Aluminium nanofoam under tension: Influence of porosity

Gašper Krivic, Sandeep Patil

March, 2021

Abstract

Aluminium foams are very attractive for the industry due to their light weight and high stiffness. Their mechanical properties can be investigated using molecular dynamics simulations. Aluminium nanofoam models were created through the process of deleting the atoms, binding, clustering, annealing and relaxing. Created nanofoams with desired porosity were then used in tensile tests to determine their elastic modulus and strength. Results indicate that more porous aluminium nanofoams show nonlinear decrease in mechanical properties according to power law.

1 Introduction

Metal foams are a new class of materials with low density and great mechanical properties [1]. These foams consist of 5 to 25 % metal and 75 to 95 % of gas. Among others, aluminium foams are especially attractive for many applications like architectural design, light weight construction, orthopaedic, automotive industries, energy absorption, acoustics and thermal applications [2]. There are many experimental [3] and simulation [4, 5] studies researching different properties of aluminium foams. For a better understanding of macroscopic properties Molecular Dynamics (MD) simulations are used to investigate aluminium foams with nanoscale porosity, so called nanofoams [6, 7].

In this project method for creating MD model of aluminium nanofoam with desired porosity was investigated. Furthermore the affect of a porosity on mechanical properties was researched.

2 Method

All MD simulations in this project were carried out using LAMMPS [8], while OVITO [9] was used for visualization.

MD model of a Lennard-Jones (LJ) meta-material was created as proposed in [10], taking into account LJ properties of an aluminium presented in Table 1. All MD simulations used periodic boundary conditions and LJ potential with cut-off radius $2.5\,\sigma$, as it provided most stable results.

In the first step crystal of aluminium with FCC structure and 4.05 A lattice constant was created. Its energy was first minimized with conjugate gradient (CG) algorithm and then equilibrated to 300 K with NVT ensemble followed by NPT ensemble at same temperature and 0.0 bar pressure. Density of a solid aluminium at this point served as a reference for a porosity calculation later on.

In the next step certain number of atoms ranging from 25 to 70 % of total atoms were deleted to induce porosity. Number of atoms deleted at this point however does not represent the final porosity of the material. Final porosity is later determined as the ratio between final density of a nanofoam and density of a solid aluminium from previous step.

Table 1: LJ parameters of aluminum in metal units [11].

σ [A]	2.62
ϵ [eV]	0.3920
mass [g/mol]	26.982

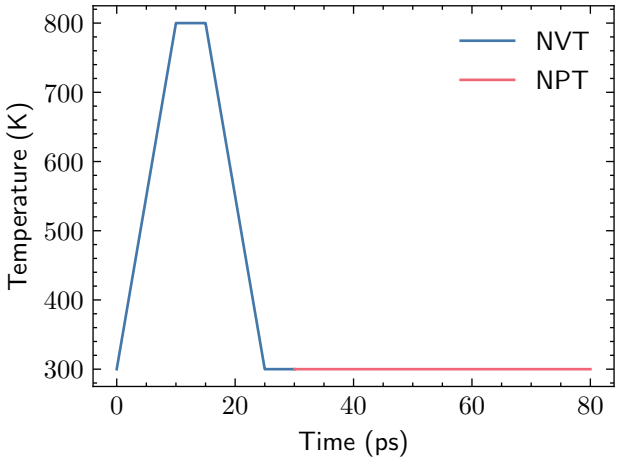


Figure 1: Annealing cycle.

In the third step atoms were let to interact with a high binding energy $\epsilon_{LJ} = 20\,\epsilon$ to make particles stick together. Again NVT ensemble at 300 K was used for 30 ps with addition to *temp/rescale* to counteract a high energy increase due to change in the interatomic potential, to prevent system from exploding.

Next cluster detection algorithm was used to select the largest group of connected atoms to get foamy structure without individual atoms within voids. Density-based spatial clustering of applications with noise (DBSCAN) [12] algorithm implemented in Python sklearn library [13] was used. In short, first random atom is selected and it's neighborhood area is determined using specified maximum radius. If there is at least one other atom in the neighborhood they formed a cluster and the neighborhood is increased by maximum radius area around new atom. This process is continued until no new atom is added to the cluster. When no more atoms are left to check, the biggest cluster forms a interconnected spongy structure and is therefore kept. At this point we were left with an unstable foamy structure due to the absence of atoms within a starting volume, which needs to be relaxed in the next step.

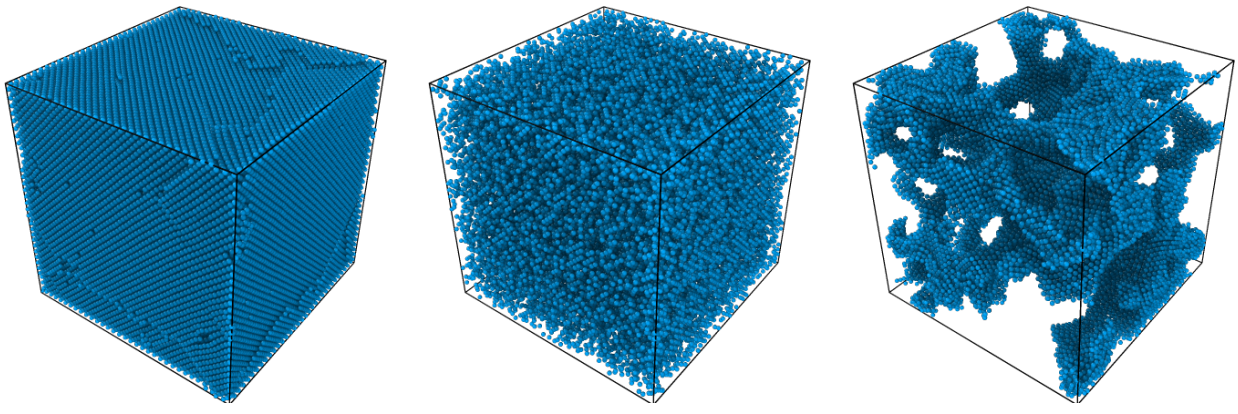
The relaxation is done through an annealing process. First structure energy was minimized using CG algorithm followed by equalibration at 300 K in NVT ensemble again with addition of *temp/rescale* to compensate the change in the interatomic potential. After that annealing cycle in NVT ensemble started with heating the structure to 800 K at 50 K/s heating rate. Then structure was held at 800 K for a 5 ps until it was cooled down to 300 K again with 50 K/s cooling rate and stabilized for 5 ps at that temperature. Now we were left with high internal compressive stresses, which were relaxed using NPT ensemble. Temperature was kept at 300 K and pressure at 0.0 bar for 50 ps until stable structure was reached. Described process can be seen on a Figure 1. At this point real porosity ϕ of an aluminium nanofoam, defined as the ration of the volume of voids over the total volume, was determined as:

$$\phi = 1 - \frac{\rho}{\rho_0}, \tag{1}$$

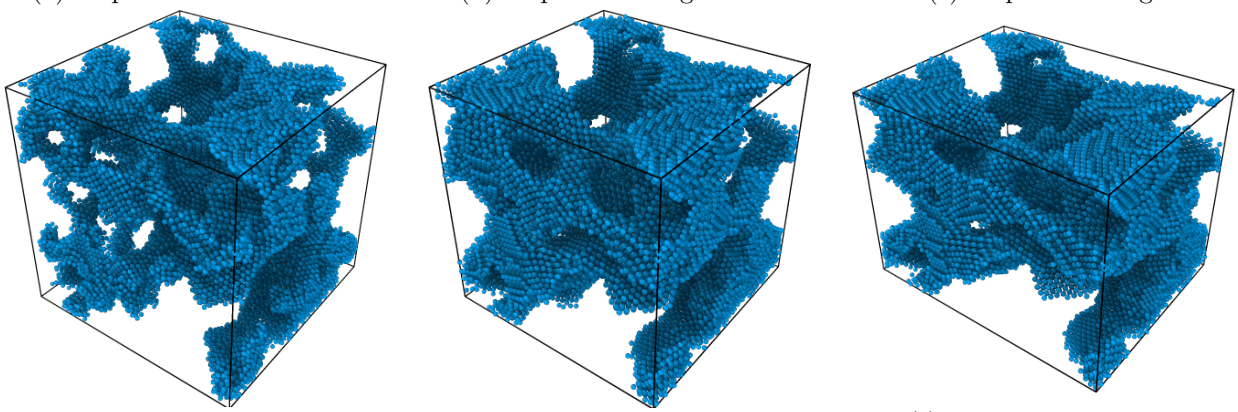
where ρ represents the density of a structure at this point and ρ_0 density of a solid aluminium at the end of a step 1.

Finally uniaxial tension test was carried out. First structure energy was minimized with CG followed by equalibration in NVT for 5 ps and NPT for 2 ps at 300 K and 0.0 bar respectively. Tensile test was performed in combination of NVE and NPT ensemble with additional *langevin* and *temp/rescale* thermostat to keep temperature at 300 K and pressure at 0.0 bar. Deformation was induced using *deform* command with engineering strain rate of 0.02 ps^{-1}. Tensile test was performed in all three directions independently with the same structure to minimize the effect of voids shapes and directions.

Snapshots of a structure with 0.60 porosity at each described step can be seen on a Figure 2.



(a) Step 1: Lattice creation. (b) Step 2: Deleting atoms. (c) Step 3: Binding.



(d) Step 4: Clustering. (e) Step 5: Relaxing. (f) Step 6: Tensile test.

Figure 2: Snapshots of an aluminium nanofoam MD model with 0.60 porosity at each creation step.

3 Results and discussion

Creating a stable foam structure was the biggest challenge. Stability was monitored through a density during a relaxation process in step 5. Figure 3 shows density during relaxation process for each aluminium nanofoam. In the beginning sudden change in the density can be observed, due to a built up compression stresses in previous treatments. Then density slowly converges towards a final value of a stable structure. Density increase is higher for more porous structures, owing to a higher deficit of atoms. In the case of structures with a lower amount of deleted atoms, which correlates to a lower porosity, stable structure was reached during relaxation time. However for structures with a higher porosity that was not the case. In the cases of structures with highest porosity simply increasing the relaxation time did not lead to a stabilization in density. It was steadily increasing but stable point was not reached, which indicates that other parameters need to be adjusted as well. Varying annealing temperature, cooling rates and number of cycles should lead to a stable foam structures even at higher porosities. In this project though same relaxing process was used for all structures, due to limited computational resources. Still one can see that in most cases change in the density towards the end is minimal. With that it was concluded that structures are at least quasi stable.

Next relation between percentage of deleted atoms from starting structure and final porosity was investigated. As shown in a Figure 4 the relation seems to be nonlinear. Where higher percentage of deleted atoms has higher effect on the porosity and vice versa. Mainly due to the fact, that if small number of atoms is deleted tiny voids are formed in the structure. Those voids then tends to be closed by attractive forces among atoms resulting in lower porosity. This process is nonlinear due to nonlinearity of an interatomic potential itself. On the other hand, when deleting high percentage of atoms more clusters get created after binding. Whereas only the largest connected group of atoms is kept after clustering, which results in nonlinearly higher porosity.

All created aluminium nanofoam MD models after relaxation can be seen on a Figure 5. Porosities are ranging from 0.23 to 0.66. All analysis are concluded using those structures.

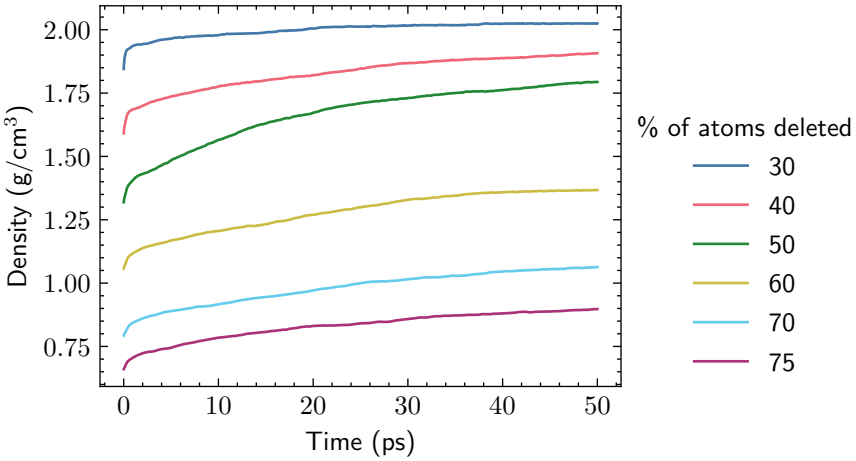


Figure 3: Density during relaxation process.

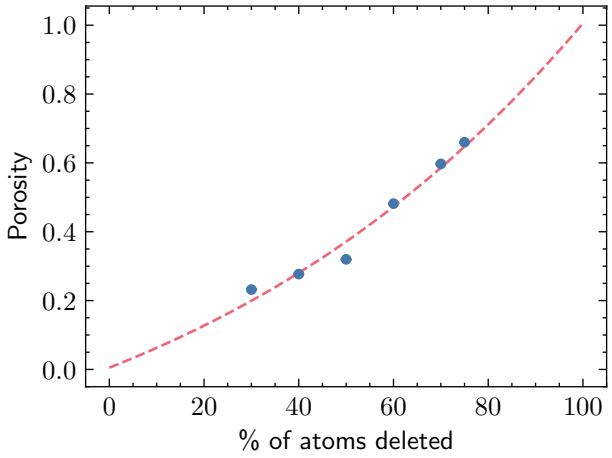
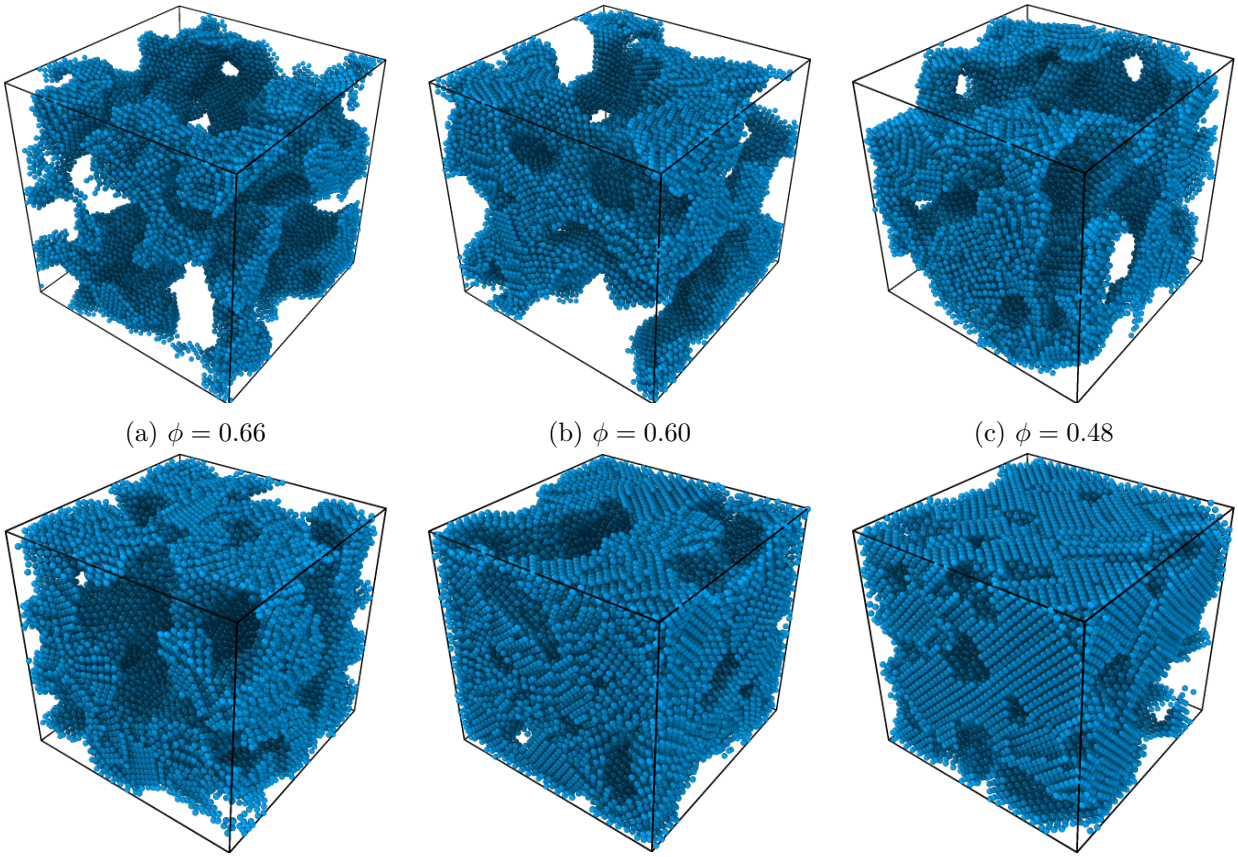


Figure 4: Porosity as a function of percentage of atoms deleted from starting structure.

Figure 6 shows obtained stress strain curves from uniaxial tensile tests. All the structures display high ductility. Aluminium on its own is a highly ductile material and this only increases with porosity. All porous structures behave nonlinearly. At very low strains, below 0.03, they show linear behaviour, which then transition into highly nonlinear that can undergo large deformation, above 0.2 strain, before failure. From the linear part elastic modulus was calculated. Results in relation to porosity are shown on Figure 7. Also ultimate stress was gathered as the highest stress during tensile test. Its relation to the porosity can be seen on Figure 8. Both elastic modulus and ultimate stress show a power relationship with porosity as proposed in [14, 15]. Higher porosity leads to lower elastic modulus and ultimate stress, due to increase in voids. Both then increase nonlineraly with a lower porosity. It is important to note that orientation of the structure plays important role in determination of properties. A different orientation might lead to a different behaviour under the load. Theoretically the more random the structure, the less the influence of its orientation to the direction of loading. Therefore to get a better estimation of properties more porous structures need to be created.



(a) $\phi = 0.66$ (b) $\phi = 0.60$ (c) $\phi = 0.48$

(d) $\phi = 0.32$ (e) $\phi = 0.28$ (f) $\phi = 0.23$

Figure 5: MD models of aluminium nanofoams with corespondent porosity.

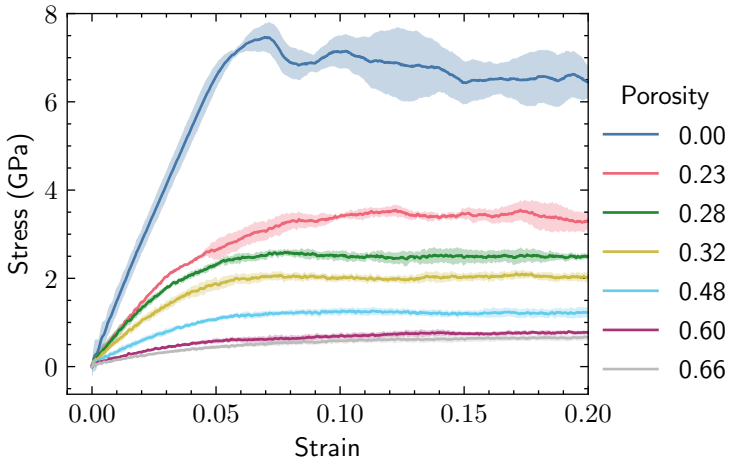


Figure 6: Stress-strain curves of aluminium nanofoams at strain rate 0.02 ps^{-1}.

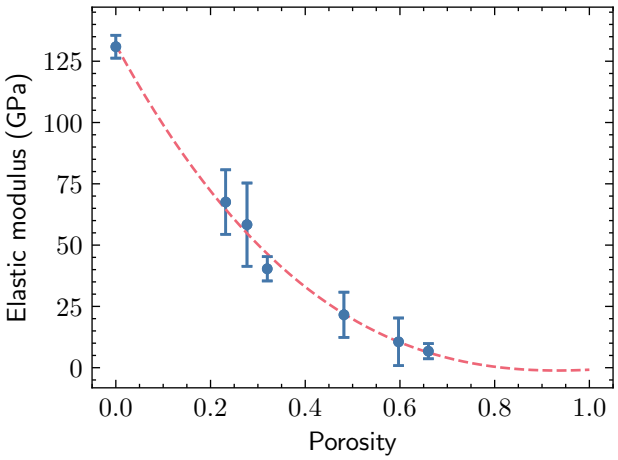


Figure 7: Elastic modulus vs. porosity of aluminium nanofoams.

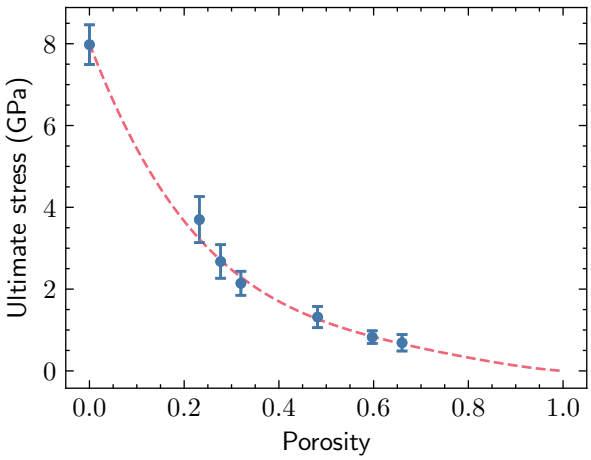


Figure 8: Ultimate stress vs. porosity of aluminium nanofoams.

4 Conclusions

In this project MD models of aluminium nanofoams with different porosity were created. Tensile tests were carried out to analyse their mechanical properties. Following conclusion were drawn from the project.

The results show a lower actual porosity in comparison to the percentage of atoms deleted from original structure. In order to obtain nanofoam with desired porosity more atoms should be deleted.

Elastic modulus and strength decrease significantly with increasing porosity according to power law.

In future simulations steps towards stable structure should be taken. Affect of the annealing time and temperature should be further researched. Also more nanofoams with same porosity should be tested to minimize the effect of a voids orientation.

References

[1] Michael Ashby, Tony Evans, and N. A Fleck. *Metal Foams: A Design Guide.* Elsevier, Burlington, 2000.

[2] J. Dineshkumar, T. Jesudas, and R. Elayaraja. Characteristics, applications and processing of aluminium foams – A Review. *Materials Today: Proceedings*, 2021.

[3] Lijuan Su, Haiqing Liu, Guangchun Yao, and Jinlong Zhang. Experimental study on the closed-cell aluminum foam shock absorption layer of a high-speed railway tunnel. *Soil Dynamics and Earthquake Engineering*, 119:331–345, April 2019.

[4] P. J. Tan, J. J. Harrigan, and S. R. Reid. Inertia effects in uniaxial dynamic compression of a closed cell aluminium alloy foam. *Materials Science and Technology*, 18(5):480–488, May 2002.

[5] Ying Zhao, Zhaohan Yang, Tianlai Yu, and Dabo Xin. Mechanical properties and energy absorption capabilities of aluminium foam sandwich structure subjected to low-velocity impact. *Construction and Building Materials*, 273:121996, March 2021.

[6] Nina Gunkelmann, Eduardo M. Bringa, and Yudi Rosandi. Molecular Dynamics Simulations of Aluminum Foams under Tension: Influence of Oxidation. *J. Phys. Chem. C*, 122(45):26243–26250, November 2018.

[7] Nina Gunkelmann, Yudi Rosandi, Carlos J. Ruestes, Eduardo M. Bringa, and Herbert M. Urbassek. Compaction and plasticity in nanofoams induced by shock waves: A molecular dynamics study. *Computational Materials Science*, 119:27–32, June 2016.

[8] Steve Plimpton, Axel Kohlmeyer, Aidan Thompson, Stan Moore, and Richard Berger. LAMMPS Stable release 29 October 2020. Zenodo, October 2020.

[9] Alexander Stukowski. Visualization and analysis of atomistic simulation data with OVITO–the Open Visualization Tool. *Modelling and Simulation in Materials Science and Engineering*, 18(1):015012, December 2009.

[10] Y Rosandi and B Wijatmoko. Generation of nanoporous model using sequential annealing and largest cluster selection method. *J. Phys.: Conf. Ser.*, 1080:012027, August 2018.

[11] Haiyan Zhang, Li Cunhui, Meiwen Zhao, Yingmin Zhu, and Weidong Wang. The influence of interface wettability on normal and explosive boiling of ultra-thin liquid films on a heated substrate in nanoscale: A molecular dynamics study. *Micro & Nano Letters*, 12, July 2017.

[12] Erich Schubert, Jörg Sander, Martin Ester, Hans Peter Kriegel, and Xiaowei Xu. DBSCAN Revisited, Revisited: Why and How You Should (Still) Use DBSCAN. *ACM Trans. Database Syst.*, 42(3):1–21, August 2017.

[13] Sklearn.cluster.DBSCAN — scikit-learn 0.24.1 documentation. https://scikit-learn.org/stable/modules/generated/sklearn.cluster.DBSCAN.html.

[14] M.F Ashby. The properties of foams and lattices. *Phil. Trans. R. Soc. A.*, 364(1838):15–30, January 2006.

[15] L. J. Gibson. Cellular Solids. *MRS Bulletin*, 28(4):270–274, 2003.