A Comparison Study of Metals Mechanical Properties Under Tensile Loading Using Molecular Dynamics Simulations

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Abstract

Molecular dynamics simulations have become essential in material science research. An important first step in molecular dynamics is to become familiar with Lammps - Large-scale atomic/molecular massively parallel simulator. This study employs the Lammps application to conduct simulations of tensile loading on different metals, including aluminum (Al), iron (Fe), nickel (Ni), and copper (Cu). The objective is to collect stress-strain data for the purpose of determining material's strength including Young's modulus and Ultimate Tensile Strength (UTS). It was found that out of the four metals, Ni exhibits significantly higher Ultimate Tensile Strength (UTS).

Introduction

The material strength is determined by its greatest load-bearing capacity. The Young's modulus and yield strength can be calculated by determining mechanical stress and strain using a tensile test. Computational methods such as molecular dynamics simulations, Monte Carlo simulation and discreteness simulation facilitate the visualization of metal deformation at the atomistic level. The Stress-Strain Curve can demonstrate mechanical qualities such as ductility and brittleness. Hook's Law states that stress and strain have a direct proportionate relationship. The modulus of elasticity can be determined by utilizing the proportional limit in the Stress-Strain curve.

$$Stress(\sigma) \quad \alpha \quad Strain(\varepsilon)$$

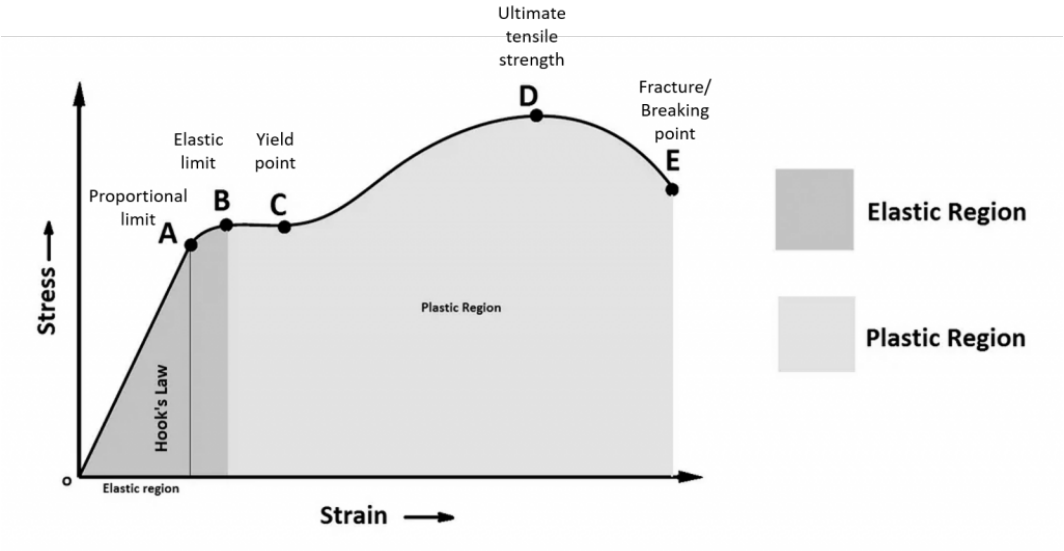


Figure 1: Stress-Strain Curve

The ultimate tensile strength (UTS) refers to the highest level of stress that a material can endure when subjected to stretching or pulling through tensile loading. Materials with higher ultimate tensile

strength have greater ductility, whereas brittle materials have ultimate tensile strengths that are closer to their yield points.
This study utilizes atomistic simulations to examine the modulus of elasticity and ultimate tensile strength of four selected metals.

Methodology

The simulation was performed using large-scale atomic/molecular massively parallel simulator (LAMMPS) [1] with a constant timestep of 1 fs. LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales. A cubic shape was taken using the respective lattice parameters units 10 in x, y, and z directions. The size of the cube varied with respect to the lattice parameter of metals Al, Fe, Ni and Cu; but the total number of atoms were constant at 4000. A periodic boundary condition was imposed in three directions to imitate infinite shape. The interaction potential was described by the embedded-atom method (EAM) potential developed by Y. Mishin *et al* (Al [2], Fe [3]), X. W. Zhou *et al* (Cu [4], Ni [4]). To initiate velocities, Maxwell-Boltzmann distribution was applied. Prior to tension loading, energy minimization using conjugated gradient method was applied, using Nose/Hover isobaric isothermal ensemble the cube was relaxed for 20 picoseconds. The tension load was performed in the x direction [100] using $1 \times 10^{10} s^{-1}$.

Results

Mechanical property analysis:

In Figure 2: Stress - Strain Curve Comparison, stress vs strain data has been plotted for Al, Fe, Ni and Cu. The elastic region (where stress is proportional to strain) is much smaller for Fe, conversely, Ni has the highest plastic region. From the graph, it can be inferred that Ni is more ductile than the other three materials. Materials with higher modulus of elasticity will be stiffer than those with lower modulus of elasticity. As shown in Table 1, Fe with 128.19 GPa of young's modulus will be stiffer material than Cu with only 46.07 GPa.

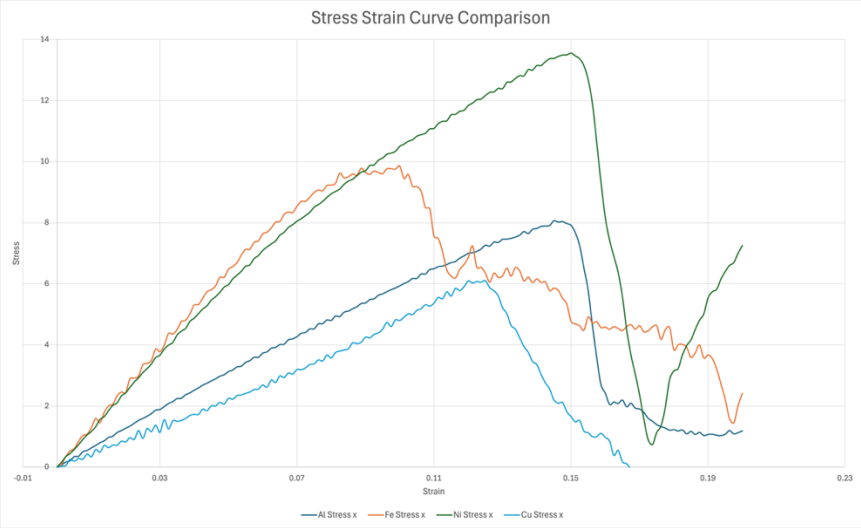


Figure 2: Stress - Strain Curve Comparison

In general, materials with high young's modulus withstands higher tensile load. However, Ni has lower elastic modulus of 116.61 GPa than Fe, it was found that it can withstand more tensile load than the

other materials including Fe. In the figures Figure 4 and Figure 5, the comparison is shown by using column graphs.

Table 1: Mechanical Properties of metals

Metals	E (GPa)	UTS (GPa)
Al	58.94	6.49
Fe	128.19	7.64
Ni	116.61	8.05
Cu	46.07	4.25

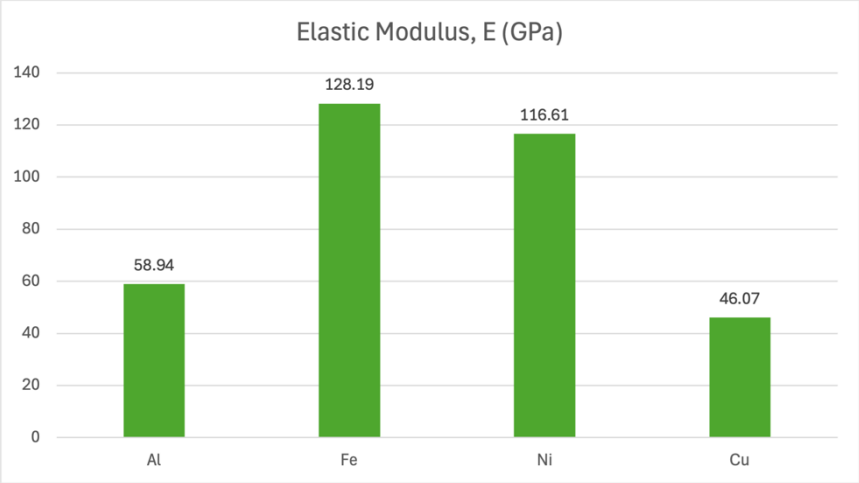


Figure 3: Elastic Modulus Comparison among Al, Fe, Ni and Cu

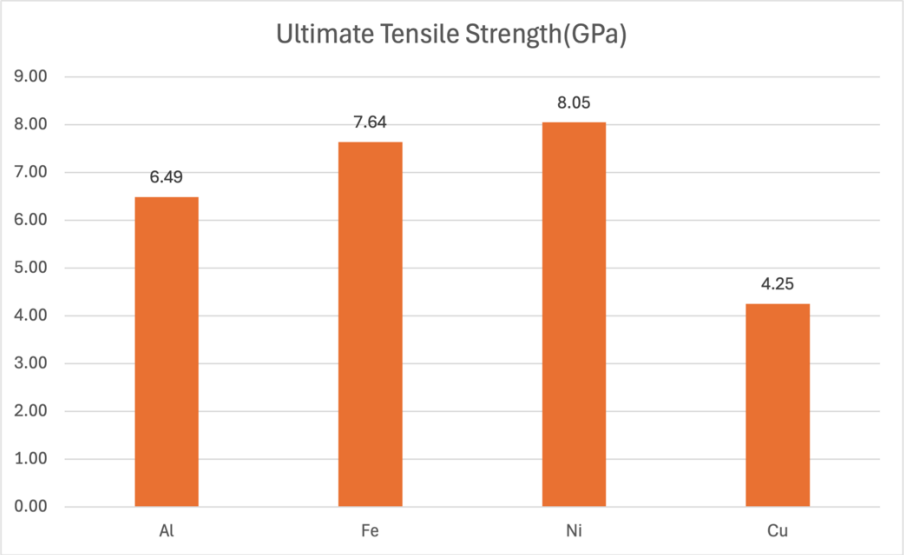


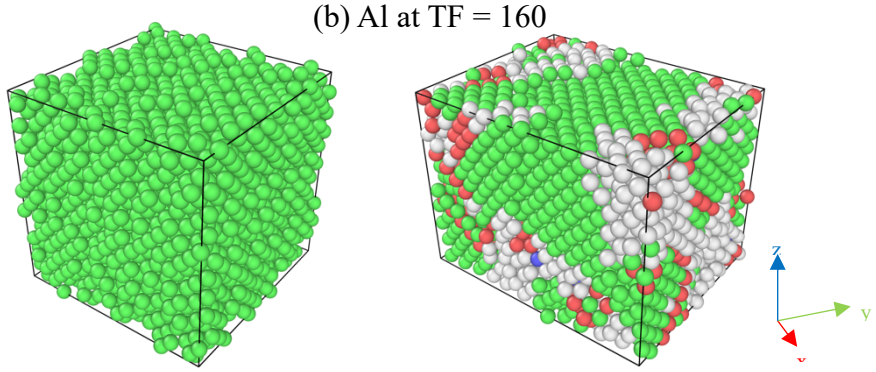
Figure 4: Ultimate Tensile Strength comparison among Al, Fe, Ni and Cu

Analysis of atomistic deformation:

The deformation was observed using OVITO [5] for all 4 materials. Although the tensile loading was directed at x direction, Ni deformed mostly in y direction whereas, Cu did in the z directions. Ni and Cu both formed twin at the end of the simulations.

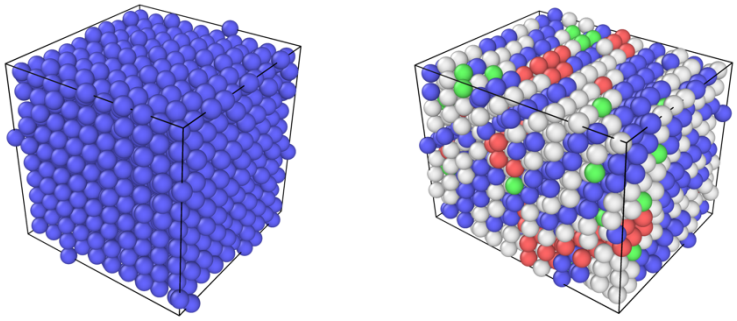
(a) Al at TF = 0

(b) Al at TF = 160



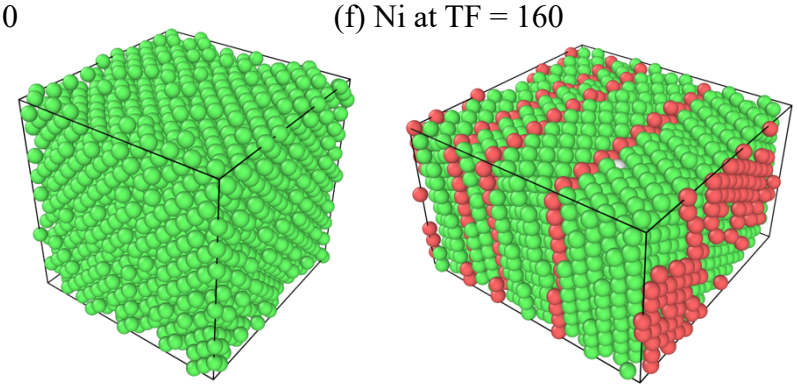
(c) Fe at TF = 0

(d) Fe at TF = 160



(e) Ni at TF = 0

(f) Ni at TF = 160



(g) Cu at TF = 0

(h) Cu at TF = 160

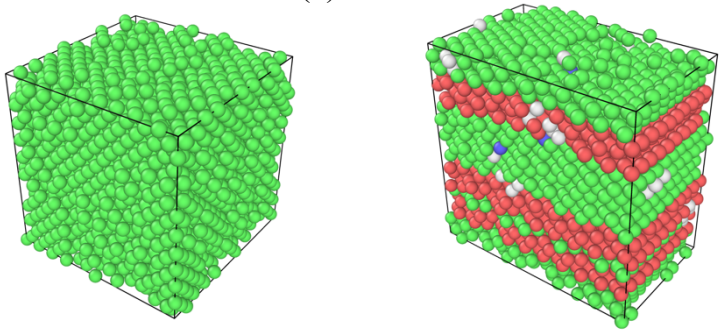


Figure 5: Atomic Visualization using OVITO of timeframe start (0) and end (160) of Al, Fe, Ni, and Cu

Using Common Neighbor Analysis modifier in OVITO, the metals were visualized in Figure 5 at timeframe (TF) 0 and 160.

Conclusion

The high strength of Ni can be used for machining components which are subjected to high stress, and as for Fe, is more suitable for rigidity. Here, Cu provides a good balance of stiffness and strength, makes it a good material to use for electric conductors. On the other hand, Al has moderate strength and stiffness. Being a lightweight material, Al can be a good choice for aircraft materials where moderate stiffness is required.

Acknowledgement

This study was solely focused on gaining hands-on experience with Molecular Dynamics Simulations, and skills of related tools like LAMMPS and OVITO to further practice the researcher's learning from the workshop "Elements of ICME Research Workshop" by Professor Andrew L. Ferguson in 2014.

Reference

[1] S. Plimpton, "Fast Parallel Algorithms for Short-Range Molecular Dynamics," *Journal of Computational Physics 117,* p. 117, 1995.

[2] D. F. M. M. a. D. P. Y. Mishin, "nteratomic potentials for monoatomic metals from experimental data and ab initio calculations," *Physical Review B,* vol. 59, no. 5, pp. 3393-3407, 1999.

[3] N. P. Y. M. a. D. P. H. Chamati, "Embedded-atom potential for Fe and its application to self-diffusion on Fe(100)," *Surface Science,* vol. 600, no. 9, pp. 1793-1803, 2006.

[4] R. J. a. H. W. X.W. Zhou, "Misfit-energy-increasing dislocations in vapor-deposited CoFe/NiFe multilayers," *Physical Review B,* vol. 69, no. 14, p. 144113, 2004.

[5] A. Stukowski, "Visualization and analysis of atomistic simulation data with OVITO–the Open Visualization Tool," *Modelling and Simulation in Materials Science and Engineering,* vol. 18, no. 1, p. 015012, 2010.

[6] Z. T. a. C. B. L.M. Hale, "Evaluating variability with atomistic simulations: the effect of potential and calculation methodology on the modeling of lattice and elastic constants," *Modelling and Simulation in Materials Science and Engineering,* vol. 26, no. 055003, 2018.