Novel Method to Create Lighter and Stronger Porous Materials using Nanorod Reinforcements

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ABSTRACT

Maintaining the strength and stiffness of a material while decreasing its density remains a fundamental challenge in materials science, and also a desirable requirement for many applications. For example, a stronger but less dense biological implant whose properties match that of a bone will prolong life by not degrading the surrounding bone. My novel solution is to reinforce these lightweight but weaker porous materials with strong nanorods. I hypothesized that nanorods counter the collapse of pores, thus strengthening and stiffening the foam. I test this by reinforcing a porous copper foam model with silver and niobium nanorods. I used Large-scale-Atomic/Molecular-Massively Parallel-Simulator (LAMMPS) to systematically compare deformation characteristics of a porous copper model system with various pore-geometries and nanorod reinforcements as a proof of principle. Under tension, multiple pores brought outward from the center improved the strength by 13% compared to a one-pore reference system of the same porosity. During testing, the silver nanorod disintegrated and coated the copper pore. Niobium, with a much higher melting point than silver, made the system stronger by staying stable and reinforcing the pore. Under compression, the modulus of niobium reinforced porous copper was 44% above that of the non-porous perfect copper. These results support my hypothesis that reinforcing metal foams with nanorods is a novel and effective way to engineer strong but exceedingly light alloys.

I.   Introduction

Maintaining strength in a material while decreasing its density remains a fundamental problem of materials science. I discovered a method in which to make materials lighter but stronger, especially solving the following issues.

With the increasing population of senior citizens, the need for reliable prosthetics and other biomaterials increases significantly. Indeed, there have been exciting advances, especially in bone implants over the years, but these implants still face challenges. The overlying reason

lies in the fact that the implant must integrate and become part of the body. This requirement, also called biocompatibility, is an implant's ability to blend in with the conditions of the recipient body. Any implant must generally meet the following challenges: the immune system must not attack and reject it, the body cells must grow into the implant and bond intimately, and it should be able to withstand the corrosive attacks of body fluids in addition to the daily strain on the bone. Alloys such as titanium (Ti) don't fulfill this role because of their less-than-ideal biocompatibility.[5]

Although titanium alloys are currently the preferred material for implants because of their high strength, their modulus of elasticity and density are appreciably greater than that of natural bone, according to the Table 1a above. As defined, the modulus of elasticity or stiffness of a material is a positive number that measures a material's resistance to non-permanent deformation under an applied load.[7] Stiffer materials have higher elastic moduli. This property is defined mathematically as the slope of its stress–strain curve in the linear elastic region (**see Figure 1**). Strain, is a value used to depict the deformation of a metal with respect to the change in length of the cell (See **Figure 2).** Stress is the materials response to the

Figure 1 – A schematics stress-strain graph shows how to calculate the strength and modulus[6]

strain deformations.[8] *Modulus mismatch* is a biomechanical term that measures the difference in the stiffness of a biomaterial implant against the bone on which it rests. Modulus mismatch is

detrimental since mechanical loads **promote** bone regeneration and repair.[5] A Ti implant, due to its larger modulus and density (Heaviness), will carry a disproportionate amount of the biological loads and the surrounding bone experiences abnormally low levels of stress. This "stress shielding" leads to loosening of the implant caused by degrading of the surrounding bone.[5]

Figure 2 – Diagram of strain on an object. Because of the force on both sides that alter the length of the object, strain is calculated from the side dimensions.[9]

A secondary application that lightweight but simarly strong structures serve better are moving vehicles. Scientists have proven that lighter cars produce better fuel efficiency and speed. Similarly, any other type of transportation will benefit in the same way because the force required as output of the engine is a lot less, a direct application of Newton's Second Law: Force = Mass x Acceleration. The lowered mass with the lighter material will exceedingly lower the force required by the engine, and boost fuel economy, all without any decline in safety since the material is similarly strong.[10]

Metal foams or porous materials are a feasible and promising approach to lower the density and modulus of heavy, conventional metallic materials. However, such a lowering of modulus and density comes with a massive loss in their strength as shown in Ashby's Plot (**Figure** 3). According to **Figures** 3 and 4, foams have a linear relation with metals in respect to modulus, density, and strength. The advantageous properties strength and modulus are lost because the atoms that lie on the surface of pores initiate deformation: their missing neighboring atoms cause weak bonding. The surface atoms deform at lower stresses because of their weaker bonds, thereby decreasing the strength of porous materials. These atoms also possess higher potential energy, striving to lower their

Figure 3 – Graph of Modulus vs density. Porous materials, also called foams, decrease in modulus in a direct proportion with density.[6]
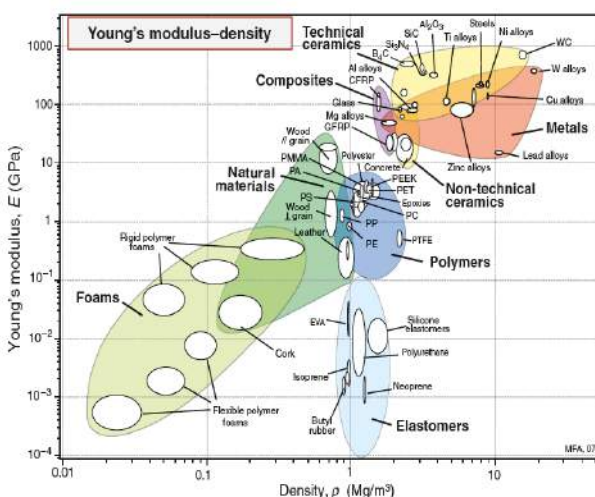
energy state by bonding with other atoms. As they trigger deformation, they fail at much lower stresses than their fully dense counterparts. Such a process leads to the collapse of pores under stress.[11,12]

Figure 4 – Graph of strength vs density. Porous materials also have significantly lower strength and density than their dense counterparts.[6]

The challenge presented, therefore, is to engineer the material to meet the properties of bone, which means decreasing the density and modulus, perhaps by increasing porosity, all without losing strength. My novel solution is to reinforce these engineered porous materials with nanorods, which possess exceptional strengths[13,14]. Theoretically, these structures will take up the least amount of volume, barely adding to the modulus and density. My *hypothesis* is that the addition of nanorods will appreciably increase the strength of the porous metals by impeding the collapse of pores. I will first test this hypothesis by fabricating a model porous metallic system (to be used as a reference) and testing its properties such as density, modulus, and strength. Copper will be my model surrogate system for ease of computational simulations. Computational experimentation rather than lab experimentation was used in my case because this method was new and complicated to test first in the lab. If the principle is proved by my experimentation, lab tests can use my results that already have been proven and implement them into their specific applications (bone implants or vehicle bodies). I propose to first carry out atomistic simulations on normal dense and porous copper that will be used to compare my experimental systems to. I will benchmark their deformation behavior and identify the mechanisms causing the deformations to happen. Next, I will test the mechanical response of porous copper by adding nanorod reinforcements to determine how/whether these nanorods impede pore collapse and enhance strength compared to the reference system. These simulations will allow us to test my hypothesis, which will provide guidance for future experimentation for engineering strong and lightweight reinforces porous metals whose moduli match that of natural bone. Not only will this improve the quality of life for the disabled, but it also will benefit the environment by reducing the use of natural resources in vehicles. I will use large-scale molecular dynamics simulations to study this problem. This approach will not only help us evaluate
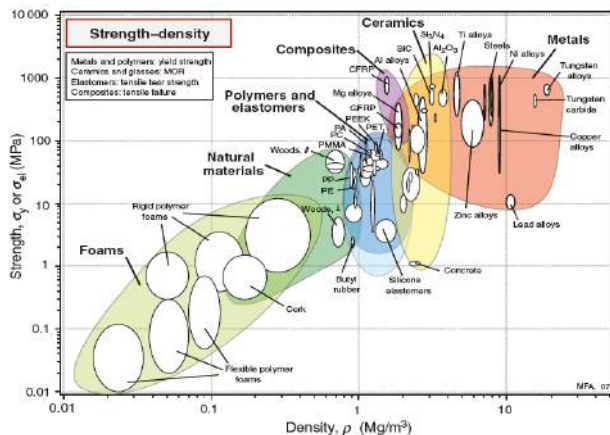
mechanical properties mentioned above, but it will also provide an picture of how these materials deform and fail on the atomic scale.

Before I reinforce the pores with nanorods, I will also test the effects of pore geometry, content, size, and placement within the simulation cell to see if the simple arrangement of pores influences modulus, strength, and deformation mechanisms of the system. The presence of the nanorods should aid the system in resisting the deformations, mainly by keeping the pores from collapsing. I'll test nanorod placement within the pore and the different nanorod compositions: Face-centered Cubic (FCC) silver and Body-Centered Cubic (BCC) niobium (See **Figure** 5).

The actual alloys used in applicable materials such as titanium are highly complex. I will, therefore, create a simple model copper system that will stand as a proof of principle. The findings can be translated to other materials, with my results and methodology as a guide to further research on this important problem.

Figure 5 – Face Centered Cubic Unit cell (left) in comparison to a Body Centered Cubic Unit Cell. The atoms for FCC are centered on the face while the atoms BCC are centered on the body.[15]

This report is organized as follows. Section II describes the methodology used in this study. Section III and IV present results and discussions, and how they correlate to my hypothesis. Lastly, Section VI will present the conclusions and some ideas for extending this work.
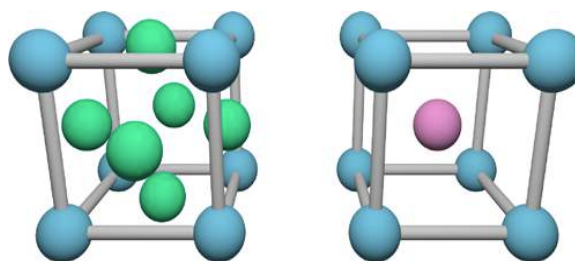
II.   **Methodology**

a.   **Simulation Method**

I used LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator), an open source molecular dynamics (MD) simulator from Sandia National Laboratories, to simulate the deformation of the copper system.[16] In MD simulations, Newton's equations for a system of interacting atoms are numerically solved over a number of time steps. At the start of these simulations, each atom is initially given a position based on a crystal structure and velocities based on desired temperature. The forces between atoms are based on an interaction potential appropriate for the material that is studied. Choosing the interaction potential is crucial for replication of the studied system. An Embedded atom method (EAM) model is generally used by

LAMMPS to approximate the interaction between atoms. I used the copper-silver and copper-niobium potentials in this study because the nanorod compositions I tested, silver and niobium, were interacting with the copper system.[17, 18, 19] Computational resources for this experiment were provided by UNT's High Performance Computing Services. I ran the MD simulations on my University's Talon 2 supercomputer cluster that has around 5000 processors.[20] The Talon 2's Unix interface required a thorough knowledge of the Unix command language. Each of my simulations required anywhere from 16 to 256 processors to complete in 6 hours of wall clock time.

I used this atomistic computational approach to deform and test the material under tensile conditions and compressive stress conditions since these are the two major types of deformation in nature (Figure 2). I used periodic boundary conditions, which translate the one simulation cell to an infinite number of neighboring unit cells, approximating a much larger system from just one simulation unit cell.[18] Periodic boundary conditions erased the experimental error of wrongly concluding certain properties just from how a small portion of the system reacts. My methods are not unique since there is a number of different ways to run this simulation. In the first step, I used either a perfect or porous system of copper with 15 initial unit cells along X and Y dimensions and 25 unit cells along Z. Next, I minimized the system's energy state and equilibrated my system at 500K and 10K for 500,000 iterations and 250,000 iterations respectively, totally approximately 750 picoseconds in real time.

Finally, I tested the material under a *uniaxial* tensile or compressive strain along the z-axis. Uniaxial strain is a commonly used experiment to test the deformation of a material by stressing it along a particular axis. It is important to not deform the material rapidly but allow it to happen as a slow process just as in reality. After consistent trials, I found that a time step of 0.001ps is the most ideal for gathering results and producing consistent deformations based on observing whether energy of the simulation system is conserved. The material is annealed dynamically and stressed at a strain rate of $\sim10^7$ /second and at a temperature of 10 Kelvin for 500ps. Respective dump files, that contain snaps of atomic coordinates of the system at a particular time instant, are produced every 10,000 time steps. These dump files help in visually observing the deformation over time. Importantly, these simulations help track the evolution of stress and strain in the system over time, showing how atoms respond in the process. During the tension runs, the material is pulled along the z-axis. Under compression, the material is squeezed

uniaxially in the opposite direction (Opposite direction from arrows in **Figure** 2). I repeated each run at least 3 times to make sure that the results were consistent. In addition, using similar systems and getting similar results was also a way of showing consistency.

b. Pore Geometry and System Description

Using my knowledge of geometry, I created 18 different systems, basing each one on previous pore systems deformed. Although my first geometries were systematic, my later tested systems were solely based on how the previous ones reacted. The geometries close to the 18th stopped reacting differently so I concluded this part of my experimentation after that system. The values that I altered were the placement of pores, size and number of

Figure 6- Schematic pore geometry of the systems tested in my study.
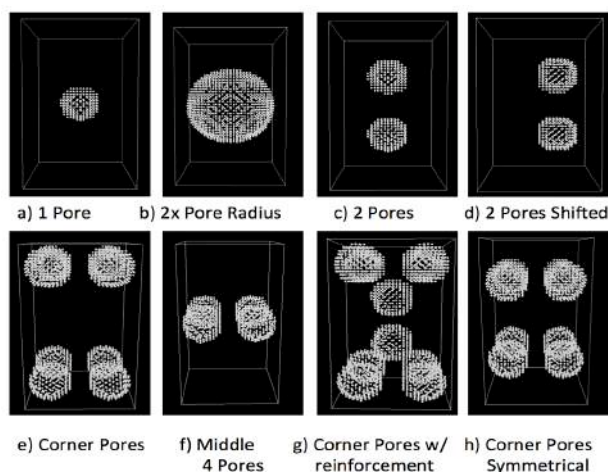
pores (porosity), and the size of the system in case I wanted to maintain the same fraction of porosity while increasing the pores' sizes. After gathering sufficient data about how the systems react, I identified the best responding pore organization: the system in which the visual deformations are minimal, resulting in a higher strength and significant change in modulus. I started out increasing the size of the pore by doubling its radius as seen in **Figure** 6b. Next, I kept the porosity constant and increased the dimensions of the pore in the same proportion as I did with the dimension of the simulation cell. Afterwards, I incorporated more pores and different placements according to the statistical and visual deformation values, as seen by **Figures** 6c-h. In assessing a model, I first look for the peak stress (strength) in the stress-strain curves of the model under study. Then, I calculate the modulus from the slope of the stress-strain curve shown in **Figure** 1 to see how it changes. The strength and modulus are the two dependent variables that I'm testing: these indicate whether material has maintained its strength or stiffness after density loss. Previous studies have shown that the steep fall in the stress levels beyond strain that yields the peak stress is due to the formation of defects in the crystal. Therefore, lastly, I correlate the atomic picture of deformation at various times, as shown in **Figures** 4 and 5, with the corresponding stress-strain values. First, my plan was to find the best orientation for the

pores. I kept the control as a perfect block of copper and calculated its stress-strain curves. Compared to the control, my goal was to create a porous, lower density system with a peak stress closer to perfect system.

After experimenting with pore placement, determining whether the arrangement of pores influences the systems properties, I reinforced the model with nanorods and systematically tested the effects on the metal in the same way as I did in the pore placement simulations, seeing if they bring back the properties lost by the low density. With nanorods, I altered orientation, size, and makeup to see the change in properties that occur with each alteration. Size was the first problem. Silver nanorods are not stable enough because they have a large fraction of atoms with unfulfilled bonds because of their proximity to the crystal surface. So, I increased the square cross sections of the rectangular prismatic nanorod until I found one that didn't immediately break apart and form a lower surface area sphere. Next, I increased it a little more and tested 3 larger sizes to see their effects. Next, I tried different orientations of the rod inside the pore to understand its effect on peak strength and modulus. Finally, I tested how material properties influenced performance by replacing FCC silver nanorod with BCC niobium nanorod.

c. **Data Analysis**

I analyzed stress-strain value and created their plots using Microsoft Excel. The stress along the z-axis was plotted as a function of uniaxial strain. From these plots, I calculated the modulus and primary peak stress as shown in **Figure** 1. Ovito, the Open Visualization Tool, was used to visualize the deformation process with respect to time and strain[21]. To identify the local atomic arrangement and how they deviated from ideal crystal structure, I always ran a common neighbor analysis (CNA) algorithm[22]. OVITO can take the output of CNA runs and color-code the displayed atoms by their local bonding environment (By Atom Type: FCC, BCC, etc). This allows us to clearly see the nucleation and interaction of various crystal defects produced during the deformation. To simplify the analyses, we often display only those atoms that lie in defected regions as shown in **Figures** 7 and 8. Besides visualization, I also used OVITO to create the input atom configurations for my simulations, deleting atoms out of the super-cell to make voids and nanorods.

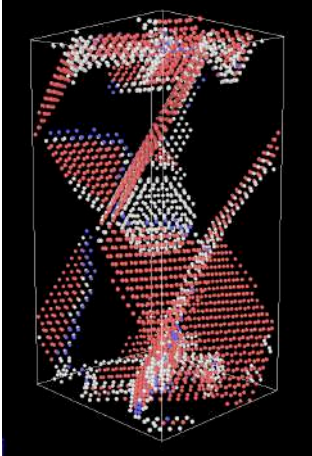## III.   Results

a. Pores Under Tension

Under tensile deformation, the perfect copper system always had the highest modulus and strength compared to porous copper. The strength of porous metals under tensile deformation test decreased as the porosity increased. Generally, the way I increased the porosity was to create larger pores or increase the number of pores. The standard pore system I used was a spherical shape with a 9-angstrom radius.

The system with one pore in the center had a 7% decrease in peak stress from its initial value of 10,700. Crystalline line defects called dislocation loops formed as sheets of non-fcc atoms near the pore's surface and expanded into the crystal. Cooperative displacements of atoms create such loops and provide a pathway to relieve elastic strain energy that builds initially in the crystal during tensile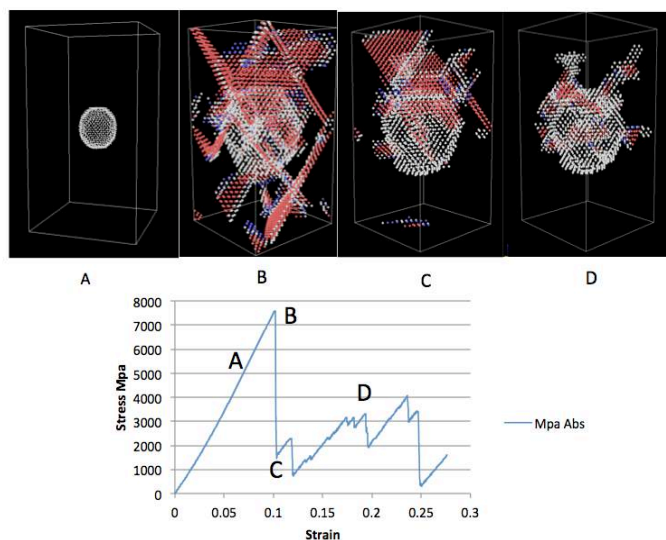 deformation. This explains the drop in stresses after peaking. At that point, the dislocations cleared up to a minimal amount. Next, I systematically observed how the system responded to larger pore sizes, which is modeled with a single centric pore, that increases in size.

First I kept the system size constant at [15,15,25] and increased the pore radius by 50% thus going from a nine angstrom radius pore to a 13.5 angstrom radius all the way to a 22.5 angstrom radius (**Figure** 3b: Any pore bigger than that would have been too large and have overlapped the box). As the pore sized increased by 50% each time, the peak

Figure 7-Deformation of 1 Pore System- Dislocation loops form as sheets around pore

Figure 8 – Visuals by point in stress
A) Before Peak of Deformation B) At Peak C) At the lowest point after peaking D) at Second Peak

stress and modulus dropped consistently 10-20% each run the porosity rose from 1.16% to 3.93% to 9.31% to 18.18%. The atomic mechanisms of deformation via dislocation loop formation are similar to the single small pore system discussed above. However, these processes occurred at lower strains and smaller peak stresses.

Tension System	Porosity	Peak Stress	Modulus
Perfect Copper	0%	10746	91265
1 Pore	1.16%	10035	91155
1.5x Radius Pore	3.93%	8736	85154
2x Radius Pore	9.31%	7608	76325
2.5x Radius Pore	18.18%	6539	61140
2x Radius Pore Constant Porosity	1.16%	8752	89402
2x Radius Pore Constant Porosity w/ 2 Pores	2.33%	8558	87444
3x Radius Pore Constant	1.16%	7364	87097
4x Radius Pore Constant	1.16%	6611	85654
5x Radius Pore Constant	1.16%	6281	85013
2 Pores	2.33%	9839	89097
2 Pores Bottom Pore Shifted	2.33%	9878	89138
2 Pores Both Pores Shifted	2.33%	10010	89160
Corner Pores	9.31%	8589	76526
Corner Pores w/ Middle Support	11.64%	8062	72323
Corner Pores Symmetrical	9.31%	8592	76287
Middle 4 Corner Pores	4.65%	8566	82964

Next, I kept the porosity constant by increasing both the pore radius and simulation box dimensions commensurately. The beginning porosity was 1.16% and this stayed constant throughout. Just as above, the peak stress decreased by 10% with each doubling of pore radius. However, the modulus had an independent trend as it only decreased 2.3% with each 100% increase in pore size. The addition of another pore, symmetrically placed on top of one another in the center did not raise the modulus or peak stress but slightly decreased the peak strength and modulus by a factor of 2.2%. The porosity for this 2 pore system was 2.32% and although it doubled the porosity compared to the 1 pore system, it decreased the strength by only 2.2%. This allows for smaller incremental changes since the 13.5 radius pore system starts at a 6.5% decrease in strength after tripling the porosity of the reference system.

I then tested systems in **Figure** 3:c-d to understand how increasing number of pores influence deformation. This system had the same dimensions as the first system, but I placed 2 similarly sized pores in different orientations. **Figure** 3:c and d depict the 2 pores lined up in the center and then the one on the bottom shifted, respectively. I noticed that the system in which both pores were shifted from the center had the highest peak strength by 1.3%. But the modulus of this system was still 2% lower than the 1 Pore System, just like the other 2 Pore configurations.
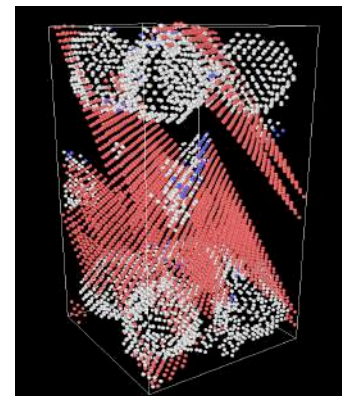

Figure 10– Corner Pore Deformation – Dislocations nucleate at each pore.

Since shifting the pores outwards increased the strength of the material, I accordingly arranged the pores into a different system: The pore sizes stayed the same but the placement and number of pores changed. I first placed the pores at corners of the simulation box (See **Figure** 3e), increasing the porosity to 9.31% with 8 pores, one in each corner. Although the modulus was similar to the 2x radius pore system (shared similar porosity of 9.31%), the peak strength was 13% higher, indicating that a higher number of pores that are placed outside the center is a beneficial arrangement for higher strength. The visual deformation seemed to be gathering in the middle of the corner pores so I placed two pores in the middle to try to combat this mechanism (**Figure** 3g). However, the material became weaker with a 6% decrease in strength and much lower modulus. With the periodic boundary condition, the cells are not symmetrical since the corner pores are closer to the pores in the next cell than they are with the ones in the same cell. So, I tested the effect of arranging the pores so that the z length is similar between the pores in the same cell as well as the pores in the neighboring cells (**Figure** 3f and h). This change had no influence in the values of

Figure 9- Tension Porosity vs Modulus and Stress Graphs – Downward Trend as modulus and stress decrease with increasing porosity with the exception of the systems such as corner pore that increased strength and modulus with the techniques of numerous unsymmetrically brought out pores

modulus and peak strength. However, when I removed the four corner pores in the bottom and moved the top corner pores to the middle with respect to the z-axis, the peak stress remained constant but the decrease in porosity increased the stiffness. Figure 9 and the corner pore system (Figure 6e) show that altering pore geometries can influence the properties of the system when under tension.
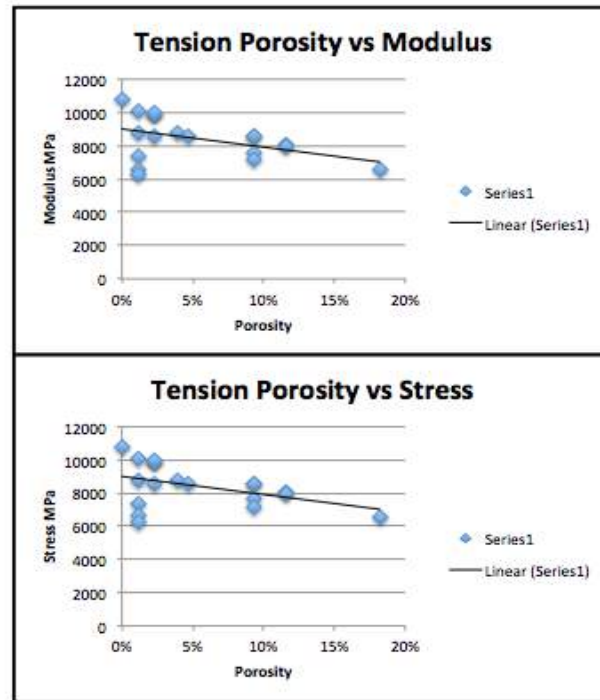
b. Pore Placement Compression

Compression, the squeezing of the two ends of the simulation cell, is an important deformation mode for biological load bearing implants and so is valuable to determining the validity of my method. Under compression, the copper system's peak stress acted in a similar way as the tension, decreasing with the increasing porosity. Starting with the one pore system, it drops 20% in peak strength from the perfect copper. However, while in the tension the modulus had a direct relationship with the peak stress, the modulus here in compression seems to have an inverse one as the material became stiffer as I went down in porosities. But as I started testing the models with larger pores, which increased the porosity, the modulus decreased with each 50% pore radius increment by 7%. The peak stress was more of an exponential model as it decreased by 5%, at first, then 10%, and finally 20%. Notably, the strength is on average 55% lower in compression than tension since the highest peak for the perfect copper is 10746 during tension but 4857 during compression. The compression of the system with the increasing pore size with constant porosity shows no particular trend. The peak stress increases slightly at first, and then decreases 12% when increased to a 300% size system. With the next 100% increase, the peak stress decreases 5% and finally increases 5% at 500% size. The modulus did not change appreciably in these model pore systems. However, in realistic porous metals this is

Table 3– Results of Compression

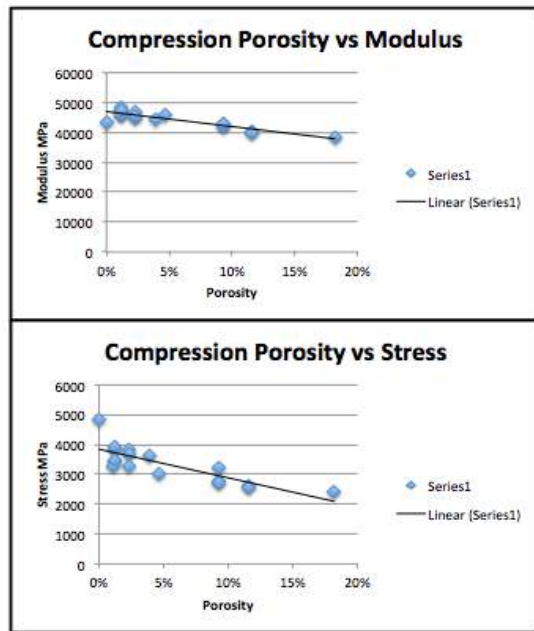| Compression System	Peak Stress	Modulus
Perfect Copper	4857.98	43585
1 Pore	3830	46044
1.5x Pore	3624	44423
2x Pore	3212	41958
2.5x Pore	2428	38255
2x Pore Constant Porosity	3910	46038
2x Pore Constant Porosity w/ 2 Pores	3296	47004
3x Pore Constant	3449	47479
4x Pore Constant	3281	48216
5x Pore Constant	3461	47482
2 Pores	3817	45005
2 Pores Both Pores Shifted	3692	45314
Corner Pores	2758	42684
Corner Pores w/ Middle Support	2633	40485
Corner Pores Symmetrical	2744	42825
Middle 4 Corner Pores	3045	45777

Figure 11 – Compression Porosity vs Modulus and Stress (Measure of Strength) – Downward trend seen in modulus and strength; properties stick to the trend much more than they do in tension, because simple pore techniques don't influence system properties.

not true, as seen from the charts in **Figures** 3 and 4 because of much larger porosity fraction and greater interconnectivity of pores. The tactics I used for tension didn't apply in the same way during the compression run. The trend strictly followed as the modulus and strength always decreased with an increase in porosity. However, it can be noted that shifting the pores from the center increases the stiffness of the material even though it decreases the strength.
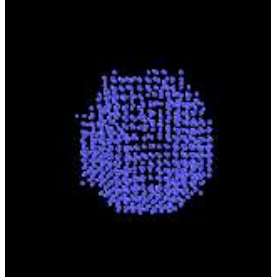

Figure 12–Silver nanorod minimized its energy by transforming into a sphere

c. Nanorod Reinforcement

The first test involved how different orientations of nanorods affected the system's deformation behavior. Nanorods are unstable below a threshold of cross-sectional dimensions given the weaker bonding of atoms lying near the large surface area of these materials. Thus, I needed to study the thermal stability of nanorods as a function of their cross-sectional area to identify the smallest stable rod. Starting from a 1x1 angstrom cross sections, I tested silver and niobium nanorods with up to 11x11 Angstrom cross section, and found that 9x9 cross section was

Nanorod C.S. in Angstroms	Tension Modulus	Compression Modulus
3x3	90668	50537
4x4	90742	50532
5x5	90528	53425
6x6	90250	54164
7x7	90249	62797

Table 4 – Results for porous copper reinforced by niobium nanorods. The tensile modulus remain the same, but the compression modulus increases up to 62.797 MPa

the smallest Ag nanorod to stay stable in a separate test before being placed in the porous system.

After these preliminary tests to ensure that the nanorods are stable enough, I ran the simulation starting with the 9x9 angstrom nanorod in the 2x Pore Radius system. I used this system for the future tests as well. However, the silver nanorod disintegrated in all the runs even when no stress was applied and the silver atoms coated the walls of the copper pore. By this process of reconstruction it was able to minimize the system energy. Nevertheless, I tested this silver-coated pore system under compression to understand how the pore surface coating influences the deformation. I found that modulus and peak stress of this system did not measurably change from that of the reference porous system.
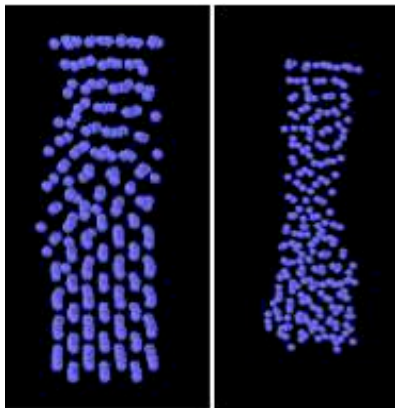
Figure 13 – Deformation of Niobium Nanorod – 4x4 Nanorod thins and weakens

After observing that silver wasn't stable, I chose niobium because it has a lower surface energy, thus making it more stable and allowing me to test my hypothesis. Since niobium has a body centered cubic crystal structure and different properties compared to silver, we use a Cu-Nb interaction potential to study its deformation.[23] In the initial runs, I tested a 3x3 and 4x4 angstrom nanorod, and they performed very well in the annealing stage as they did not collapse. However, at larger tension, around 9%, the nanorod collapsed right before the peak, thus not affecting the strength. So I moved on to test a larger 6x6 angstrom nanorod cross-section. As I increased the cross section size, the systems performed well. The highest cross section I tested was 7x7 angstroms cross-section and it had a 44% higher modulus than that of perfect copper during compression (**Table 4**).

IV. Discussion

The tensile runs had a common trend of decreasing modulus and strength as porosity increased. Although this problem could not be completely reversed by adjusting pore arrangement, I found a few geometries that allow us to tune the deformation process. The first is to increase the number of pores, which in turn decreases the modulus but hardly affects the strength. Therefore, a system with a larger pore and 2.32% porosity, when compared to a system with two smaller pores with the same porosity, has a significantly lower modulus.

Figure 14 – Niobium Nanorod sustains deformation The initial deformation is a lot less than in Figure 8, as niobium nanorod supports the pore and increases the strength.

For a system with fixed modulus but higher strength, the pores can be moved outward from the center. The system with two pores equally spaced on top of one another in the center
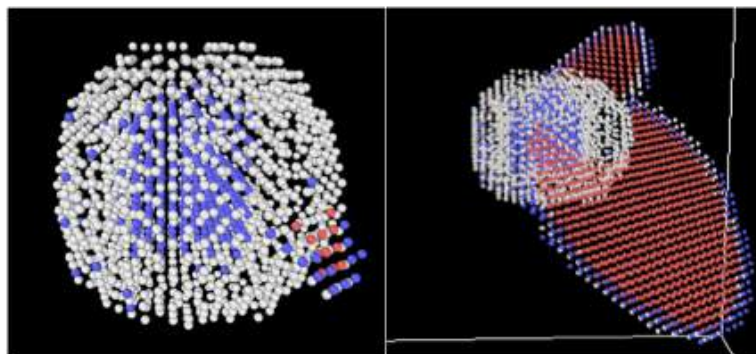
had a 2% lower strength than a system with the two pores moved outward. The copper system retained its stiffness but its strength increased when the pores were moved outwards.

The final technique came up when I combined the first two methods to create a system with a larger number of off-centered pores. This system with 8 pores, one in each corner, had a porosity of 9.31%, which is similar to that of the 18-Angstrom radius pore system. When compared, the modulus stayed the same but the peak stress or strength was an incredible 13% higher. These findings supported the conclusion that dispersing the pores from the centers and increasing the number of them can lead to a higher strength while maintaining similar modulus.

Reinforcing dispersed pores with ones in the center does not help, but in fact decreases the modulus and strength since more pores were present, after an increase in porosity. However, the same strength can be maintained if the porosity is cut in half but has a similar arrangement. The corner pores contrasted to the middle 4 pores illustrates this observation as the strength stayed the same but the modulus increased as with any system in which the porosity increases.

The first silver FCC structure failed to be of any help to the material since it collapsed. This can be explained by silver's lower melting point (962°C) and much higher surface energy than Niobium (2468°C) [24]. For this reason, the silver nanorod collapsed to reduce surface energy by forming a sphere of low surface area. Because of niobium's lower surface energy and higher melting point, it is more stable during the test. In fact, niobium strongly supported my hypothesis by increasing the modulus of the material by 44% in 7x7 Angstrom Cross-Section configuration. Since one nanorod tremendously stiffened a one-pore system (44% increase), the modulus of foams with more than one pore can be tuned by strategically reinforcing a certain portion of pores. Strength was maintained when the pore didn't collapse under niobium reinforcement.(**See Figure 14**).

As the cross section size of the niobium nanorod increased, the modulus increased as well, showing that the stiffness of a nanorod-reinforced system can be manipulated by changing the size of the nanorod. Niobium is an excellent nanorod material since it maintains incredible stiffness even after a significant decrease in density. The strongest and least dense pore geometries can be reinforced with these nanorods based on the individual results to produce a system tailored to the specific properties modulus, density, and strength. For implants, foams will decrease the density as shown in **Figure** 3. With nanorod reinforcements and a pore geometry depending on the desired properties, a composition with the perfect properties can be

engineered. By using my method, the strength, modulus, and density of a nanorod reinforced foam can be exactly that of bone. In addition to bone implants, any alloy of the same structure can be engineered to be stronger and lighter with the insertion of Niobium nanorods to reinforce the collapsible pores. However, significant changes only occurred during the compression stage of the experiment. This means that under tension, the material will act normally, only gaining strength and stiffness under compression.

V. Conclusions and Future Research

Our simulation results of the nanorod reinforcement during tensile and compression runs are promising. They indicate that my hypothesis, that porous material properties such as strength, stiffness, and density can be tailored with the help of nanorod reinforcement, is reasonable. Simple pore placement techniques can influence how a material deforms, as shown by the porous runs and as proven by multiple tests on differently organized systems. Nanorods give incredible strength and stiffness to the system, just as envisioned. These simulations present a proof of concept and encourage us to experiment with fabrication techniques to enable us to synthesize such configurations in the laboratory.

In the future, I must move from this perfect copper model system and aim to replicate these findings in a more complicated, irregular system. Here, the starting material will look more similar to porous copper in reality. Instead of centric spherical pores, there will be random pores that were grown in the material and I'll translate these techniques in this system to the other. Nanorods should also be tested in greater detail. Other materials such as the ultra-strong carbon nanotubes should be used as reinforcements. My model system showed a definite change in properties as the system proportionately increased in size, so the variability in nanorod strength must be tested. Variability includes the difference in performance between compression and tension, which seems to be a weak point to the otherwise perfect material. Perhaps by considering nanorod composition and reinforcing stronger pore geometries with nanorods, one can engineer a system that will perform just as well under tension as compression. Aside from this computational research, the lab portion of this research requires several tests. Porous microstructure must be grown and tested with emphasis on tension and compression, replicated especially to the methods used here. My computational research will guide the laboratory and experimentation to follow.

References

[1]- "Mechanical Properties of Bone." *Dissemination of IT for the Promotion of Materials Science*. University of Cambridge, Apr. 2006. Web.

[2]-"Density of Bone", The Physics Factbook™, Edited by Glenn Elert -- Written by his students, An educational, Fair Use website, Oct 2010, they got their value from the source: Cameron, John R.; James G. Skofronick & Roderick M. Grant. Physics of the Body. Second Edition. Madison, WI: Medical Physics Publishing, 1999: 96.

[3]- "Modulus of Elasticity - Young Modulus for Some Common Materials." *The Engineering Toolbox*. The Engineering Toolbox, n.d. Web. 19 Sept. 2014. <http://www.engineeringtoolbox.com/young-modulus-d_417.html>.

[4]-Materials Properties Handbook: Titanium Alloys, R. Boyer, G. Welsch, and E. W. Collings, eds. ASM International, Materials Park, OH, 1994.

[5]- Thelen, Sarah, Francois Barthelat, and L. Catherine Brinson. "Mechanics Considerations for Microporous Titanium as an Orthopedic Implant Material." *Journal of Biomedical Materials Research* 69A.4 (2004): 601-10. Web.

[6]- M. F Ashby. *Materials Selection in Mechanical Design*. Oxford: Pergamon, 1992. Print.

[7]- B. J Alder, T. E. Wainwright (1959). "Studies in Molecular Dynamics. I. General Method". Journal of Chemical Physics. American Institute of Physics. 31 (2): 459.

[8]- Truesdell, C., and W. Noll. The Non-linear Field Theories of Mechanics. Berlin: Springer-Verlag, 1992. Print.

[9]- Crouse, Bryce. "Stress and Strain." *NDT Resource Center*. National Science Foundation, n.d. Web. 22 Sept. 2014.

[10]- Koffler, Christoph, and Klaus Rohde-Brandenburger. "On the Calculation of Fuel Savings through Lightweight Design in Automotive Life Cycle Assessments." The International Journal of Life Cycle Assessment 15.1 (2010): 128-35. Web.

[11]- Farkas, Diana, Alfredo Caro, Eduardo Bringa, and Douglas Crowson. "Mechanical Response of Nanoporous Gold." *Acta Materialia* 61.9 (2013): 3249-256. Web.

[12]- Erhart, Paul, Eduardo Bringa, Mukul Kumar, and Karsten Albe. "Atomistic Mechanism of Shock-induced Void Collapse in Nanoporous Metals."*Physical Review B* 72.5 (2005): n. pag. Web.

[13]- Ta, Na, Jingyue (Jimmy) Liu, Santhosh Chenna, Peter A. Crozier, Yong Li, Aling Chen, and Wenjie Shen. "Stabilized Gold Nanoparticles on Ceria Nanorods by Strong Interfacial Anchoring." *Journal of the American Chemical Society* 134.51 (2012): 20585-0588. Web.

[14]- Zengin, Gülis, Göran Johansson, Peter Johansson, Tomasz J. Antosiewicz, Mikael Käll, and Timur Shegai. "Approaching the Strong Coupling Limit in Single Plasmonic Nanorods Interacting with J-aggregates."*Scientific Reports* 3 (2013): n. pag. Web.

[15] - "Out-of-Plane Nesting Driven Spin Spiral in Ultrathin Fe/Cu(001) Films"
J. Miyawaki, A. Chainani, Y. Takata, M. Mulazzi, M. Oura, Y. Senba, H. Ohashi, and S. Shin
Physical Review Letters 104, 066407, published online 12 February 2010

[16]- Plimpton, Steve. "Fast Parallel Algorithms for Short-Range Molecular Dynamics." *Journal of Computational Physics* 117.1 (1995): 1-19. Web.

 [17]- H.H. Wu and D.R. Trinkle, "Cu/Ag EAM potential optimized for heteroepitaxial diffusion from ab initio data," Computational Material Science 47, 577-583 (2009).

[18]- M. J. Demkowicz, R. G. Hoagland. "Simulations Of Collision Cascades In Cu–Nb Layered Composites Using An Eam Interatomic Potential." International Journal of Applied Mechanics 01, no. 03 (September 2009): 421-442.

[19]- Honeycutt, J. Dana., and Hans C. Andersen. "Molecular Dynamics Study of Melting and Freezing of Small Lennard-Jones Clusters." *The Journal of Physical Chemistry* 91.19 (1987): 4950-963. Web.

[20]-"High-Performance Computing." *Talon 2.0*. University of North Texas, n.d. Web. 28 Sept. 2014. <http://hpc.unt.edu/>.

[21] - A. Stukowski Visualization and analysis of atomistic simulation data with OVITO - the

Open Visualization Tool Modelling Simul. Mater. Sci. Eng. 18 (2010), 015012

[22] - Honeycutt and Hans C. Andersen. The Journal of Physical Chemistry 1987 91 (19), 4950-4963

[23] - C.J.Ruestes, E.M. Bringa, A. Stukowski, J.F. Rodríguez Nieva, G. Bertolino, Y. Tang, and M.A. Meyers. "Atomistic Simulation of the Mechanical Response of a Nanoporous Body-centered Cubic Metal." *Scripta Materialia* 68.10 (2013): 817-20. Web.

[24]- Bentor, Yinon. "Periodic Table: Melting Point." *ChemicalElements.com*. Pair Networks, 1996. Web. 22 Sept. 2014.