with the $Cu$ addition. Similar trend is found for the $<110>$ direction. This direction shows a unique result that addition of $Cu$ reduces the hardness of the alloy and pure $Al$ shows maximum hardness for this direction. The reduced modulus are generally higher for the $<111>$ direction. Reduced modulus in the $<110>$ is lower than the $<001>$ direction for the different percentage of $Cu$ addition.

**Effects of $Cu$ percentage and loading direction on $Al$-$Cu$ alloy von Mises stress distribution**

In Fig. S5 and S6, von Mises stress distribution are shown for different percentage of $Cu$ and for different direction. As it can be seen that the stress field are symmetric for $<001>$ and $<110>$ direction. But there is significant stress anisotropy when the alloying elements are added in (111) direction. Moreover, the localized stress distributions are found for the $Cu$ add atoms. After unloading, $<110>$ and $<111>$ direction of alloying retain more residual stress compared to the $<001>$ direction.

**Effects of $Cu$ percentage and loading direction on $Al$-$Cu$ alloy surface imprint**

The surface imprints after indentation in $Al$–$Cu$ alloys are shown in Fig. S7. The pile up effect is more prominent for the pure $Al$ in all directions of loading. With the higher amount of $Cu$ addition, there are less pile up phenomena visible and the critical indentation depth reduces. Among the three directions, the $<111>$ direction shows the less critical depth.
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