Thesis Stage - II

Hugoniot Characterzation of alloys using molecular dynamics simulation

Ayush Tripathi

(ME22MTECH02001)

Thesis Supervisors: **Dr. Prakhar Gupta**
Dr. Syed Nizamuddin Khaderi

SUCSHM Lab || **Impact mechanics Lab**

Department of Mechanical and Aerospace Engineering

भारतीय प्रौद्योगिकी संस्थान हैदराबाद
Indian Institute of Technology Hyderabad

Presentation Outline

1. **Recap**

2. **Simulation Results**

3. **Interatomic Potential I: (V)**

4. **Interatomic Potential II: (P)**

5. **Tungsten Heavy Alloy 90W-7Ni-3Fe**

6. **Results and Conclusion**

7. **Future work**

Recap
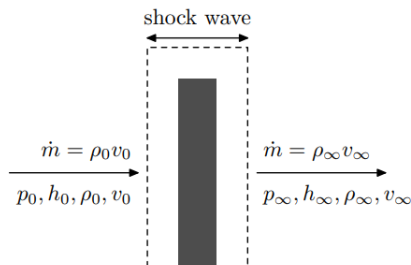
Hugoniot curve

Charactrestics described by Hugoniot relation

- Equation of state
- Phase transition
- Material strength (Shock compressibility)

under **extreme conditions**

$$\dot{m} = \rho_0 v_0$$
$$p_0, h_0, \rho_0, v_0$$

$$\dot{m} = \rho_\infty v_\infty$$
$$p_\infty, h_\infty, \rho_\infty, v_\infty$$

shock wave

Passing of a shock wave

Hugoniot curve

Conservation equations

$$\rho(u_s - u_p) = \rho_0 u_s$$
$$P - P_0 = \rho_0 u_s u_p$$
$$E - E_0 = \frac{1}{2}(P + P_0)(V_0 - V)$$

Under **wide range** of pressure , the relation between u_s and u_p is linear

$$\boxed{u_s = C_0 + \lambda u_p}$$

Hugoniot curve

$$\boxed{P_H(V) = \frac{\rho_0 C_0^2 (1 - V/V_0)}{[1 - \lambda(1 - V/V_o)]^2}}$$

Objective

- Relation between Us and Up for SC-Al and WHA

- Obtain Hugoniot Curve for SC-Al and WHA

- MD Framework for material characterization and validation

Simulation Results

The science behind MD simulations

- Each of N particle is a point mass

- Particles interact via empirical force laws
  - **all physics** in energy potential
  - many-body forces (EAM)

- Numerical integration Newton's equations of motion
  - $F = ma$
  - set of 3N coupled ODEs

- Properties obtained via time averaging

- Seed velocity; Zero Force

Simulation setup

- Single crystal fcc micro structure

- Simulation box of dimension 10a x 10a x 200a

- Lattice parameter(a) = 4.05 Å

- Equilibriated at 300K and 0 bar

- Time step 1 femto second

- Computation time 8 pico second

Stress - Strain plot for Aluminium

Uniaxial tension test Al(V)

$E_{vel} = 44.2 \; GPa$

Uniaxial tension test Al(P)
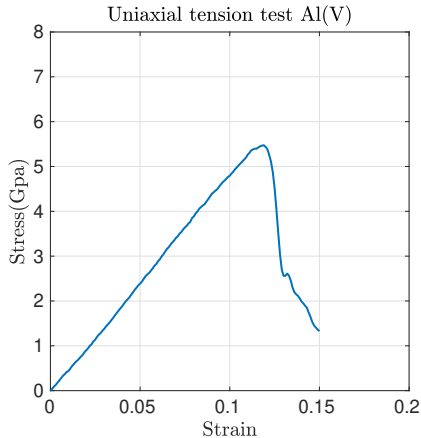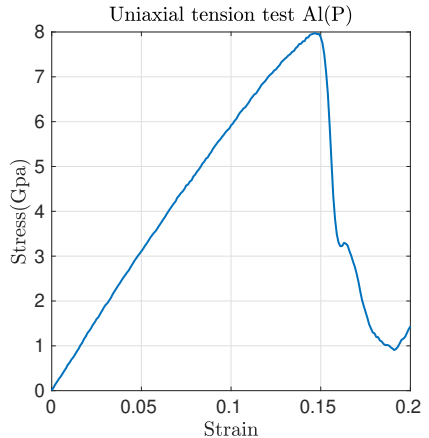
$E_{pres} = 69.1013 \; GPa$

Interatomic Potential I: (V)

Velocity EAM
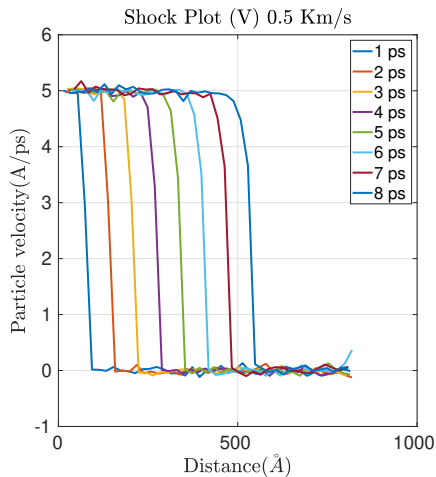
Shock Plot (V) 0.5 Km/s

$U_s = 6.5 \ km/s$
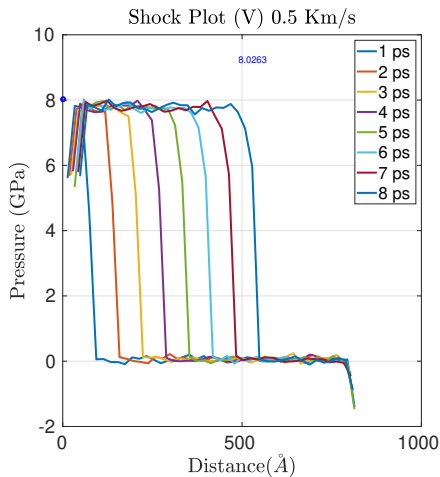
$P_{max} = 8.0283 \ GPa$

Velocity EAM
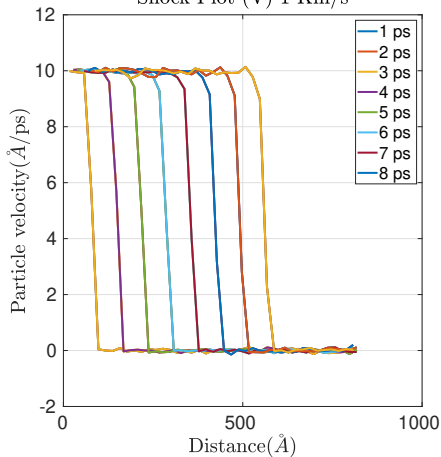
Shock Plot (V) 1 Km/s

Shock Plot (V) 1.0 Km/s

$$U_s = 7 \ km/s$$
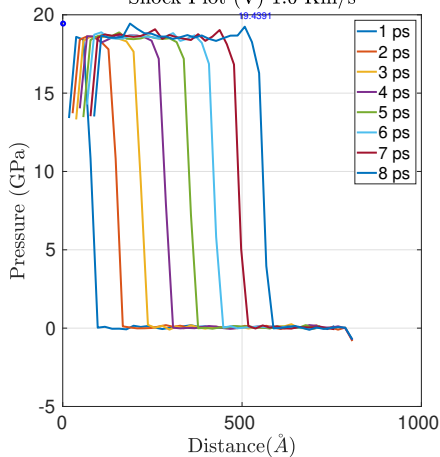
$$P_{max} = 19.4391 \ GPa$$

Velocity EAM

Shock Plot (V) 1.5 Km/s
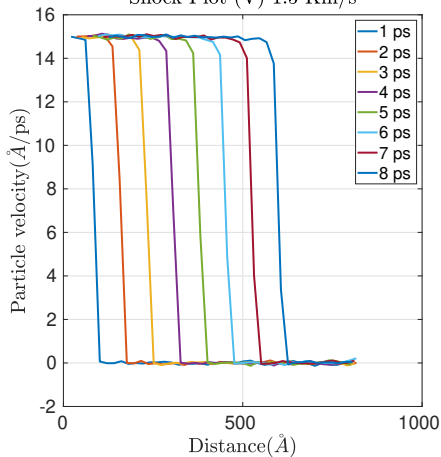
$U_s = 7.4985 \; km/s$
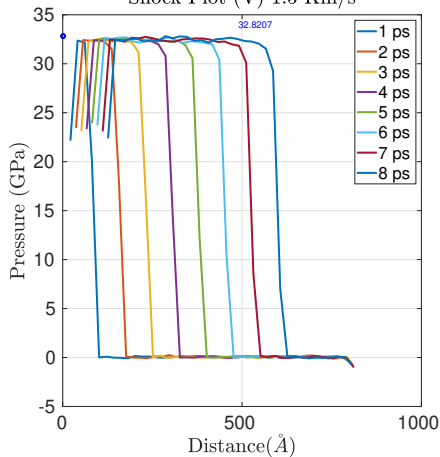
$P_{max} = 32.8207 \; GPa$

Velocity EAM

Shock Plot (V) 2 Km/s
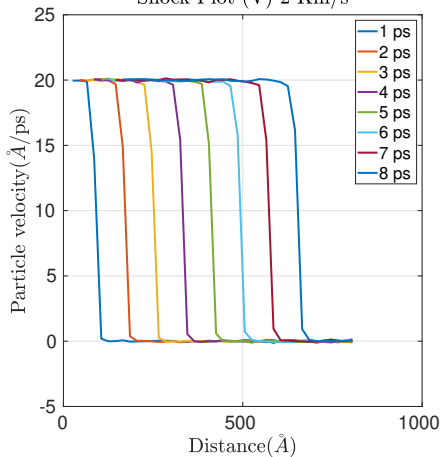
$U_s = 7.9225 \ km/s$
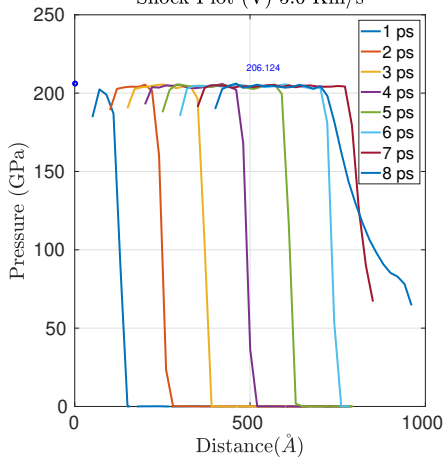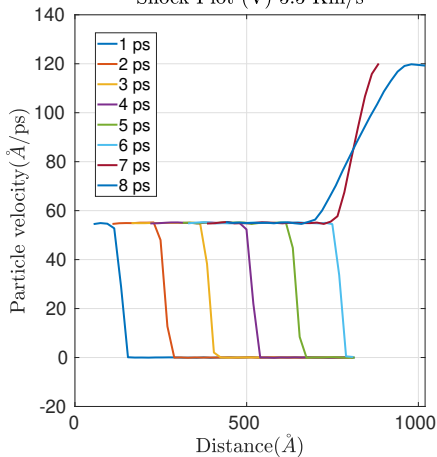
Shock Plot (V) 2.0 Km/s
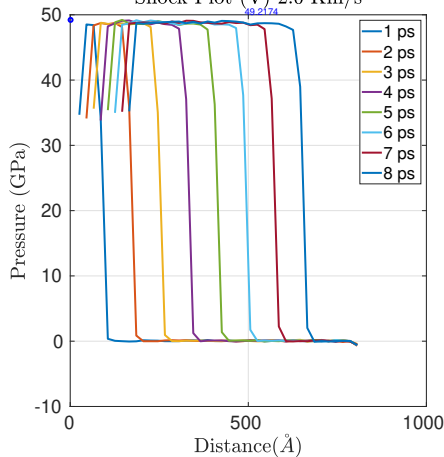
$P_{max} = 49.2174 \ GPa$

Velocity EAM

Shock Plot (V) 2.5 Km/s
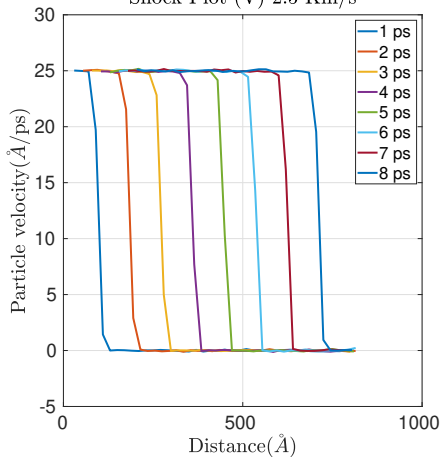
$U_s = 8.756 \ km/s$

Shock Plot (V) 2.5 Km/s
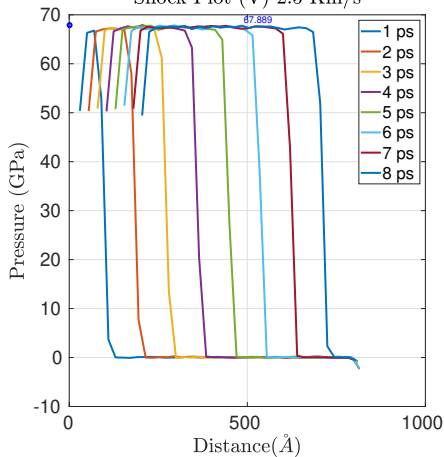
$P_{max} = 67.889 \ GPa$

Velocity EAM

Shock Plot (V) 3.0 Km/s
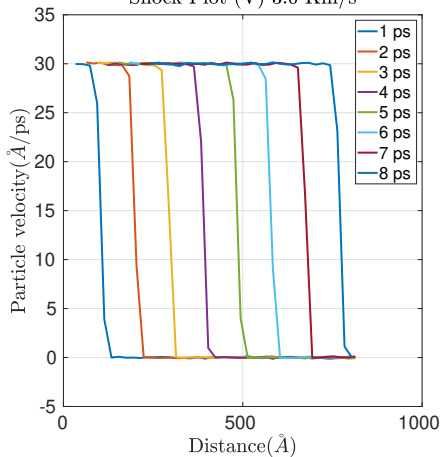
$U_s = 9.5 \ km/s$
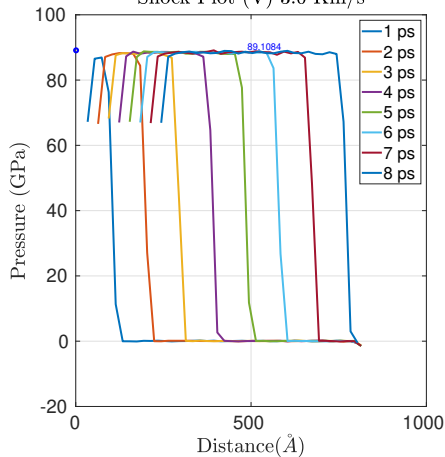
$P_{max} = 89.1084 \ GPa$

Velocity EAM

Shock Plot (V) 3.5 Km/s
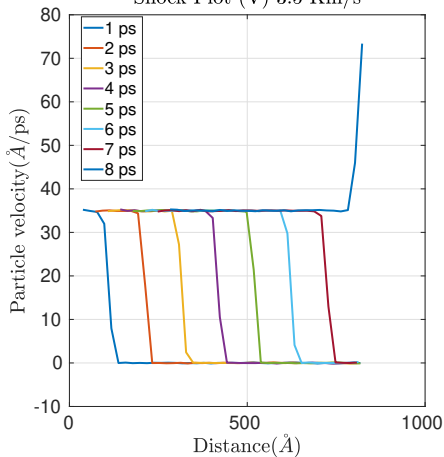
Shock Plot (V) 3.5

$U_s = 10.14 \ km/s$
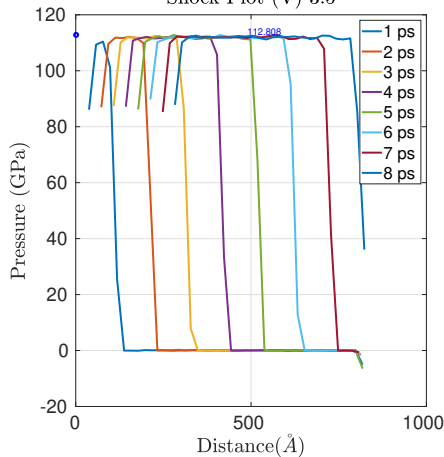
$P_{max} = 112.808 \ GPa$

Velocity EAM

Shock Plot (V) 4.0 Km/s
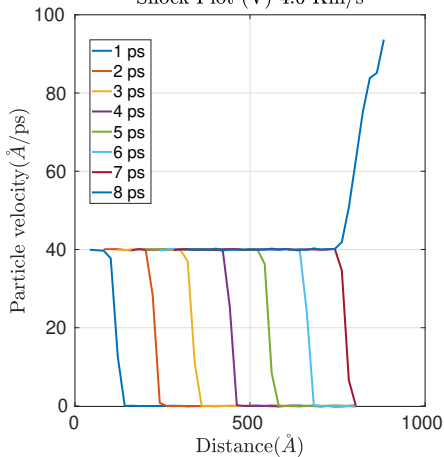
$U_s = 10.86\ km/s$
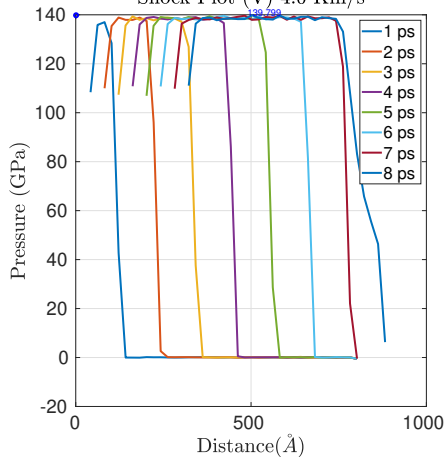
$P_{max} = 139.799\ GPa$

Velocity EAM
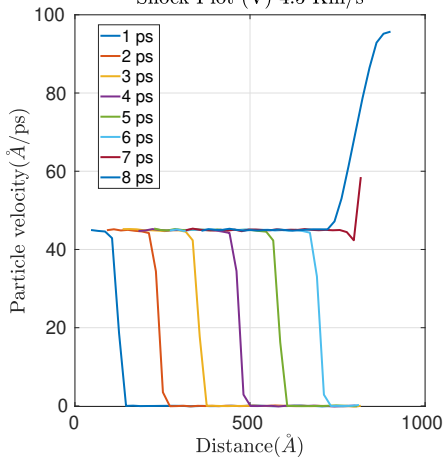
$$U_s = 11.5 \ km/s$$
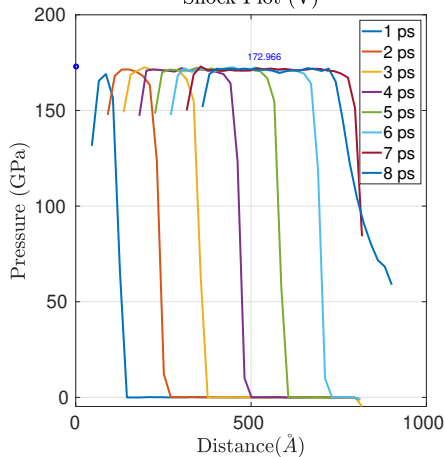
$$P_{max} = 172.966 \ GPa$$

Velocity EAM

Shock Plot (V) 5.0 Km/s
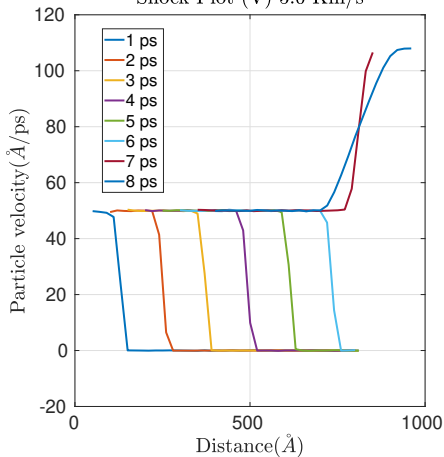
$U_s = 12.14\ km/s$

$P_{max} = 206.124\ GPa$

Velocity EAM

Shock Plot (V) 5.5 Km/s

$$U_s = 12.785 \ km/s$$
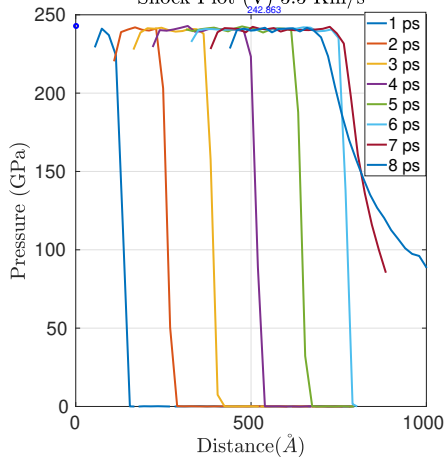
$$P_{max} = 242.863 \ GPa$$

Interatomic Potential II: (P)

Pressure EAM
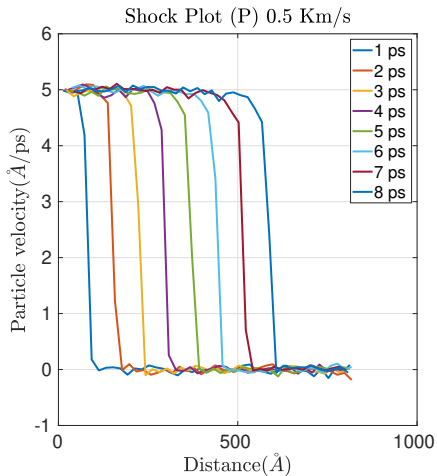
$$U_s = 6.5 \ km/s$$
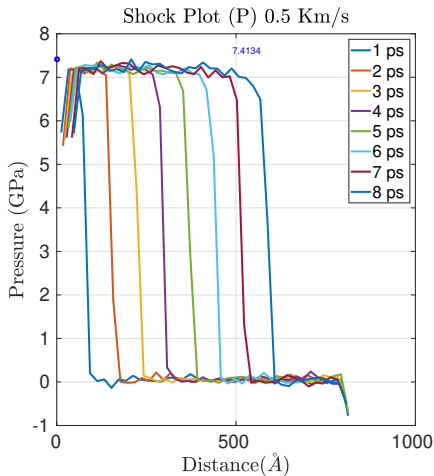
$$P_{max} = 7.4134 \ GPa$$
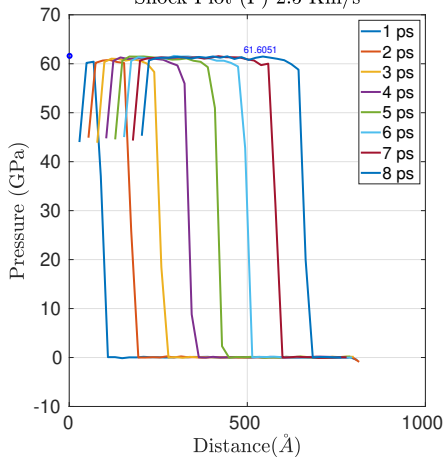
Pressure EAM

$U_s = 7.286 \ km/s$

$P_{max} = 18.954 \ GPa$

Pressure EAM

Shock Plot (P) 1.5 km/s
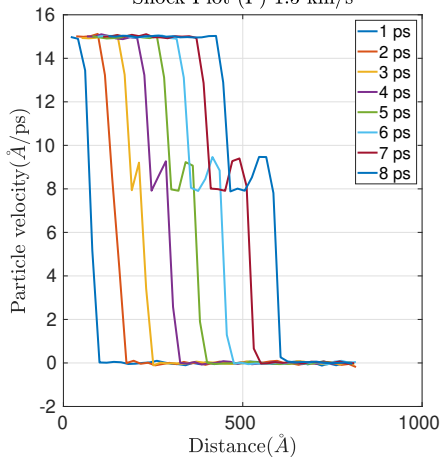
$U_s = 7.499\ km/s$

Shock Plot (P) 1.5 Km/s
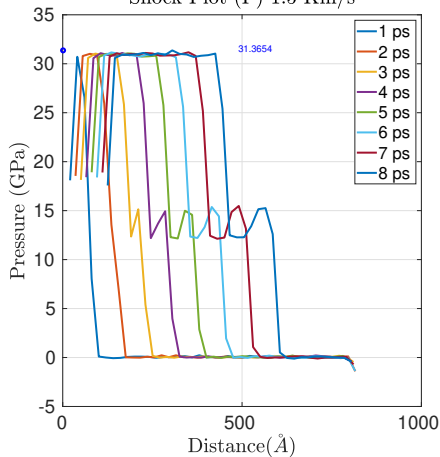
$P_{max} = 31.3654\ GPa$

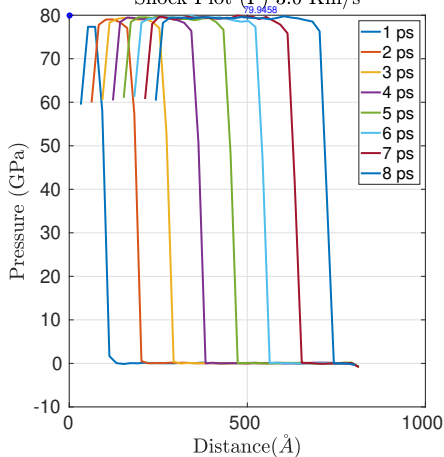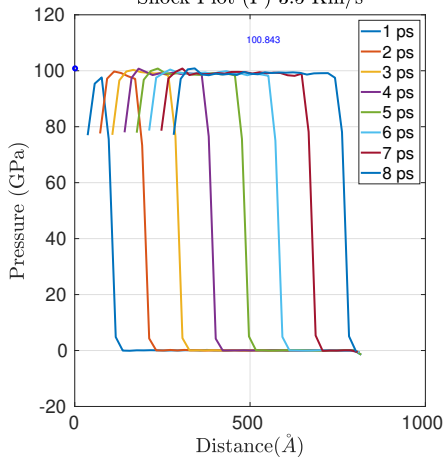# Pressure EAM

Shock Plot (P) 2.0 Km/s
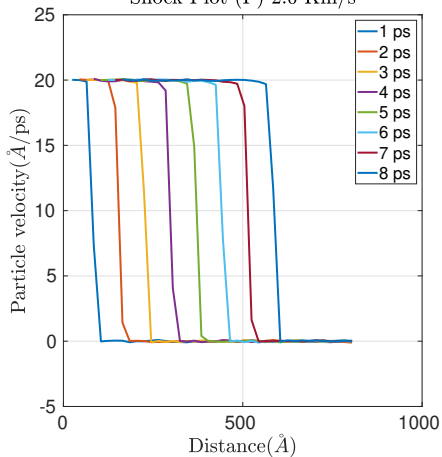
$U_s = 8.0 \ km/s$
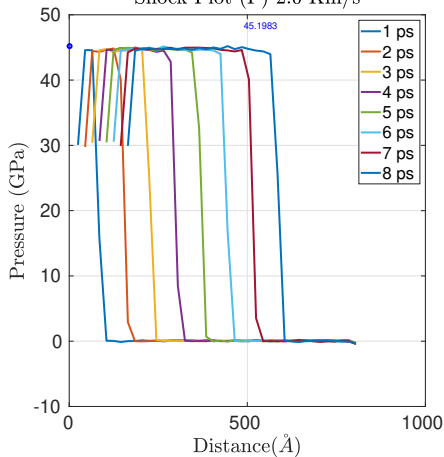
$P_{max} = 45.1983 \ GPa$
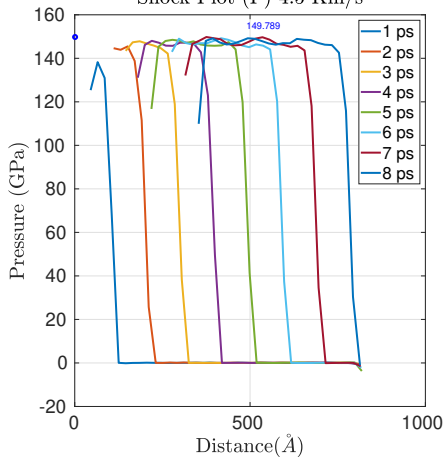
Pressure EAM

Shock Plot (P) 2.5 Km/s
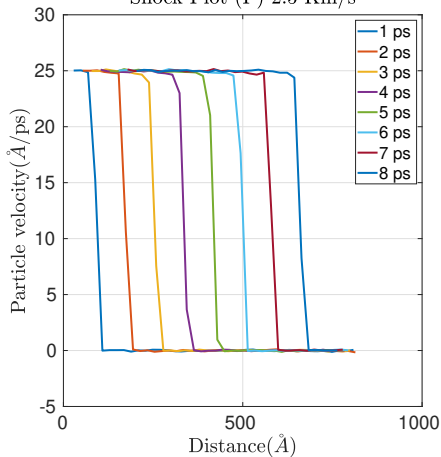
$U_s = 8.2107\ km/s$

$P_{max} = 61.6051\ GPa$

Pressure EAM

Shock Plot (P) 3.0 Km/s
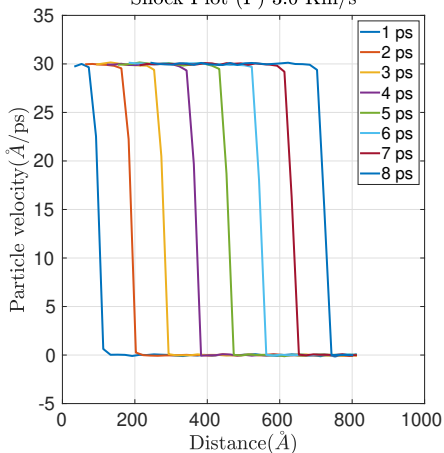
$U_s = 8.998 \ km/s$

$P_{max} = 79.9458 \ GPa$

Pressure EAM

Shock Plot (P) 3.5 Km/s
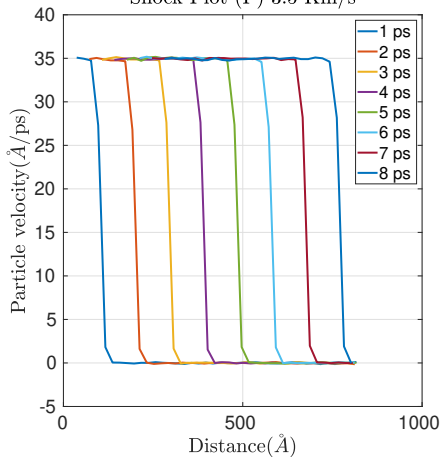
$U_s = 9.5 \ km/s$

$P_{max} = 100.843 \ GPa$

Pressure EAM
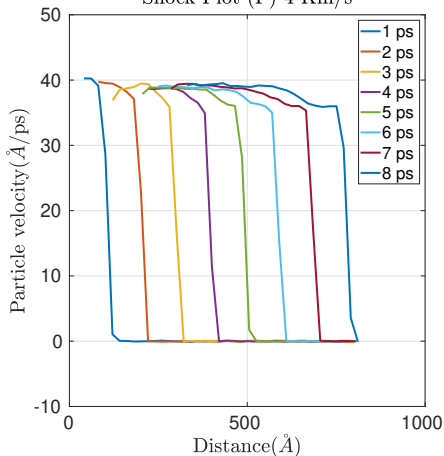
Shock Plot (P) 4 Km/s

Shock Plot (P) 4.0 Km/s

$U_s = 9.767 \ km/s$
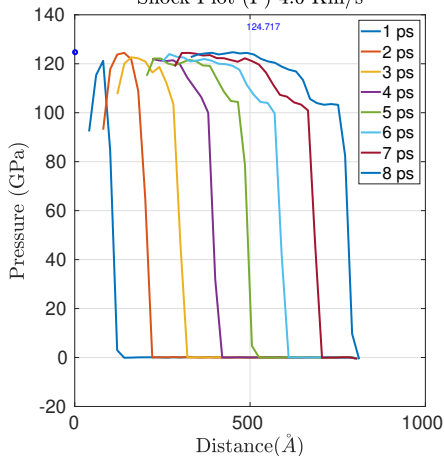
$P_{max} = 124.717 \ GPa$

Pressure EAM
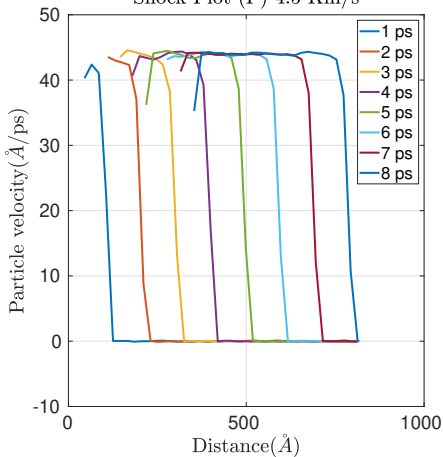
$$U_s = 9.824 \ km/s$$
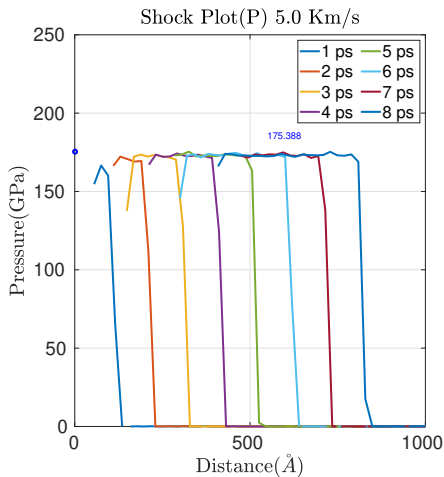
$$P_{max} = 149.789 \ GPa$$

Pressure EAM
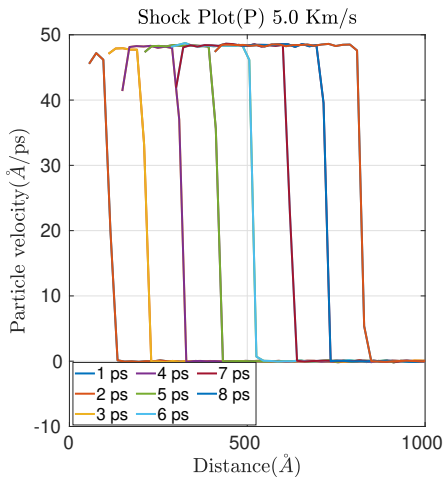
$$U_s = 10.3 \ km/s$$

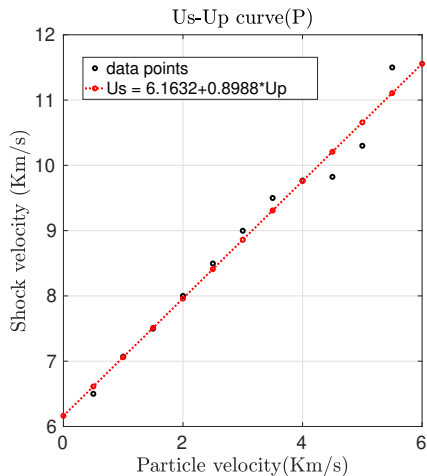$$P_{max} = 175.388 \ GPa$$

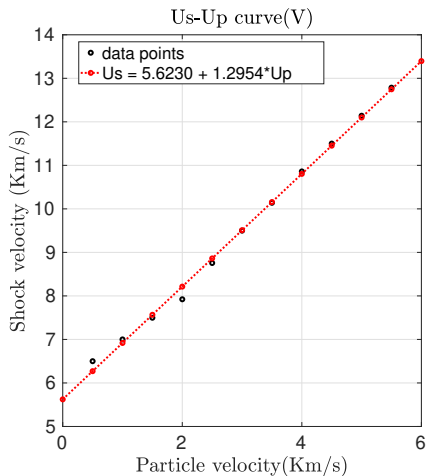# Pressure EAM

Shock Plot(P) 5.5 Km/s
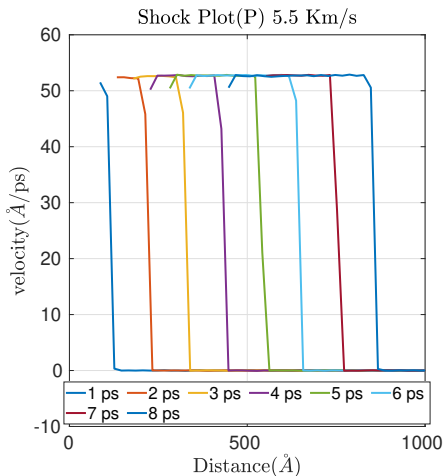
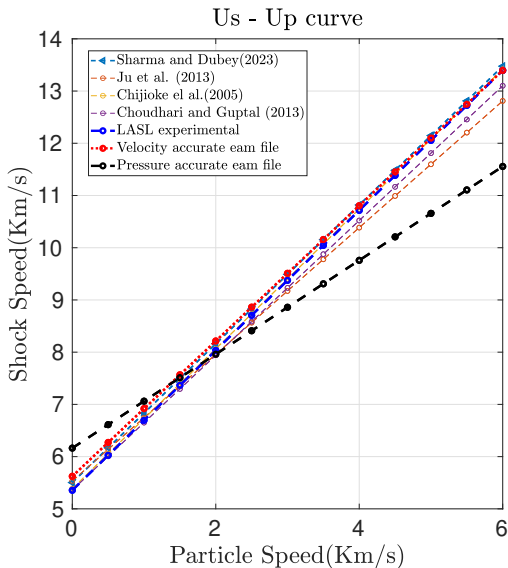$U_s = 12.785 \ km/s$
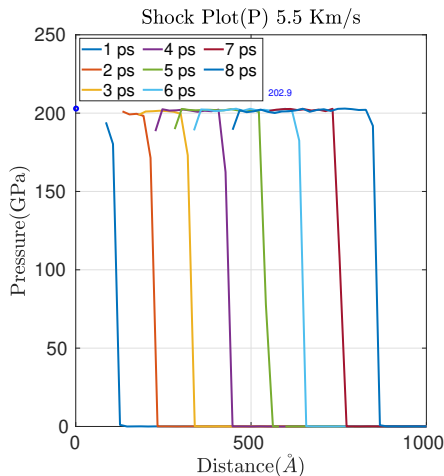
$P_{max} = 202.9 \ GPa$
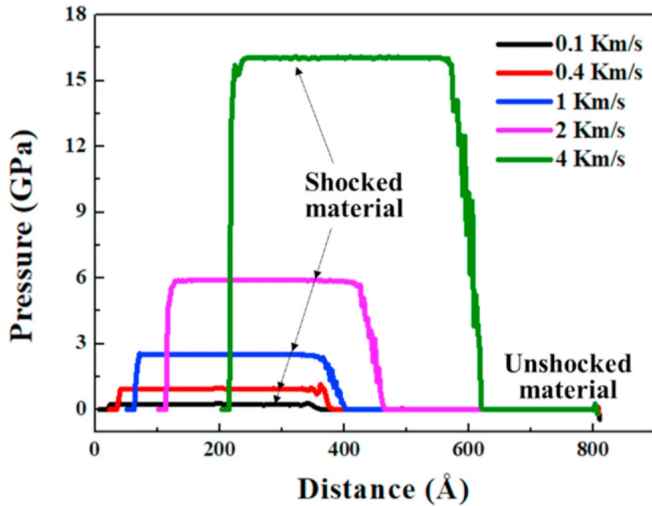
Us – Up curve

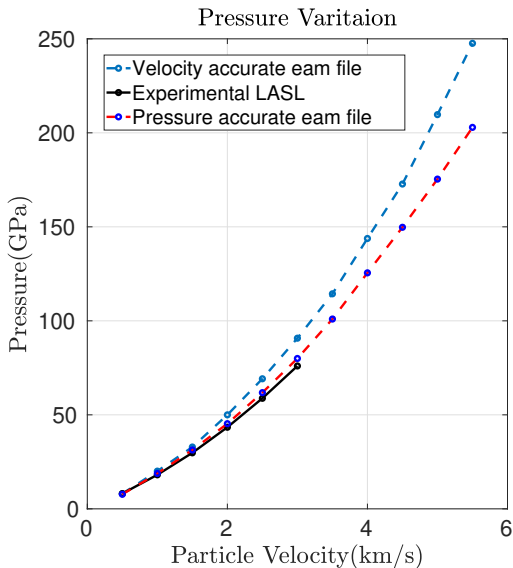
R-square = 0.9777
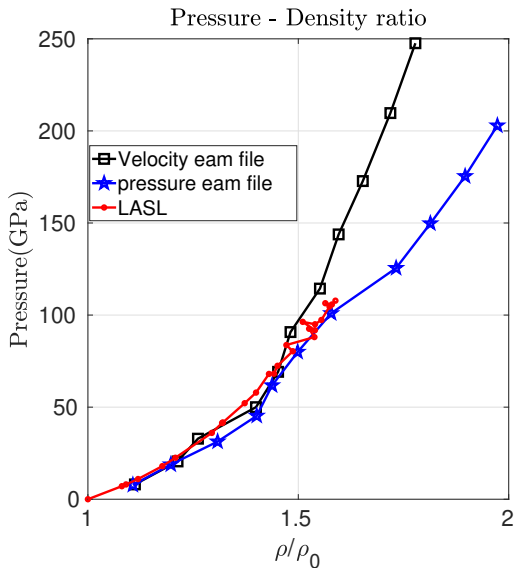
R-square = 0.9964

Us – Up Curve

Pressure Profile

Sharma and Dubey (2023)

Pressure Variation

Hugoniot curve

Tungsten Heavy Alloy 90W-7Ni-3Fe

Why Tungsten heavy alloys

- distinctive combination of yield strength, elongation and density

- better ductility under compression and tension

- **WHA foams** supposed to have better strength to weight ratio

Simulation setup

- Single crystal bcc micro structure

- Simulation box of dimension 30a x 30a x 400a

- Lattice parameter(a) = 3.165 Å

- Equilibriated at 300K and 0 bar

- Time step 1 femto second

- Computation time 5 pico second

Stress - Strain curve for WHA
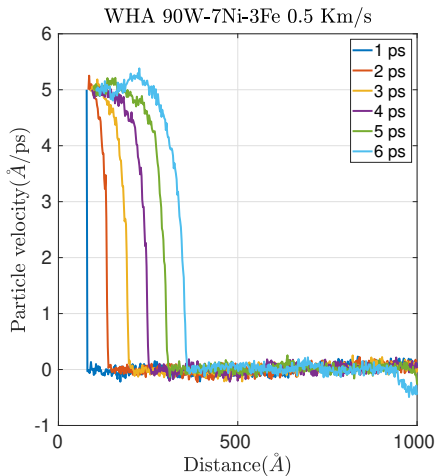

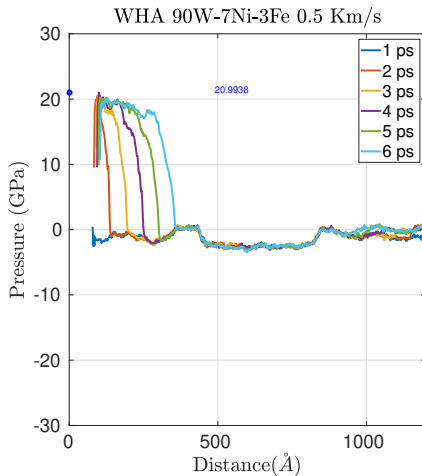Uniaxial tensile test 90W-7Ni-3Fe
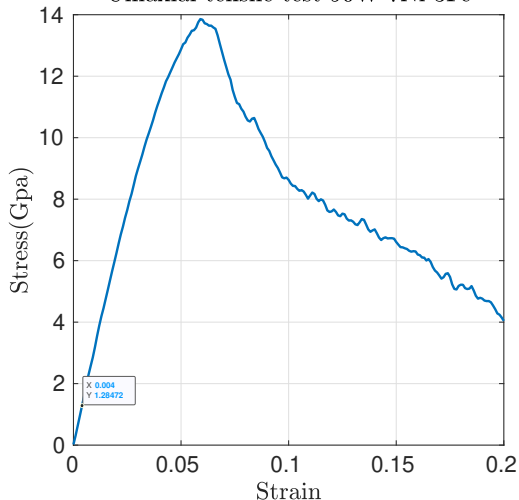
$$E_{Sim} = 321.85 \ GPa$$
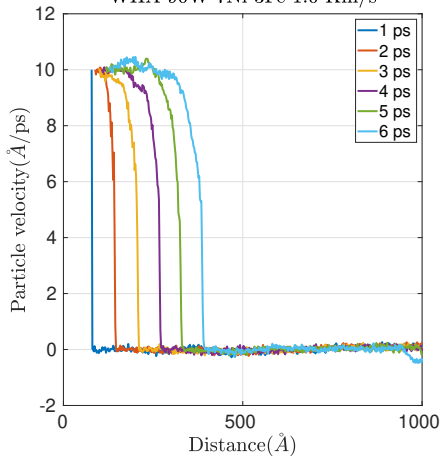$$E_{exp} = 310 \ GPa$$
$$\% \ Error = 3.8$$
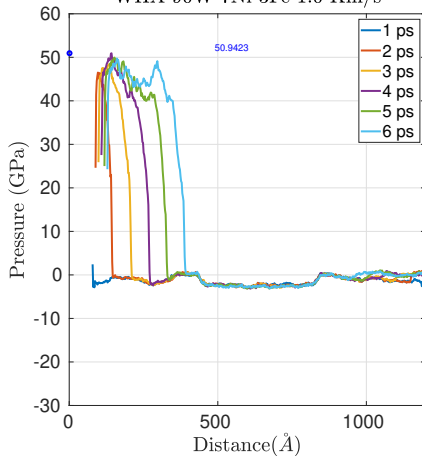
WHA

$U_s = 5.49 \ km/s$

$P_{max} = 20.9938 \ GPa$
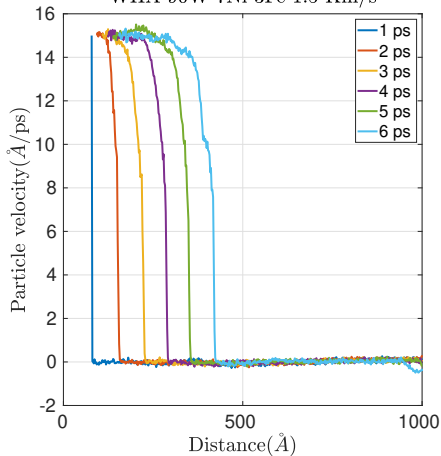
WHA

WHA 90W-7Ni-3Fe 1.0 Km/s

$U_s = 6.133\ km/s$

$P_{max} = 50.9423\ GPa$

WHA

WHA 90W-7Ni-3Fe 1.5 Km/s

$U_s = 6.649\ km/s$
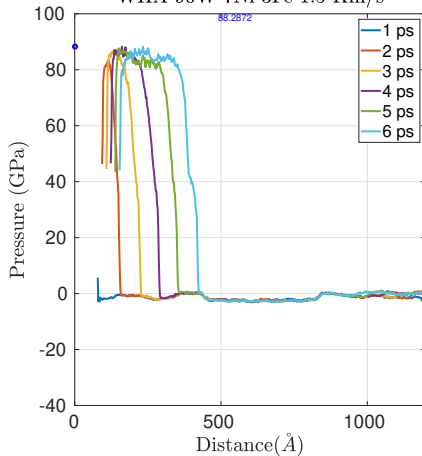
$P_{max} = 88.2872\ GPa$

WHA

WHA 90W-7Ni-3Fe 2.0 Km/s

$U_s = 7.2\ km/s$
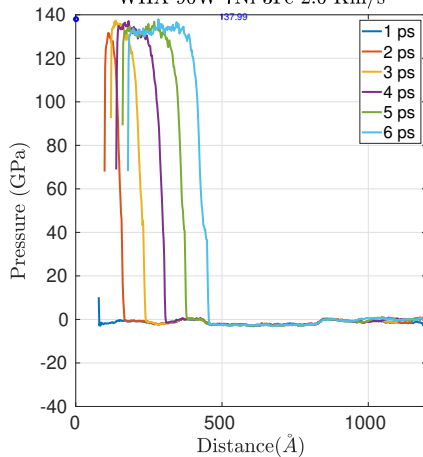
$P_{max} = 137.99\ GPa$

WHA

WHA 90W-7Ni-3Fe 2.5 Km/s

$U_s = 7.7 \ km/s$
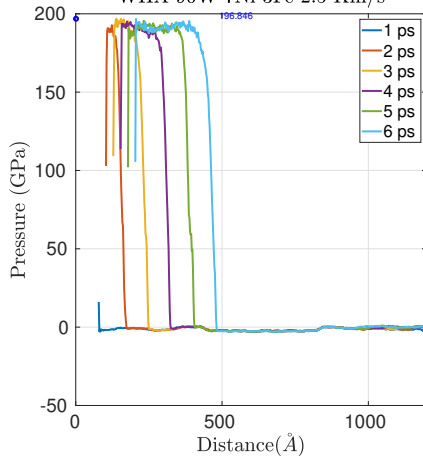
$P_{max} = 196.846 \ GPa$
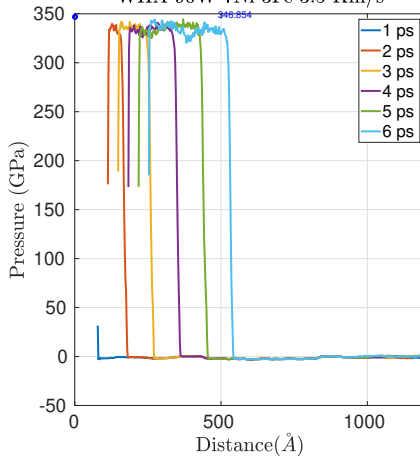
WHA

WHA 90W-7Ni-3Fe 3.5 Km/s

$$U_s = 9.14 \ km/s$$

$$P_{max} = 346.854 \ GPa$$

WHA

WHA 90W-7Ni-3Fe 4.0 Km/s

$U_s = 9.697 \ km/s$
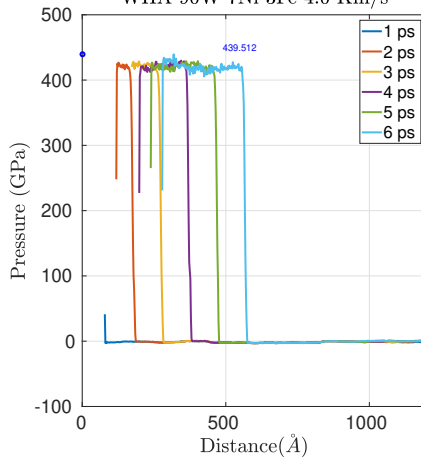
$P_{max} = 439.512 \ GPa$

WHA

WHA 90W-7Ni-3Fe 4.5 Km/s

$U_s = 10.45 \; km/s$
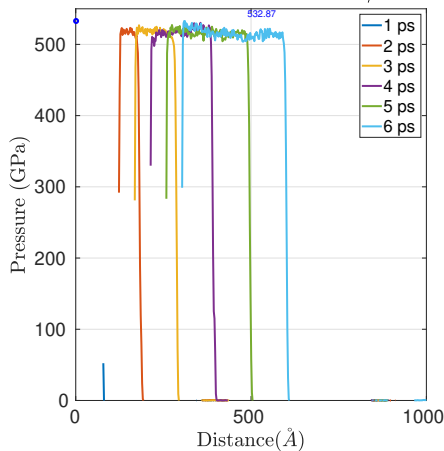
$P_{max} = 532.87 \; GPa$

WHA

WHA 90W-7Ni-3Fe 5.0 Km/s

$U_s = 11.245 \ km/s$
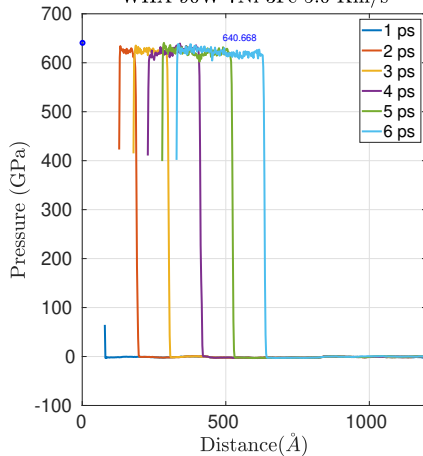
$P_{max} = 640.668 \ GPa$

WHA

WHA 90W-7Ni-3Fe 5.5 Km/s

$U_s = 11.78\ km/s$
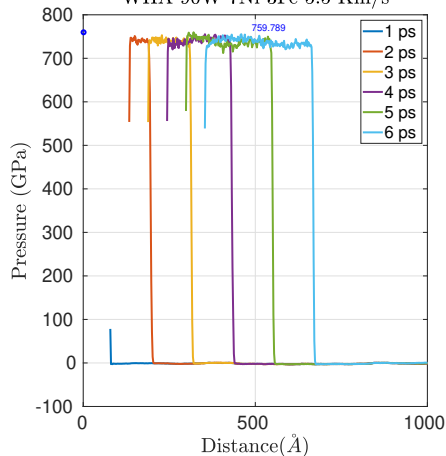
$P_{max} = 755.21\ GPa$

Us-Up Curve

WHA 90W-7Ni-3Fe Us-Up curve
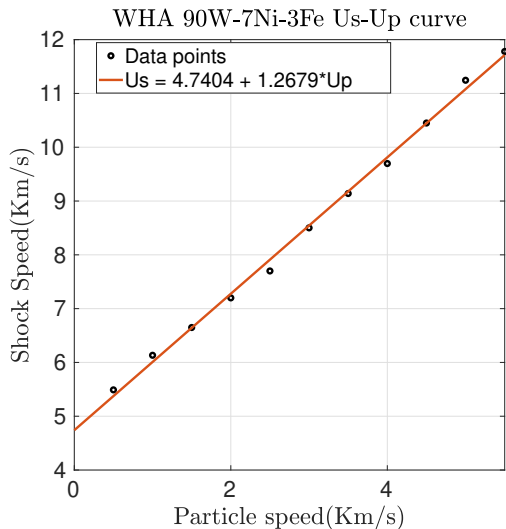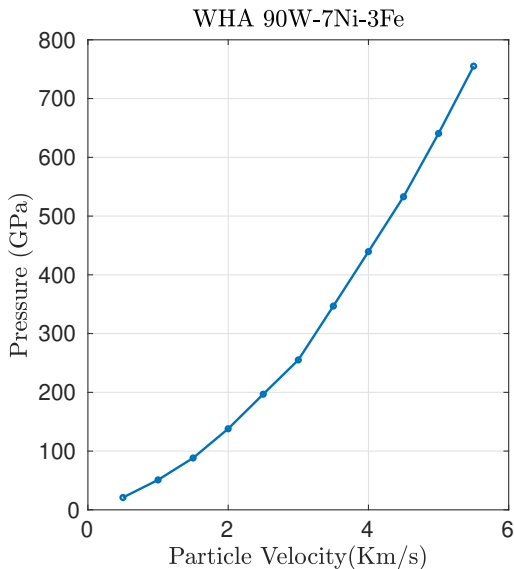
Pressure Variation

Results and Conclusion

Results and discussion

- LAMMPS code for shock loading has been developed

- Linear relationship for Us - Up has been reproduced
  - found to be in close agreement with theoretical and experimental results

- Hugoniot curve has been reproduced
  - found to be in close agreement with LASL experimental results

- Alloys with custom composition have been successfully modeled
  - further validation required

Future work

Future Work:

- Plastic Deformation

- Metal Foams, such as:

  * Aluminium

  * Tungsten heavy alloy

- Shock propagation time

- Experimental validation.

"Thank you !"

me22mtech02001@iith.ac.in