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Utilizing LAMMPS Simulation to Assess Different Alloys under Compression

Abstract

In this experiment, LAMMPS software is used to simulate various metals and alloys under compression in order to justify the use cases of these materials as well as understand the short comings to the molecular dynamic simulation. Normally, this would be done mechanically by placing the material in a compression test machine. This, however, requires more time and funding to acquire data. While mechanical testing should not be eliminated, computer simulation software like LAMMPS will be able to identify favorable materials before testing. In this way, the utilization of this experiment will be interesting toward product developing entities whose end product is of that expecting to bear compression stress. The experiment will help them utilize similar methods to test materials computationally and thus save time and money. With computer simulation, it is important to understand the assumptions that are behind each calculation. Not understanding this and fully relying on simulation data will dismiss variable defects in the material that might otherwise cause failure at lower levels of stress. Simulations will take approximately 4-5 hours in total with data analysis taking about 3 hours following. In order to determine success of this experiment, comparisons to literature will be drawn to see if the overall rank of the compressive yield strength is similar to that found in literature as well as their percent difference in magnitude.

Introduction

In compression stress testing, a load is applied to a material in order to reduce strain instead of elongating a material like in tensile stress testing. Similar to the stress-strain curve for tensile testing, an analogous compressive yield strength and Young's Modulus can be determined for Hookean materials.

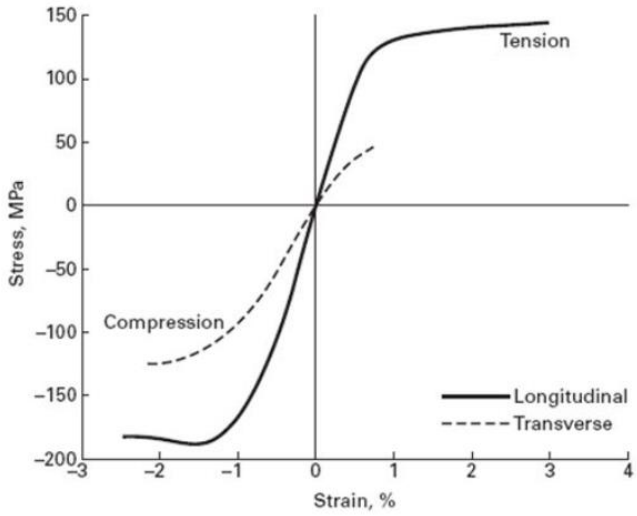

Figure 1. General Modeling of Tension vs Compression Stress Strain Curve [1]

LAMMPS is an open source software tool for molecular dynamic simulation developed by Sandia National Lab. In molecular dynamics simulations, the atom's physical movement is analyzed. By giving atoms time to interact with one another, the simulation will update atom location and continuously do so in order to observe the evolution of the system as the material is compressed.

Methods

To conduct this experiment, LAMMPS requires the use of a .in file (input file) that will be fed into the LAMMPS software thus running the molecular dynamics simulation. This will be done for samples of Aluminum (Al), Copper (Cu), Iron (Fe), and Iron-Nickel (Fe-Ni). It is important to acquire interatomic potentials to correspond to each one of these metals and alloys in order to correctly shift the atoms in the simulation for each time step. This can be found through the interatomic potential website developed by NIST [2]. It is important to note that for the simulation of the two-element alloy of Iron and Nickel the USER-MEAMC package has to be used, however the package is no longer supported as of December 2018. To utilize this package an older version of the LAMMPS repository was downloaded and utilized for Iron-Nickel from Github. In the initialization process step of setting the input file, the lattice parameter has to be set to the correct value, which is 4.05 Å for Al, 3.597 Å for copper, 2.87 Å for Iron [3], and 6.629 Å for Fe-Ni [4]. In addition, the input files have to create atomic lattices for each of the elements, in which case each were assumed to have an FCC lattice structure. Foe Fe-Ni however, two lattice structures had to be created and properly transposed within the lattice simulation box created. To acquire data to plot the stress-strain curve the values are deposited into variables that are later dumped into a text file for graphing. It is important to note that compression stress is applied in one direction, which in this case is the x -direction. As such, the stress strain curve produced in the x-direction is the only thing that is meaningful as the stress-strain curve for those created by stress in the y and z direction will represent non-parametric noise and will not be meaningful to interpret. By acquiring and plotting this data the Young's modulus can be found by extrapolating the value through a linear fit through the elastic region. In addition, yield strength can be identified in the data and validated by the graph.

Results

The stress-strain diagram for Aluminum under compression is given by the graph below.

Figure 2. Aluminum seems to be showing Hookean behavior under tensile loading.

The compressive yield strength is 5.57 GPa (we can take the absolute value since the graph is in the third quadrant due to direction of stress and strain). As seen by the elastic regime from [0, -0.108], the elastic regime can be fit to a linear model in order to extrapolate an estimate for Young's Modulus.

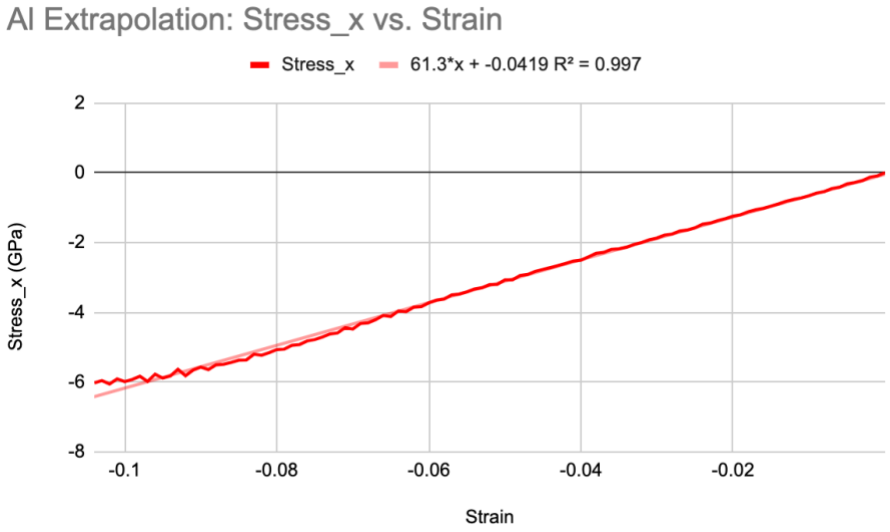

Figure 3. Aluminum extrapolation of Young's modulus from elastic regime.

Based on the fit given in the graph above. The Young's modulus was determined to be 61.3 GPa. The stress-strain diagram for Cu is given below.

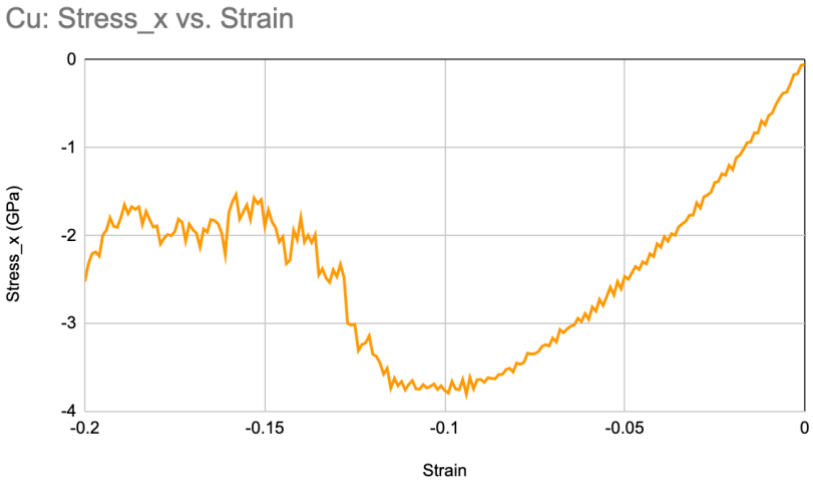

Figure 4. Compressive Hookean behavior from Copper is seen here.

Compressive yield strength is given by 3.09. The elastic regime is found to be in the range of [0, -0.082] and a linear fit is mapped to this range to extrapolate Young's modulus.

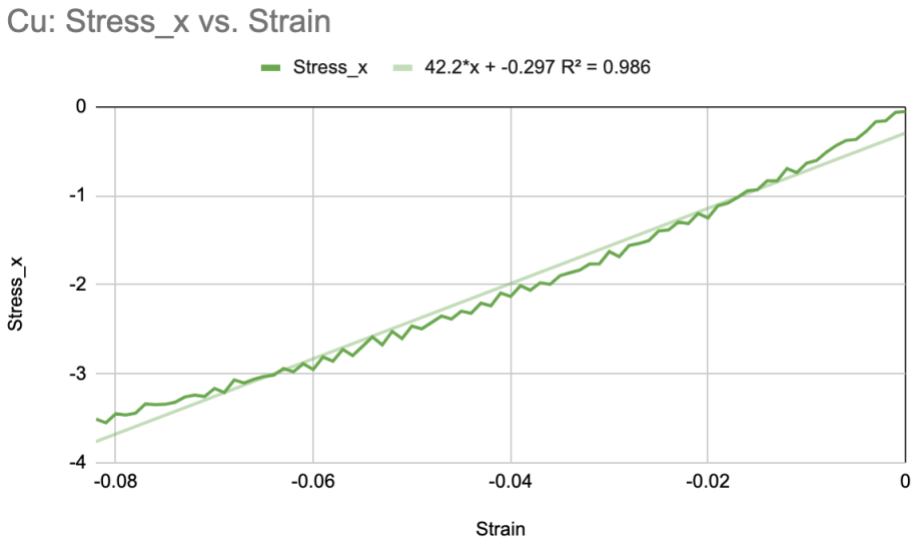

Figure 5. Copper linear fit along elastic region to extrapolate Young's Modulus

Based on the linear fit above, the Young's Modulus was found to be 42.2 GPa. The stress-strain graph for Fe is given below.

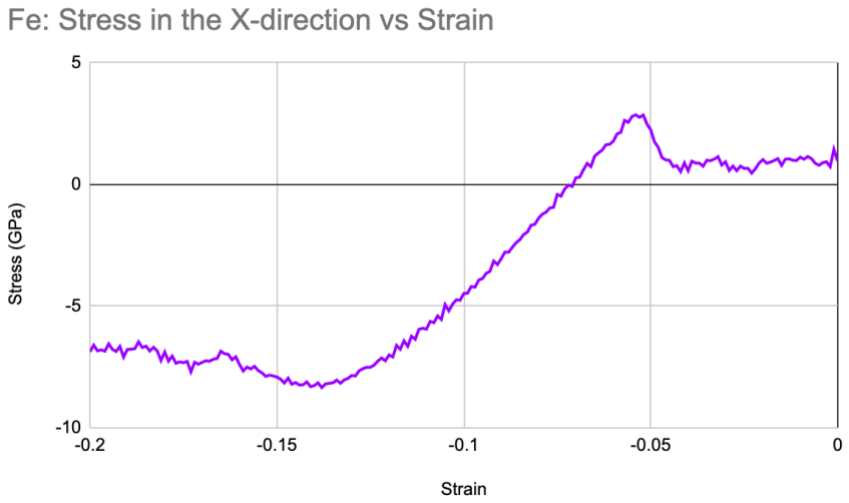

Figure 6. Iron Hookean Compressive Behavior

The compressive yield strength is found to be 7.13 GPa. In addition, the range of the elastic region is given by [-0.057, -0.122]. From this range, a linear fit is created to extract a Young's modulus estimate.

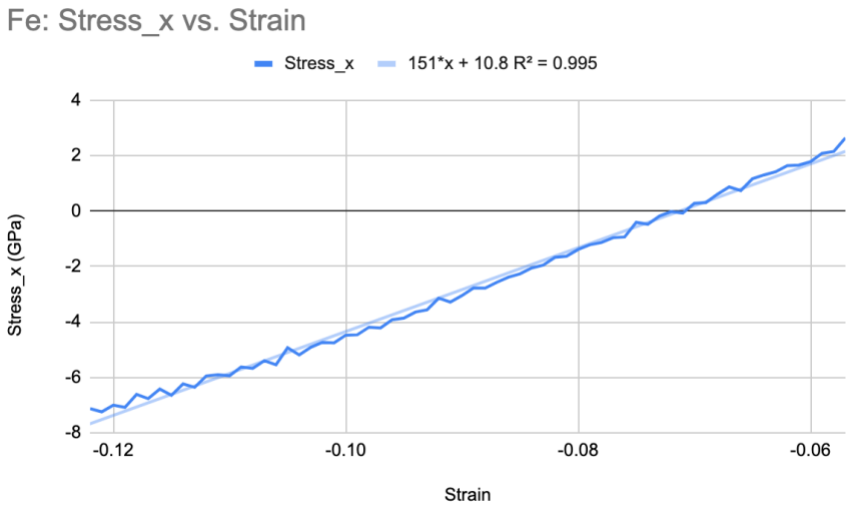

Figure 7. Linear fit along iron elastic regime.

From the produced linear fit, the Young's modulus is found to be 151 GPa. Finally, the stress strain curve for Fe-Ni is given below.

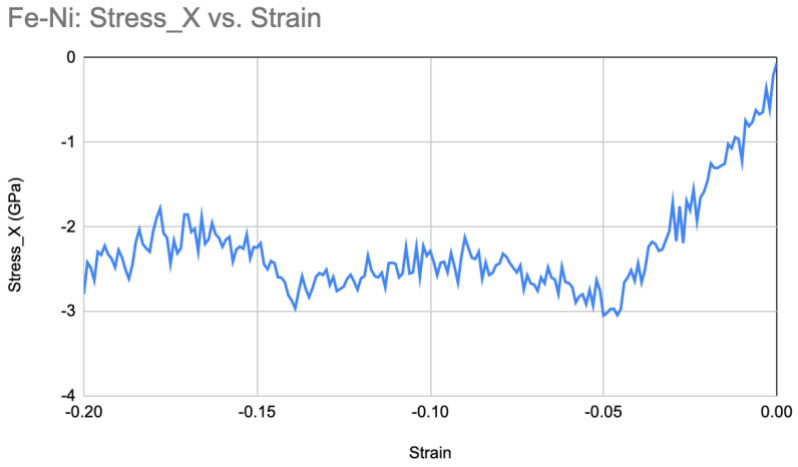

Figure 8. Hookean Compressive Behavior for Fe-Ni.

Figure 8. Stress strain curve for Fe-Ni alloy which exhibits roughly Hookean behavior

The compressive yield strength is found to be 2.66. The range of the elastic regime was estimated to be [0, -0.044]. Using the linear fit show below,

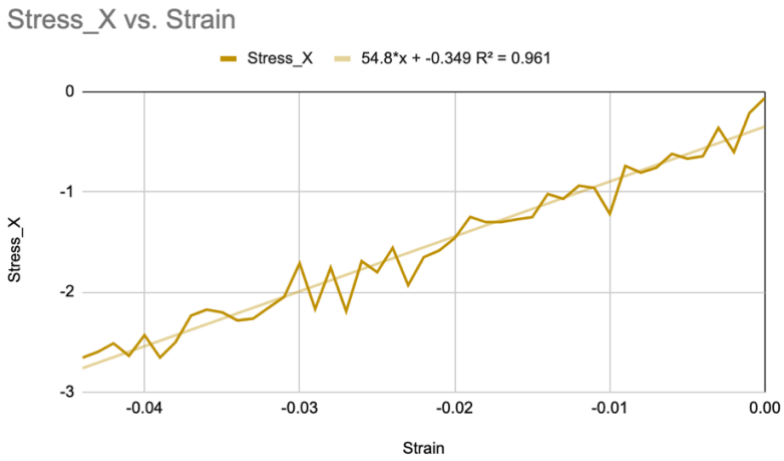

Figure 9. Linear fit to extrapolate Young's Modulus for Fe-Ni

The Young's modulus was found to be 54.8 GPa. Summarizing the data in Table 1 below, the three-key metrics of compressive yield stress, ultimate yield stress, and Young's modulus are collected as well as comparing literature values.

Table 1. Simulated and Literature values found for the following compounds. The (number) represents the rank of the Young's Modulus

Metal/ Alloy	Simulated Compressive Yield Stress	Simulated Young's Modulus	Literature Compressive Yield Stress	Literature Young's Modulus
Aluminum (Al)	5.57 GPa	61.3 Gpa (3)	330 Mpa [5]	68 Gpa [5] (1)
Copper (Cu)	3.09 Gpa	42.2 Gpa (1)	330 Mpa [6]	133 Gpa [6] (2)
Iron (Fe)	7.13 Gpa	151 Gpa (4)	220 Mpa [7]	204 Gpa [7] (4)
Iron-Nickel (Fe-Ni)	3.05 Gpa	54.8 Gpa (2)	240 Mpa [8]	137 Gpa [8] (3)

Discussion

From the collected data, it can be seen that when comparing the simulated compressive yield stress with the literature compressive yield stress, the simulated values are magnitudes above those found in literature. This highlights the tendency for the LAMMPS simulation to utilize perfect lattice structures in simulation. In this way, the simulation does not account for material defects that could arise from vacancies, interstitials, or dislocations that be located within our structure that would hinder the compressive yield stress.

The Young's modulus calculated from the compressive load can also be an effective measurement to understand how the specimen can resist change as it shows the amount of stress it can withstand per increment of strain. In addition, since the compressive yield stress for each substance can often be given by a range, the elastic modulus is a more effective measurement to determine the accuracy of the simulation. Table 2 below shows the percentage error between the simulated and literature young's modulus.

Table 2. Percent Error for the simulated young's modulus compared to the literature

Metal/Alloy	Percentage Error for Young's modulus
Aluminum (Al)	9.85%
Copper (Cu)	68.27%
Iron (Fe)	25.9%
Iron-Nickel (Fe-Ni)	60%

The large percent errors show that there are inaccuracies given by the simulation. In addition, the order of the Young's modulus for the specimens are only correct for Iron-Nickel. As such, these shortcomings should be noted as an important risk as this can when fully depending on simulated results for end product solutions.

By analyzing the literature values for the elastic modulus of the materials in order to study the use cases of the material. The Young's modulus can be thought of as the material's ability to resist strain when a force is applied. As such, the highest Young's modulus is favorable. However, it is important to not how alloying metals can achieve favorable properties like high Young's modulus and allow for the use of cheaper materials. In turn, this concept is important when developing products as this can drastically effect cost as well.

Conclusion

In conclusion, the experiment was not successful in terms of the designated metric of success initially set at the beginning of the experiment. This could be due to potential inaccuracies in the initialization of the atom. Since each of these tested specimens have different favorable lattices, configuration for the initialization was created through research and the documentation of the pseudo potentials in the repository. Straying from the favorable configuration of the specimens can result in large differences in the end result. While simulations are a helpful component in the driving force for innovation by providing a means to test without the constraint of time or funding, it is important to understand the risks of relying completely on simulated data to draw end product conclusions.

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