Failure Mechanisms and Scaling Laws of Nanoporous Aluminum: A Computational Study**

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Recent nanomechanical experiments and simulations reveal a ligament size-dependent effect on the strength of nanowires, nanocolumns, and nanofoams. Here, we show the failure mechanism and scaling laws of nanoporous aluminum (np-Al) using a molecular dynamics case study. We develop scaling laws for Young’s modulus, yield strength, ultimate strength, and toughness with respect to relative density and ligament diameter for np-Al. Our findings offer useful insights into the knowledge of nanoporous metals’ mechanical properties in order to support material scientists’ intention of developing fully comprehensive scaling laws for nanoporous metals.

1. Introduction

In 1959, Richard Feynman endorsed the advancement of nanoscience in a well-celebrated speech “There is plenty of room at the bottom.” As the ability for us to see and manipulate matter at the nanoscale continuously increases, the use of nanomaterials is moving from opportunistic to deliberate through design, creation, and implementation.[1,2] This is very evident in the case of nanoporous materials (np-materials) where control over not just the porosity but of the pore and ligament dimensions is now possible.[3–5] A class of np-materials, np-metals, has gained public interest by showing great promise in areas such as catalysis/electrocatalysis,[6,7] fuel cell technologies,[8] molecular sensing,[9] actuation,[10] surface-enhanced Raman scattering,[11] and plasmonics[12] to name a few. The most popular np-metals at the moment are made from the most chemically noble metals (gold, palladium, nickel, platinum, etc.) because they lend themselves to the easiest and least expensive chemical process used to form np-metals: chemical/electrochemical dealloying.[3,4,13–15] However, just recently the first incident of synthesized np-aluminum (not alumina, aluminum oxide, or anodic aluminum) by dealloying was reported by Suarez et al.[13] This breakthrough only incentivizes us to more closely study the properties of np-aluminum, so that this material can be used to its fullest extent.

Aluminum itself is prized for its low density, ability to resist corrosion, and large plasticity.[16,17] These qualities have made aluminum an important material in construction and transportation. The metal is also part of an important group of materials suitable for applications at cryogenic temperatures; in the most extreme of cases aluminum is used on the circuit boards of quantum computers that operate at temperatures around 500 mK.[18] Now with the advent of np-aluminum and other np-metals, it is of considerable importance to investigate their properties as we get closer to the day when bulk np-metals can be made en masse for general use.

Biener et al. found a yield strength for np-Au that was 10 times higher than Ashby-Gibson scaling laws predicted and raised the question whether the scaling laws deduced from macroscopic foams can be applied to nanoporous materials.[19] Later, Biener et al. demonstrated that the strength of metal foams can be enhanced by reducing the length-scale of ligaments and pores.[20] Volkert et al. also reported that yield stresses of gold nanocolumns increase strongly as ligament diameter decreases.[21] To et al. studied size effects in np-Al using molecular dynamics simulations on np-Al models created by deleting overlapping spherical regions in a cube.[22] Sun et al. used molecular dynamics simulations on np-Au models created by phase-field modeling in order to study failure mechanisms and scaling laws of np-Au.[23] In 2014, Suarez et al. fabricated the first sample of dealloyed np-Al.[13] Here, we further the efforts by studying the effects of density, ligament diameter, and temperature on the mechanical properties np-Al via molecular dynamics. This paper analyzes the failure mechanism of np-Al and then moves on to develop scaling equations and trends for young’s modulus, yield strength, ultimate strength, and lastly toughness.

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[**] The authors acknowledge support from the University of Georgia (UGA) Research Foundation. Calculations are performed at the UGA Advanced Computing Resource Centre.
2. Computational Models and Methods

2.1. Creation of Nanoporous Al Model

Creating a realistic atomistic nanoporous model is not an easy task; however the Cahn–Hilliard equation has recently been emerging as one of the most successful ways to create a realistic, bicontinuous, open-cell nanostructure, which is a computational method equivalent to the physical process of dealloying. Here, we make a brief introduction of the Cahn–Hilliard method used to create the np-Al models of interest (for more detail please see the refs[23,24]). The Cahn–Hilliard equation acts on a discrete volume, populated with discrete points, positioned on a simple cubic lattice called a phase field, which is expressed as follows:

\[ \frac{\partial u}{\partial t} = \nabla^2 \left[ \frac{df(u)}{du} - \theta \nabla^2 u \right] \]  

(1)

\[ \frac{df(u)}{du} = \frac{1}{4} \left( u^2 - 1 \right)^2 \]  

(2)

Here, \( u(x, y, z, t) \) is the order-parameter whose value determines whether a point represents component A or component B. The overall behavior of the Cahn–Hilliard equation is determined by the free energy functional, Equation (2), which determines what values of \( u \) are stable; in this case, there are two stable values of \( u, -1, \) and \( +1 \). To make it clear, the free energy equation determines that \( -1 \) and \( +1 \) represent particles in a domain that is pure in either component A or component B. \( \theta \) defines the thickness of the boundary layer that divides a domain pure in component A from a domain pure in component B.

Initially these discrete, regularly spaced nodes are randomly chosen and assigned a positive or negative value close to zero. The assigned value determines whether a point is component A or component B of a binary mixture. By solving the Cahn–Hilliard equation, the binary mixture is separated into domains which are pure in each component. After the separation, one component is removed and the remaining “material” is a bicontinuous, open-cell nanostructure. Figure 1a shows the dynamic evolution of the mixture separation process governed by the Cahn–Hilliard equation.

The final ratio of component A to component B in the mixture is a predictable quantity of the Cahn–Hilliard equation because it strongly depends on the initial conditions. At the beginning of each simulation, every node in the phase field is assigned an initial order-parameter value. For example, if 60% are assigned positive values at the beginning then one would correctly expect that the number of \( +1 \) nodes at the end of the separation would be close to 60% of the batch. That means, to control the percentages of positive and negative nodes at the end of the separation, which corresponds to the ratio of component A to component B in the nanoporous structure, we need to set the initial percentages of positive and negative nodes at the beginning of the separation close to that value of interest. Figure 1b shows six np-Al models with the relative density as 0.36, 0.44, 0.54, 0.65, 0.74, and 0.84 with the average ligament diameter 5.0 nm, respectively. The relative density is defined as the ratio of the porous sample’s density to the density of bulk aluminum; the average ligament diameter is calculated by taking multiple cross-sections of each sample, measuring the characteristic length of each ligament, and then averaging the measurements together.

Besides, the relative density of the nanoporous structure, the size of the pure domains in the structure is directly proportional to how long the system is allowed to separate; therefore, in order to control the average ligament diameters in the nanoporous models with a fixed relative density of interest, we need to adjust the simulation time. Figure 1c shows four models with the average ligament diameters as 3.11, 5.64, 7.47, and 9.88 nm with the relative density around 40%. After the creation of the bicontinuous domains, the Al atoms of interest are populated into the domains with positive values to generate their coordinates in the 3D structure as depicted in Figure 1b and c.

2.2. Simulation Techniques

Here, molecular dynamics simulations, based on the open-source code LAMMPS, are performed to investigate the mechanical behavior of the np-Al[25] In order to accurately show the electron cloud effect of metallic materials, an embedded atom method (EAM) potential is adopted to describe the interatomic forces between aluminum atoms in our model, which is detailed as follows[27]

\[ E_i = F_a \left( \sum_{j \neq i} \rho \beta \left( r_{ij} \right) \right) + \frac{1}{2} \sum_{j \neq i} \varphi_{ab} \left( r_{ij} \right) \]  

(3)

\( E_i \) is the potential energy of atom \( i \) where \( F_a \) is the embedding energy which is a function of the atomic electron density \( \rho \), \( \varphi_{ab} \) is a pair potential interaction, and \( a \) and \( b \) are the element types of atoms \( i \) and \( j \). The \( 20 \text{nm} \times 20 \text{nm} \times 20 \text{nm} \) model is simulated using a standard velocity-Verlet time integration with a timestep of 1fs. Periodic boundary conditions are applied in \( x, y \) and \( z \) directions in order to mimic a specimen with an infinite size. At the beginning of each simulation, an energy minimization based on the conjugate gradients method is imposed on the np-Al models. During the energy minimization process, the boundaries of the np-Al models are allowed to expand or contract freely. Afterward, a canonical ensemble NVT with a Nose–Hoover thermostat is performed for 25 ps to thermally equilibrate the np-Al. In order to mitigate the initial pre-stress in the np-Al model, an isothermal–isobaric ensemble NPT is invoked for another 25 ps (graphs of pressure vs. time and temperature vs. time during the NPT equilibration can be found in the supplemental materials, Figure S1). Then, after energy minimizations and equilibration, we apply a tensile load to the np-Al model, under an NVT ensemble, with a strain rate of \( \text{20–30 ps}^{-1} \). The uniaxial,
apparent stress was calculated based on virial stress as follows:

\[
\sigma_{ij} = \frac{1}{V} \sum_{k \in V} \left( -m^{(k)} \left( u_{i}^{(k)} - \bar{u}_i \right) \left( u_{j}^{(k)} - \bar{u}_j \right) + \frac{1}{2} \sum_{l \in V} \left( x_{i}^{(l)} - x_{i}^{(k)} \right) f_{l}^{(j)} \right) \quad (4)
\]

where \(N\) is the number of atoms in the system, \(k_B\) is Boltzman’s constant, \(T\) is temperature, \(k\) and \(l\) are atoms in the domain, \(V\) is the volume of the domain, \(m^{(k)}\) is the mass of atom \(k\), \(u_{i}^{(k)}\) is the \(i\)th component of the velocity of atom \(k\), \(u_i\) is the \(j\)th component of the average velocity of the atoms in the volume, \(x_{i}^{(k)}\) is the \(i\)th component of the position of atom \(k\), and \(f_{l}^{(j)}\) is the \(j\)th component of the force applied on atom \(k\) by atom \(l\). All the visualizations of the models are depicted using OVITO software.\(^{[26]}\)

3. Results and Discussions

3.1. Mechanism of Failure

In order to study how np-Al fails during deformation, multiple simulations have been performed to determine
the dominating failure mechanism. A representative ligament is shown in Figure 2 and 3 to illustrate the deformation evolution process of np-Al. Dislocations in our paper are defined by a common neighbor analysis calculation (CNA) that shows the packing arrangement of each atom. FCC aluminum is shown in blue, hexagonal close packed aluminum is shown in cyan, and disordered atoms are shown in red. When the CNA undergoes a shift which demarcates a change in packing arrangement, it is noted as a dislocation forming. It can be clearly observed that dislocations nucleate at the surfaces of joints; at the surface because the high surface-energy lowers the stress needed to activate a dislocation, and at the joints because torque generated during the tensile loading is largest in the ligament joints.

As strain increases, slip systems begin to develop in the thinnest segment of the stressed ligament followed by necking and rupture. The dislocation motifs seen in our np-Al simulation include Lomer–Cottrell locks inside joints and parallel slip planes. Lomer–Cottrell locks are seen to develop in ligament junctions and cause dislocation pile-ups, which may help fracture resistance in the junctions by preventing further slippage between planes. Similar failure mechanisms, specifically dislocations initiating at the joints of ligaments, have been observed via MD studies for np-gold and np-silicon. The observation of dislocations initiating at the surface of joints, using two different types of force fields (EAM for np-Al and np-gold and REAXFF for np-silicon), strengthens the validity of our result. Load-bearing ligaments, ligaments closely aligned with the loading direction, were observed to fail first but for ligaments not aligned with the loading direction shearing was observed during plastic failure and snapshots of a shearing event can be seen in supplemental materials Figure S2.

Three defining properties for the mechanical performance of np-metals are chosen as the independent variables to study the mechanical properties of np-Al: relative density, ligament diameter, and temperature. Here, we vary the relative density from 36 to 84%, using an average ligament diameter of 4.92 ± 0.34 nm and then perform tensile simulations at a temperature of 300 K. For ligament diameter studies, we create models with average ligament diameters ranging from 3.11 to 9.88 nm, with a relative density of 41 ± 0.27%, and temperature of 300 K. With respect to temperature effect, a np-Al model with a relative density of 41% and a ligament diameter of 5.64 nm is used to perform the study with temperatures from 20 to 600 K.

It can be implied from Figure 4 that there are similarities between the three stress–strain curves for np-Al, although each one has its own emphasis. For each curve, the stress increases linearly at the beginning of tensile loading until about 95% of strain-at-failure, then the slope begins and continues to decrease for the last 5% until the failure strain is reached, at which point the slope inflects again becoming negative with a gradual slope denoting the necking of np-Al ligaments before complete fracture. Aside from these similarities, the three graphs show very distinct dissimilar trends which are the focus of the rest of this paper. Using calculations from these three stress–strain graphs, we will share our findings concerning the mechanical properties and scaling laws of np-Al and compare them to previous studies on open-cell metal foams and np-metals.

As the major focus of this paper is the scaling laws of the physical properties of np-Al with respect to the relative density and the average ligament size, we will investigate four mechanical properties of interest such as Young’s modulus, $E$, yield strength, $\sigma_y$, ultimate strength, $\sigma_u$, and toughness, $K$.

### 3.2. Young’s Modulus

The first mechanical property of np-Al to be discussed is the Young’s modulus, taken as the line of best fit from on a stress versus strain graph from zero strain to 3% strain (Young’s modulus can also be determined from the second derivative of energy vs strain but this method produced less
accurate results see more detail in Figure S3). The Young’s modulus allows for determination of a material’s stiffness at ordinary working conditions; that is at low strain under elastic deformation. It is observed from Figure 5a that decreasing the relative density lowered the Young’s modulus, \( E \), of the np-Al, following a power law relationship.

\[
E = 92.07 \rho^3
\]  

(5)

Following the Ashby and Gibson’s model which states that open-cell foams classified above the nanoscale have a Young’s modulus-relative density relationship of \( E = C \rho^2 \), we have the coefficient constant \( C = 60.92 \) for our np-Al model. The variable \( \rho \) represents relative density, \( \rho = \frac{\text{Density of np-Al}}{\text{Density of bulk Al}} \) and is, therefore, unit-less, exponentials are inherently unit-less so the units of \( C \) in this relationship and in the preceding relationships will take on the units of the property being defined (Young’s modulus,
ultimate strength, and yield strength (GPa); toughness (MJ/m³)). From the data analysis and curve fitting in Figure 5a, it can be noticed that the Young’s modulus of np-Al in the study does not scale as subtly as the Ashby and Gibson’s model would predict. Sun et al. [23] also pointed out the discrepancy with the Ashby and Gibson’s scaling law for nanoporous gold (np-Au) and developed a scaling law better suited for predicting the Young’s modulus of np-Au with respect to the relative density of $E = C_a (\rho^2 + C_b \rho)$. The attempt to curve fit Ashby and Gibson’s scaling law and Sun’s scaling law is shown in Figure 5a. The curve based on Sun’s scaling law describes our simulation data well but at low densities it predicts a negative and unrealistic Young’s modulus of np-Al. This disparity stimulates us to develop a different scaling law to fit the data more accurately and predict a more reasonable Young’s moduli of np-Al for all relative densities. These findings exemplify the differences in mechanical properties between nanoscale, porous materials, and bulk, porous materials, thereby offering new insights into the mechanical property prediction of novel np-materials.

With respect to the effect of ligament size on the Young’s modulus, an intriguing phenomenon is observed in Figure 5b that the Young’s modulus almost remains, for all intents and purposes, unaffected by any changes to the average ligament diameter of np-Al. When changing ligament diameter from 3.11 to 9.88 nm Young’s modulus varies, with no trend, by less than 1% between the values of 8.1 and 8.2 GPa, a similar trend is evidenced by Sun et al. [23].

The effect of temperature on the Young’s modulus of np-Al has been shown in Figure 5c. Young’s modulus of np-Al decreases gradually as the simulating temperature increases from 20 to 300 K; above 300 K the Young’s modulus begins to decrease more rapidly, as the np-Al becomes more pliable at a high temperature due to the increased kinetic energy present in the system allowing atom debonding at lower stress. The study shows that np-Al’s resistance to deformation remains high in low temperature environments making it a good candidate for applications at or below the cryogenic temperature scale.

3.3. Yield Strength

To determine what applications a material is suitable for, it is important to fully understand how much stress it can take before failure. To this end, Figure 6a depicts the yield strength
of np-Al plotted against relative density and is curve fitted with three different scaling laws. It can be observed that the relative density exerts a dramatic effect on np-Al’s yield strength, with a 94% drop from 2.5 to 0.16 GPa as the relative density decreases from 84 to 36%. Following the first Ashby–Gibson scaling law, \( \sigma_s = C \rho \), which describes open-cell foams that predominantly fail due to axial yielding of ligaments, we have a fitted curve \( \sigma_s = 1.821 \rho \) describing the relationship between the yield strength and the relative density of np-Al. According to the second Ashby–Gibson scaling law, \( \sigma_s = C \rho^2 \left( 1 + \rho^2 \right) \), which describes open-cell foams that fail due to plastic collapse at junctions, we end up with a fitted curve \( \sigma_s = 1.261 \rho \left( 1 + \rho^2 \right) \). Neither scaling law fits the simulation data of yield strength because similar to the Young’s modulus, the yield strength for np-Al shows a stronger relationship to relative density than that which is predicted by Ashby–Gibson scaling laws. Ashby–Gibson scaling laws have been used to match the data for np-Au,\(^{23}\) but here they fail to predict the yield strength of np-Al. Therefore, we propose a new scaling law \( \sigma_s = 4.026 \rho^3 \) which accurately matches our simulation data for the yield strength of np-Al. Our scaling law supports the studies by Beiner et al., Volkert et al., and Hodge et al. who show that experimental values for yield strength are drastically different than those predicted by the Ashby–Gibson models and scale drastically different than the Ashby–Gibson scaling laws.\(^{19,21,32}\)

Volkert and Lilleodden\(^{21}\) show that yield strength is inversely proportional to ligament diameter in gold nanocolumns, \( \sigma_s \propto D_L^{-n} \). Following this idea and the data in Figure 4b, we find the same proportionality. The scaling law of the yield strength, when measured against the ligament size of np-Al, is found to be

\[
\sigma_s = 0.3671 \left( \frac{D_L}{D_{L,\text{max}}} \right)^{-0.3577}
\]

Here, \( D_L \) is the ligament diameter and \( D_{L,\text{max}} = 12.59 \text{nm} \) is the largest average ligament diameter in our simulation models.

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Fig. 6. (a) Yield strength as a function of relative density with two Ashby–Gibson scaling laws and a best fit curve fitted to the molecular dynamics data. (b) Yield strength as a function of normalized ligament diameter approaching an asymptote as the ligament diameter increases. (c) Yield strength as a function of temperature, decreasing linearly as temperature increases.

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Here, \( D_L \) is the ligament diameter and \( D_{L,\text{max}} = 12.59 \text{nm} \) is the largest average ligament diameter in our simulation models.
Figure 6b shows a trend of increasing yield strength with decreasing ligament size in np-Al, which serves as compelling evidence to frame the idea that “smaller is stronger” in np-materials. It seems relevant to point out that smaller ligaments creating stronger nanoporous structures is reminiscent of the well-known Hall–Petch relationship for grain size which parallels this finding by stating that yield strength is inversely proportional to grain size. Of course these two phenomena describe two different mechanisms of increasing/decreasing a material’s strength but the relationships, or scaling laws, are identical in form. These findings offer useful guidance in the fabrication of ever-increasingly smaller ligaments in np-materials to provide devices, in harsh environmental conditions, with the required mechanical properties.

An inversely linear relationship is found between the np-Al’s yield strength and temperature as shown in Figure 6c. The yield strength of np-Al increases as temperature decreases giving np-Al a maximum theoretical yield strength at temperatures close to absolute zero. Yield strength in np-Al increases by 23.5% as the temperature is decreased from 300 K to a cryogenic temperature of 20 K.

### 3.4. Ultimate Strength

Knowing the yield strength and ultimate strength of a material allows for more efficient implementation of metal forming processes that rely on lengthening and allows for more reliable calculations when determining the failure of a material. Figure 8a shows the ultimate strength, σ_u, to relative density relationship, which follows the power law:

\[ \sigma_u = 4.337 \rho^3 \]  

This equation is graphed along with the corresponding molecular dynamics data in Figure 7a. Ultimate strength drastically decreases by 99% when relative density decreases from 84 to 36%.

Np-Al’s ultimate strength does not follow a similar scaling law as yield strength, or Young’s modulus for that matter, with changes in ligament diameter. The relationship depicted in Figure 7b was best described as a linear function the relative ligament size as follows:

\[ \sigma_u = -0.33 \frac{D_l}{D_{l,\text{max}}} + 0.7438 \]  

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**Fig. 7.** (a) Ultimate tensile strength as a function of relative density. (b) Ultimate strength as a function of normalized ligament diameter. (c) Ultimate strength as a function of temperature.
It would be reasonable to say that this is a result of a small sample size because like yield strength, we initially predicted that ultimate strength would asymptotically approach a constant value as ligament diameter increased, whereas ligament-size effects are not observed in meso/macro-porous materials.

The effect of changing temperature on ultimate strength in np-Al is noticeably similar to the effect of temperature on Young’s modulus, compare Figure 4a and 6c. The ultimate strength of np-Al does not change much until reaching temperatures above 125 K. After reaching 125 K, the ultimate strength decreases more and more rapidly as temperature increases. Over a range of 580 K, the ultimate strength drops by 32%. This reiterates the well-known conclusion that Al is both less stiff and less strong at higher temperatures.

3.5. Toughness

The toughness of a material is a useful metric which indicates the total amount of work which a material can absorb before it fails. Thus, knowing the toughness scaling law for np-Al allows us to find suitable materials for energy/impact absorption. Toughness, \( K \), is measured as the area under individual stress–strain curves until reaching ultimate strength. With respect to relative density, np-Al’s toughness decreases following the power law

\[
K = 170.3 \rho^3
\]

and this relationship is plotted in Figure 8a. Overall, the toughness of np-Al drops by 90% from 105.85 MJ/m\(^3\) to 10.68 MJ/m\(^3\) across the range of relative density values. This is the lowest percentage drop among all the measured mechanical properties when relative density changes. Figure 9 shows an increase in strain until plastic deformation and failure. This phenomenon competes with the losses in toughness from reduction in material and dampens the effect of relative density on np-Al’s toughness.

Toughness decreases by 56.5% as ligament diameter increases by 9.48 nm, a large drop in toughness for a change in diameter equivalent to only two FCC-aluminum-crystal unit cells. Decreasing the average ligament diameter, which increases the number of ligaments if relative density is constant, increases the energy needed to break the structure.

![Figure 8](image-url)
including ligament-size effects and temperature effects. Most role in affecting the mechanical properties of np-Al when themselves. Relative density was found to play the most important junctions and encouraging dislocations in ligaments them-

ligaments stopping further dislocations from forming in the causing necking and fracture. Lomer conclude that dislocations in np-Al originate at the surface of nucleation sites.

4. Conclusions

The tensile deformation behaviors and size effects of open-cell np-Al were investigated using MD simulations. We conclude that dislocations in np-Al originate at the surface of joints and shortly after in the thinnest section of the ligament causing necking and fracture. Lomer–Cottrell locks were frequently observed to form in the junctions between ligaments stopping further dislocations from forming in the junctions and encouraging dislocations in ligaments themselves. Relative density was found to play the most important role in affecting the mechanical properties of np-Al when including ligament-size effects and temperature effects. Most importantly, a number of scaling laws were found for Young’s modulus, yield stress, ultimate stress, and toughness of np-Al. This study provides useful insights into the understanding of the fundamental mechanism and scaling laws of nanoporous materials.

Figure 8b shows the relationship:

\[ K = -41.15 \frac{D_L}{D_{L_{\text{max}}}} + 60.58 \]  \( \text{(11)} \)

which describes the effect of ligament size on np-Al’s toughness.

When the toughness of np-Al is measured at different temperatures no trend is found, as shown in Figure 8c. There are two outliers, at 125 and 600 K, which make the graph appear to have a rough trend but every other graphed point is randomly dispersed among a range of values giving no reportable trend.

Although not the focus of this paper, we also found that using a nanoporous structure that is intelligently designed lead to dramatic increases in all mechanical properties. The increases also changed the scaling law powers closer to a than the disordered counterpart used in our study, due to the even distribution of stress and the lack of obvious defect nucleation sites.