MSE 203 : Introduction To Computational Materials

- STUDY THE EFFECT OF ALLOYING ON MECHANICAL PROPERTIES OF A HIGH ENTROPY ALLOY

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Introduction

Introduction to High-Entropy Alloys (HEAs)

HEAs: Multi-component alloys with equal or nearly equal concentrations of five or more elements.

Key Features of HEAs:

High Strength & Hardness

Excellent Thermal Stability

Good Corrosion Resistance

Applications:

Aerospace, Energy, Defense

Challenges in Understanding HEAs:

Deformation mechanisms at the atomic scale remain poorly understood.

Limited data from experimental studies at extreme conditions (high temperatures and strain rates)

Motivation

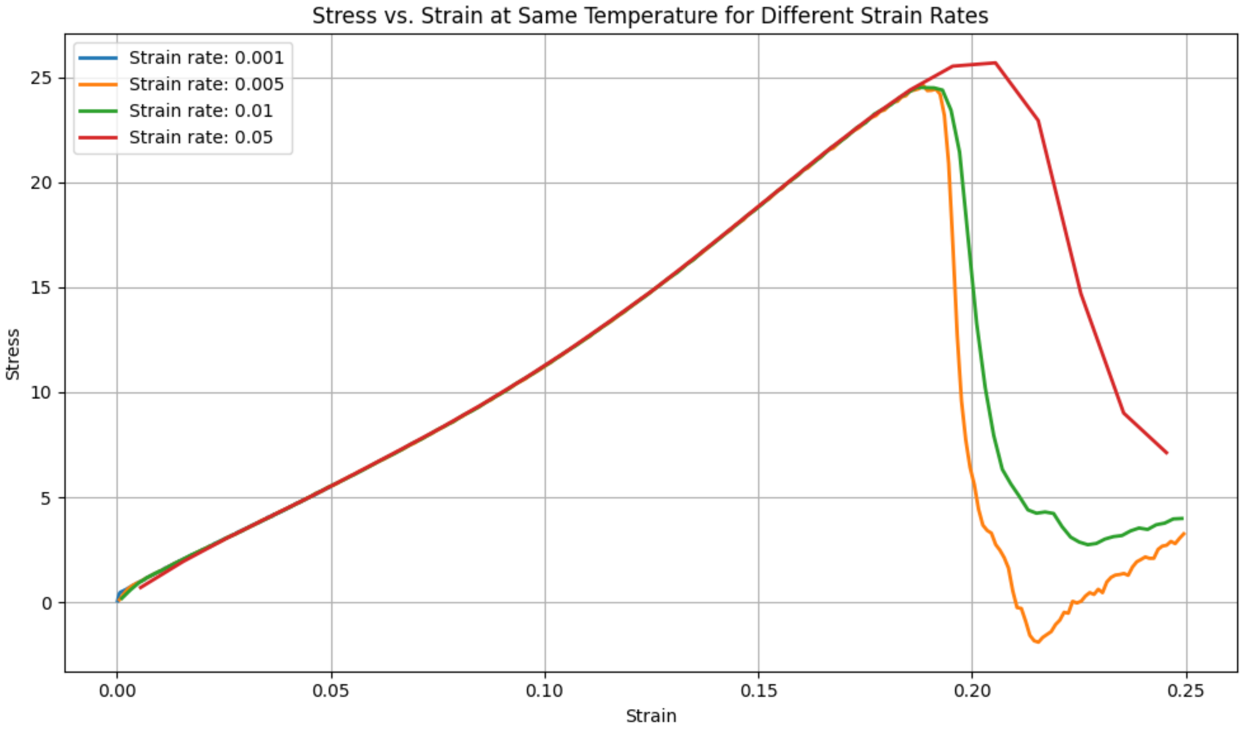
Why This Study?

- Industry Need:
  Advanced materials for extreme environments (aerospace, energy, defense).
- Challenge:
  Experimental limits hinder atomic-scale understanding of deformation at varied temperatures and strain rates.
- Our Solution:
  Use Molecular Dynamics (MD) simulations on CoCrCuFeNi HEA.
- Objectives:
  - Study effects of temperature (100–800 K) and strain rate (0.001–0.05/ps)
  - Analyze yield strength and fracture mechanisms
- Goal:
  Guide design of next-generation high-performance materials.

Simulation Methodology

- **Software:** LAMMPS (for molecular dynamics)
- **Potential Used:** EAM (Embedded Atom Method) – ideal for metals and HEAs
- **Structure & Setup:** FCC crystal; box size $100 \times 40 \times 40$ Å^3
- **Loading Conditions:**
  - **Type:** Tensile and compressive
  - **Strain rates:** 0.001 to 0.05 ps^{-1}
- **Temperature Range:** 100K to 800K
- **Visualization:** OVITO used to analyze atomic behavior and deformation

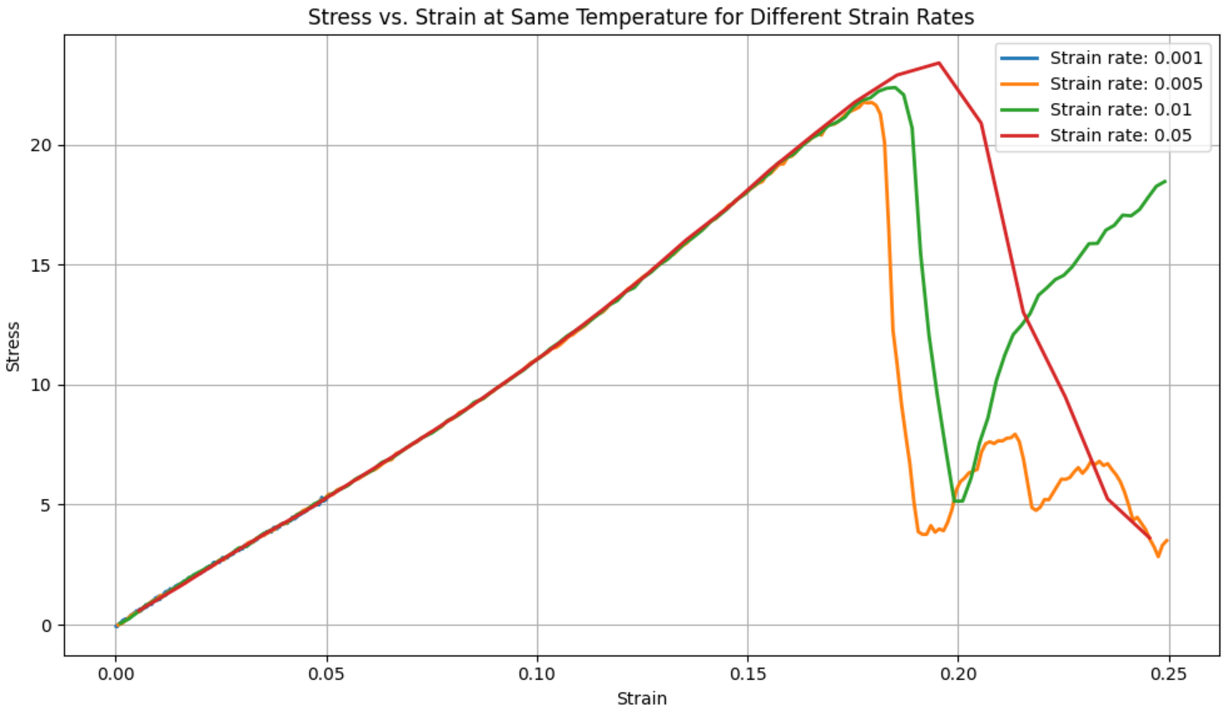
Results & Discussion



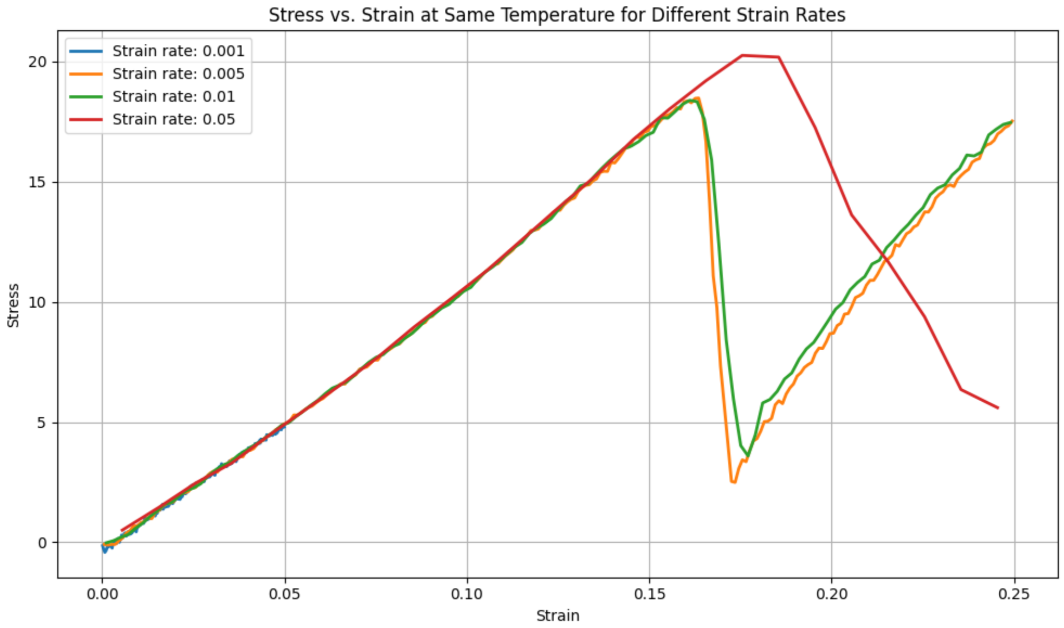
<u>at temperature of 100 kelvin</u>

- Due to very low strain rate , and the test being runned for 50 thousand simulation steps, the blue line terminating at strain of 0.05, it is end of simulation , not failure of material.
- After necking, material undergoes restructuring(slow strain rate), which is helping to bear load in the orange curve
- Very high strain rate , not allowing any recovery to take place in the red curve

At temperature of 300 kelvin

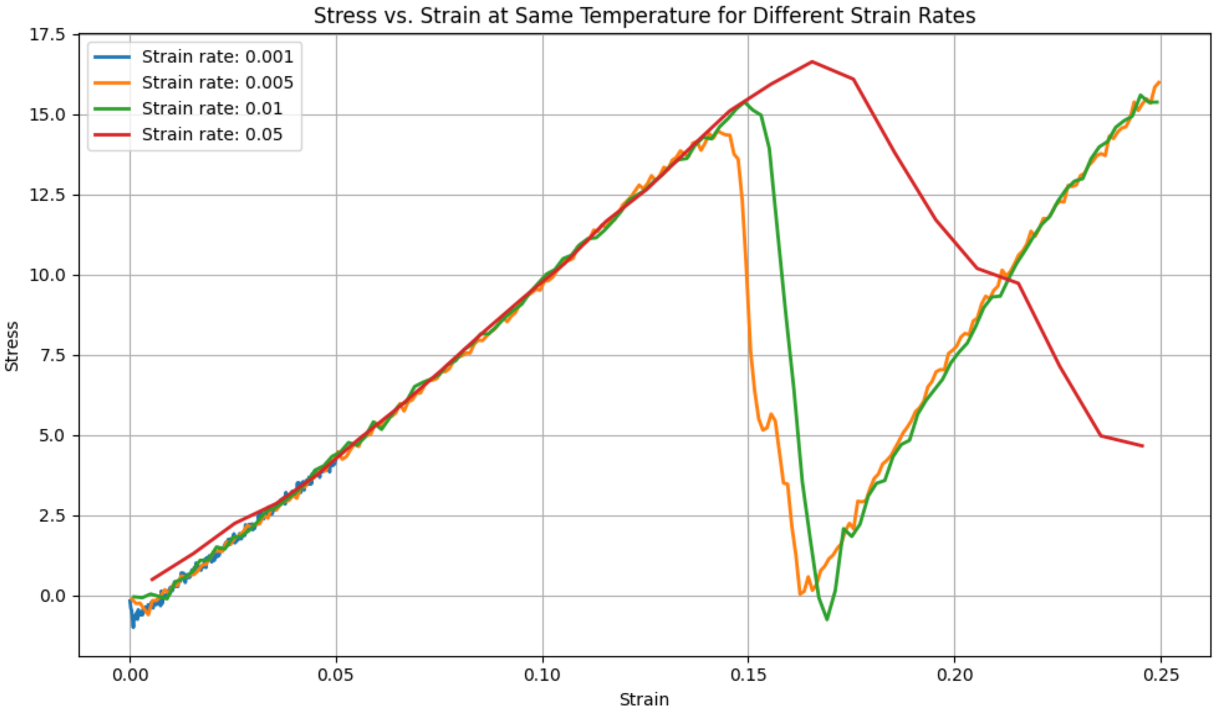


- The orange curve shows more minima and maxima than previous curve, the reason can be multiple deformation mechanisms competing with each other and their alternate dominance
- The green curve after reaching minima , shows more strength as compared to previous curve because at this temperature of 300k, this strain rate good for dislocation multiplication and interaction
- We could see a drop in maximum stress in this graph at this temperature , as compared to the previous one.



At temperature of 500 kelvin

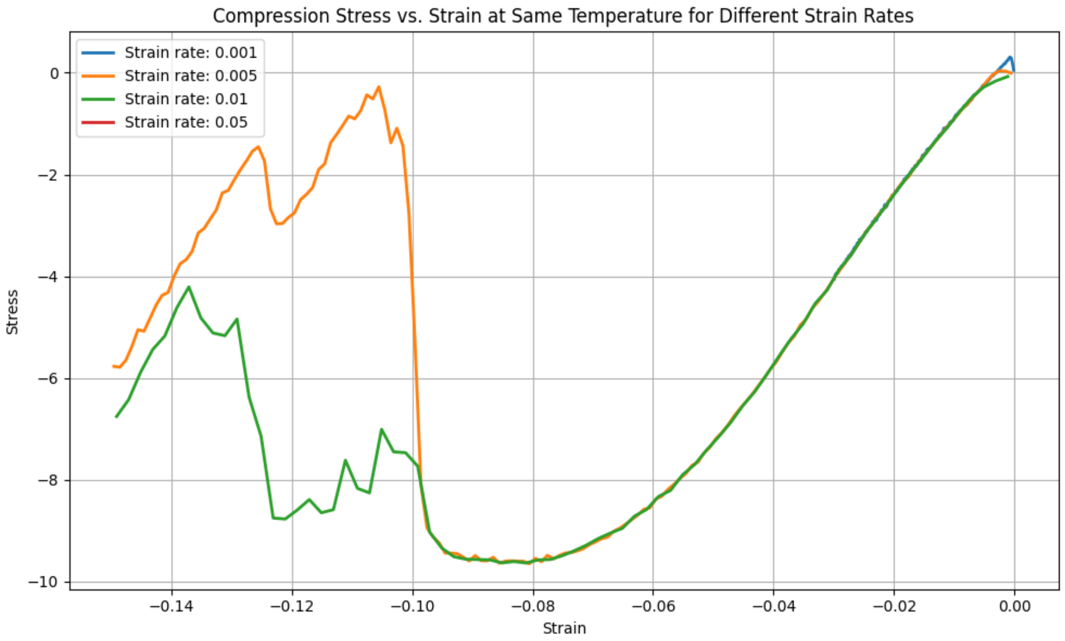
- According to literature the HEA mainly has 4 regions in stress-strain graph during compressive or tensile deformation
- Initial Elastic region
- Initial Plastic region where twin formation is dominant than dislocation mechanisms
- Final elastic and Plastic region
- As strain rate being very high, red curve does not show the same behaviour



<u>At temperature of 800 kelvin</u>

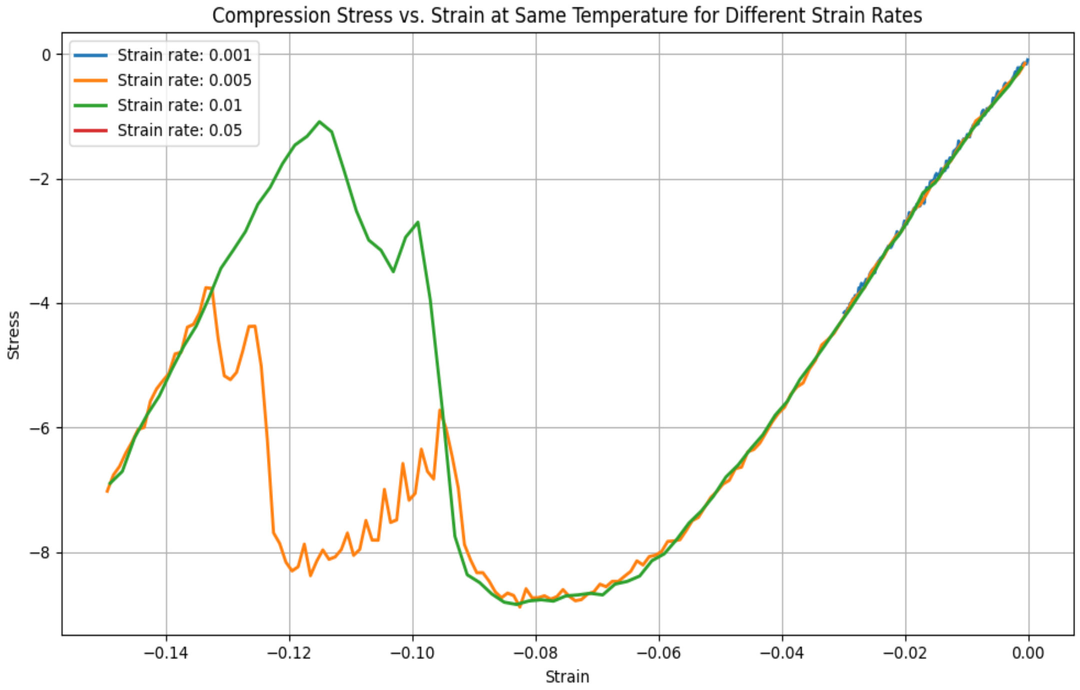
- The graph is not smooth as we have seen in the previous due to high temperature.
- The final elastic region can be seen more clearly.
- The red curve at all temperatures is deforming and breaks at this point.
- We can see from the graph the maximum stress of this graph has not decreased much. Which justifies the use of HEA at high temperature.

stress-strain behavior of pentary alloy at different temperature

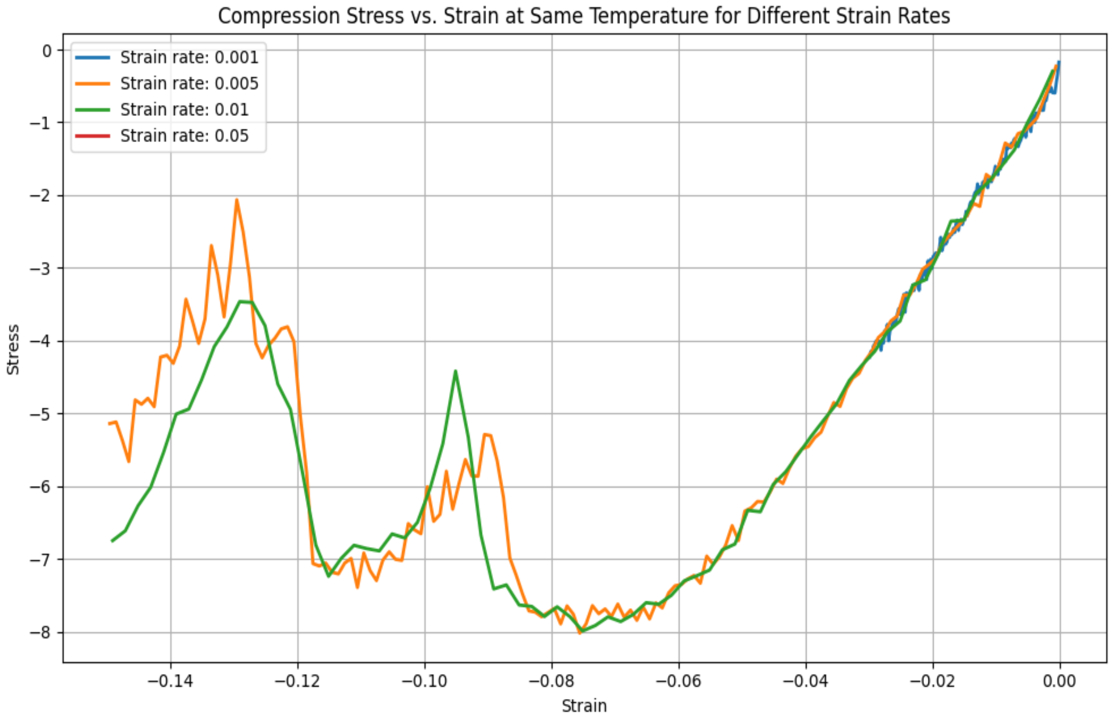


- **<u>Compression Stress-Strain Curve for different (-0.001, -0.005, -0.01) strain rate at 100 K</u>**

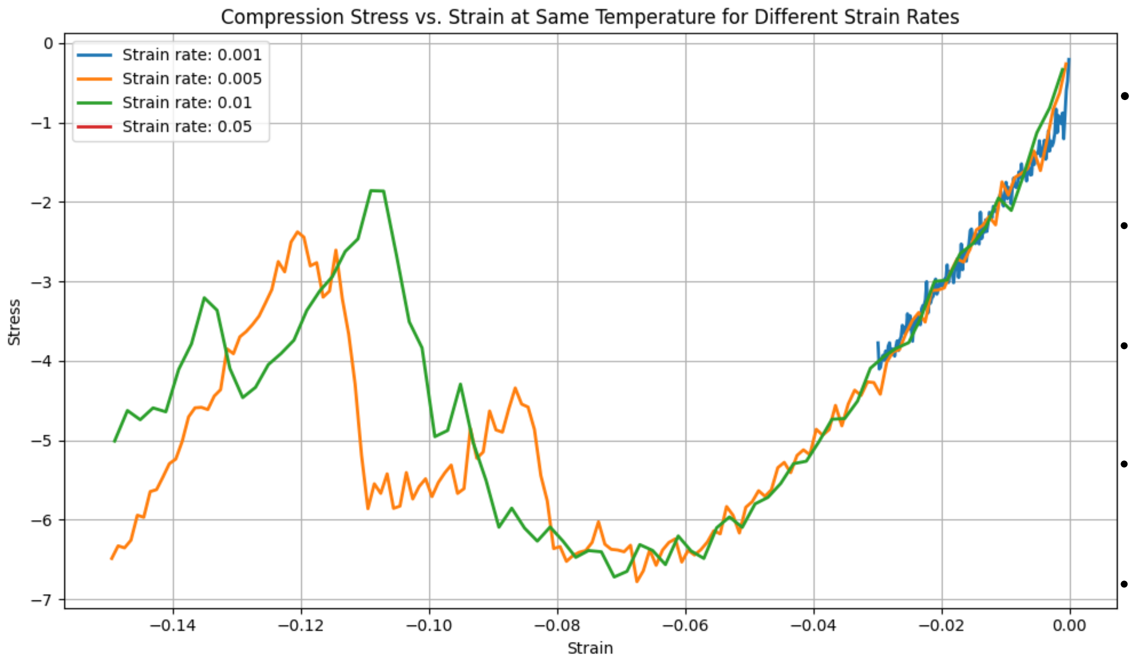
- **Higher strain rates increase peak stress**, showing more resistance before material failure.
- **Lower strain rates (0.001, 0.005)** display smoother, more gradual plastic deformation—typical of thermally activated mechanisms.
- **Intermediate strain rates (0.01)** exhibit sharp stress drops, indicating abrupt yielding or instability under rapid loading.
- Results confirm that **strain rate critically influences stress-strain response**, even at cryogenic temperatures like 100K.



- <u>**Compression Stress-Strain Curve for different (-0.001, -0.005, -0.01) strain rate at 300 K**</u>
- **Higher strain rate** (0.01) shows a higher peak stress, indicating greater resistance to compression before a sharp drop.
- **Lower strain rates** (0.001, 0.005) display more gradual deformation, especially after the initial linear region.
- **The intermediate strain rate** (0.01) exhibits a sharp stress drop around -0.10 strain, suggesting abrupt yielding or instability.
- **The results** highlight that strain rate significantly impacts the material's stress-strain response at 300K.

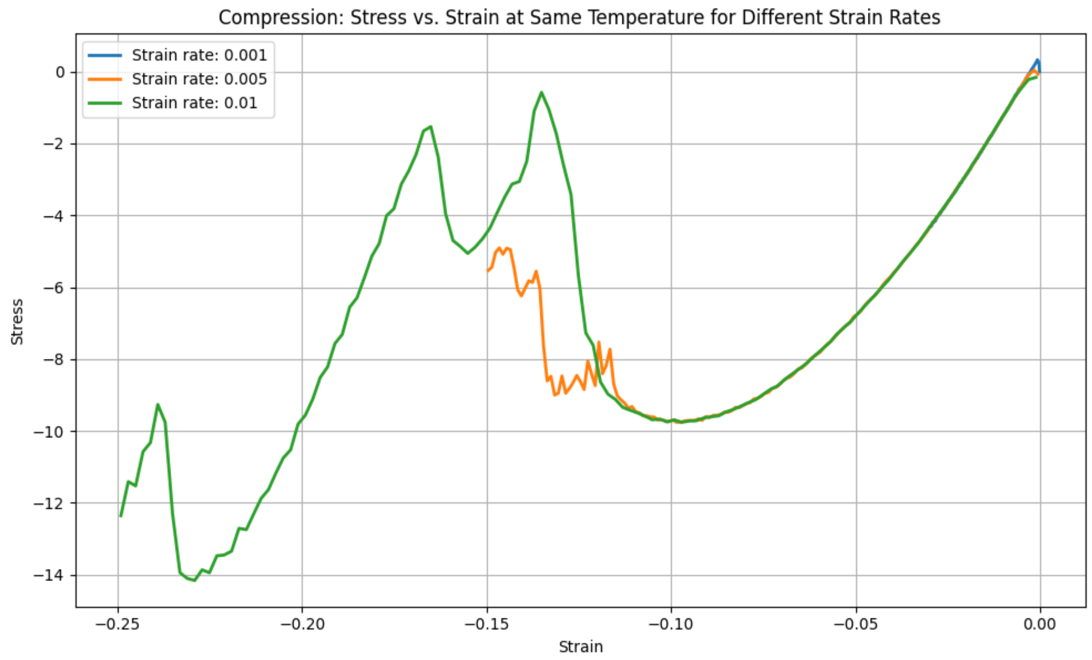


- **Compression Stress-Strain Curve for different (-0.001, -0.005, -0.01) strain rate at 500 K**
- **Higher strain rates** do not necessarily increase peak stress, the relationship is complex and depends on the specific strain rate and material properties.
- **Lower strain rates** (0.001, 0.005) display smoother, more gradual plastic deformation, which is typical of thermally activated mechanisms.
- **Intermediate strain rates** (0.01) exhibit sharp stress drops, which indicate abrupt yielding or instability under rapid loading.
- **Results** indicate that strain rate significantly affects the stress-strain response at 500K, influencing material behavior under compression.



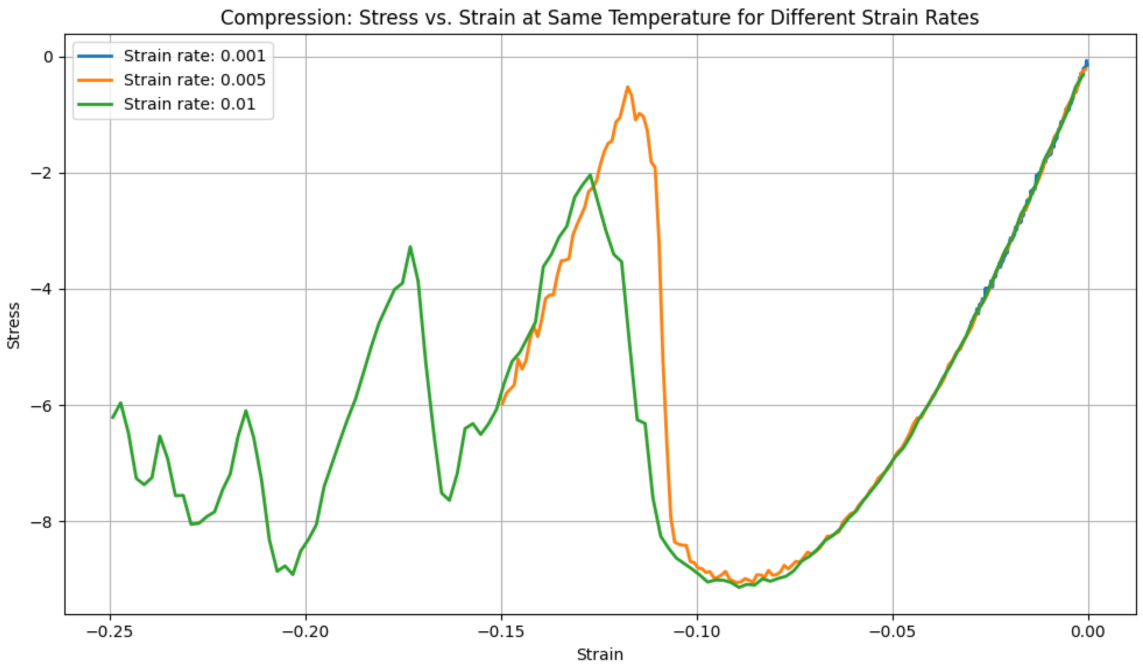
- **<u>Compression Stress-Strain Curve for different (-0.001, -0.005, -0.01) strain rate at 800 K</u>**
- **The graph** displays compression stress vs. strain at different strain rates (0.001, 0.005, 0.01, and 0.05).
- **The lower strain rates** (0.001, 0.005) show smoother, more gradual plastic deformation.
- **The intermediate strain rate** (0.01) exhibits pronounced stress drops and oscillations, indicating abrupt yielding or instability.
- **The results** confirm that strain rate influences the stress-strain response, matching the summary provided.

stress-strain behavior of ternary alloy at different temperature



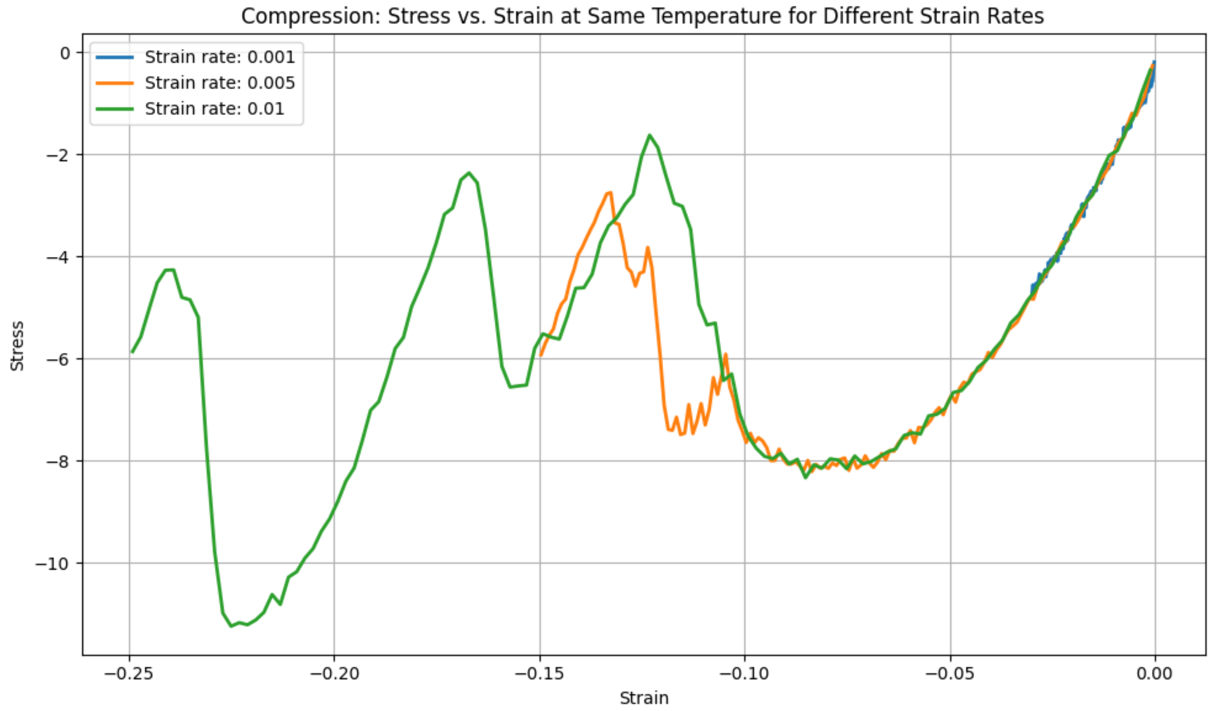
<u>Compression Stress-Strain Curve for different (-0.001, -0.005, -0.01) strain rate at 100 K</u>

- Elastic & Plastic Regions:
  - Initial linear segment: elastic
  - Beyond yield: plastic (dislocation motion and Diffusion)
- Strain Rates & Curve Termination:
  - Time and rates
- Fluctuations/Serrations:
  - Most pronounced at 100 K—caused by severe lattice distortion, strong dislocation pinning, and twinning
  - Dislocations accumulate stress, then move in bursts (jerky flow)
- Diffusion:
  - Negligible at this temperature—plasticity is not due to atomic diffusion



<u>Compression Stress-Strain Curve for different (-0.001, -0.005,-0.01) strain rate at 300K</u>

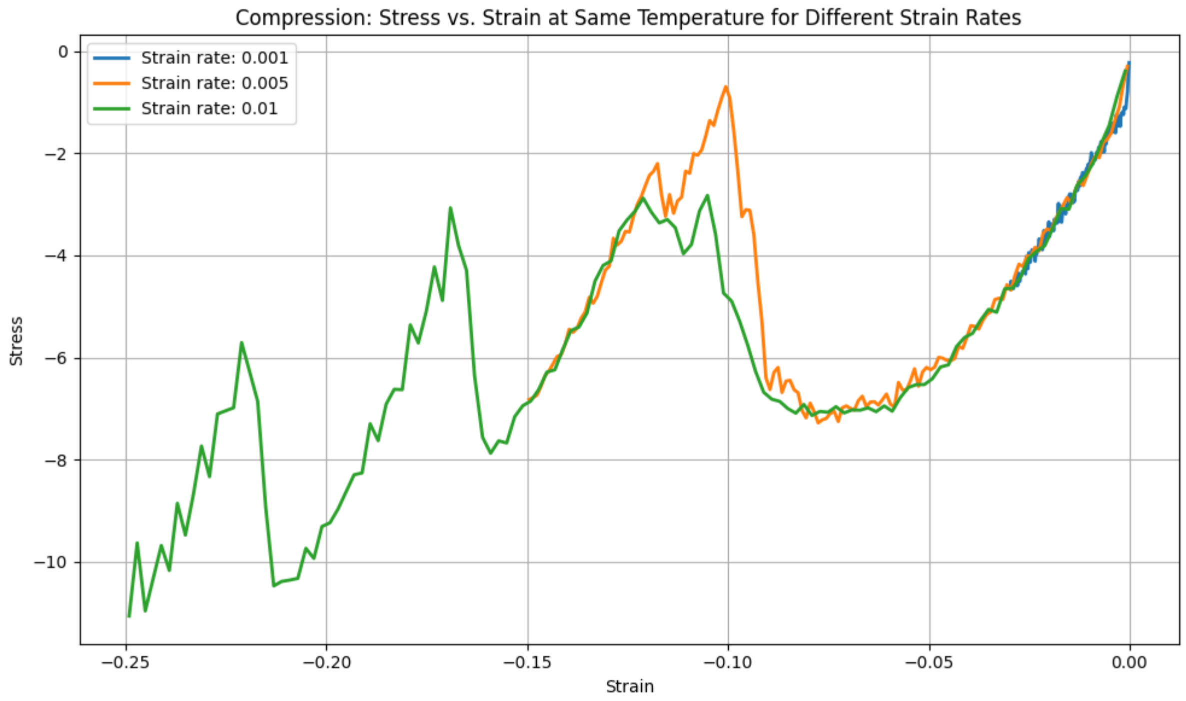
- Elastic & Plastic Regions:
  - Elastic: initial linear rise
  - Plastic: dislocation slip and diffusion
- Fluctuations/Serrations:
  - Still present, but less abrupt than at 100 K
  - Caused by dislocation avalanches and early dynamic strain aging (DSA) as diffusion begins to play a minor role
- Diffusion:
  - Still slow, but starting to influence dislocation motion and serration character



<u>Compression Stress-Strain Curve for different (-0.001, -0.005,-0.01) strain rate at 500K</u>

- Elastic & Plastic Regions:
    - Elastic: linear start
    - Plastic: smoother than at lower temperatures, dislocation slip with some diffusion
- Fluctuations/Serrations:
    - Reduced magnitude, more frequent but less abrupt
    - Caused by easier dislocation pinning as diffusion increases
- Diffusion:
    - Moderately significant—starts to assist dislocation motion, recovery processes

Compression Stress-Strain Curve for different (-0.001, -0.005,-0.01)strain rate at 800K



- Fluctuations/Serrations:
  - Minimal—high atomic mobility allows smoother dislocation motion
  - Occasional small serrations due to sluggish diffusion in HEAs
- Diffusion:
  - Now significant—enables recovery, creep, and smoother plastic flow
- HEA Special Effects:

HEAs at high temp, **dislocations may get stuck and then move suddenly** → causing **serrations**

More than one slip system active Mixed behavior (dislocation slip, twinning, local amorphization) at **high temp**

Conclusion: MD Study on HEAs

- **4-Stage Deformation:**

  Elastic → Twinning → Strain hardening → Diffusion plasticity

- **Temperature Effect:**
  - ↑ Temperature → ↑ Curve fluctuations
  - Thermal softening dominates above 300 K

- **Strain Rate Sensitivity:**

  Strong at low temperatures (100 K)

- **Tension–Compression Asymmetry (18–22%):**
  - Tension: Twin-driven
  - Compression: Diffusion-driven

- **300–500 K:** Uniform stress → Good for cyclic use

- **High T:** Fluctuated stress curves → Less stability under load