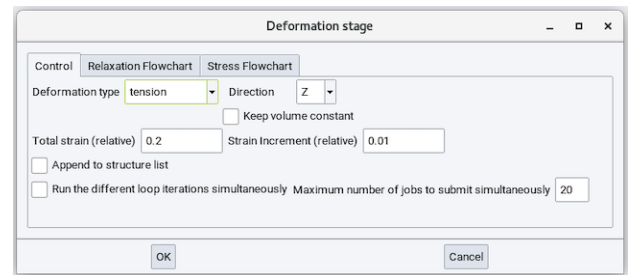# MedeA *Deformation*
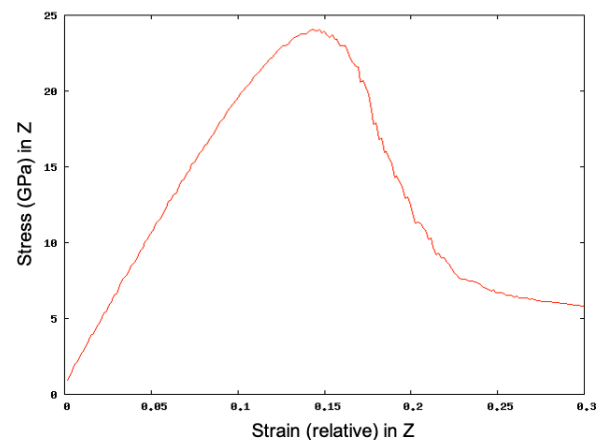Deformation and Fracture beyond the Elastic Regime

At-a-Glance

Plastic deformation and fracture occur outside the elastic regime and are not easily simulated. The *MedeA*®[1] *Deformation* module evaluates the stress-strain relationships of materials beyond the elastic regime, which can be used to extract mechanical properties of materials including Young's modulus, yield strength, ultimate strength, fracture strength, and shear strength.

Key Benefits

- Performs tension, compression, and shear deformations
- Fully automated and robust computational procedure designed to achieve utmost efficiency for the mechanical properties beyond the elastic regime
- Automated stress-strain curves for results validation
- Supports *VASP* and *LAMMPS* as the force compute engines

Computational Characteristics

- Users define the type of deformation (tensile, compression, or shear), direction (x, y, z, alpha, beta, or gamma), total strain, strain increment, and whether to keep the volume constant by shrinking/expanding the lateral dimensions

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.

- All deformed structures are saved in a structure list for easy retrieval
- *MedeA Deformation* uses *VASP* or *LAMMPS* for high-performance force computations on computers from scalar workstations, NVidia GPUs, to massively parallel supercomputers.
- Creates stress-strain plots automatically for extraction of Young's modulus, yield strength, ultimate strength, fracture strength, and shear strength.

- Works with all interatomic potentials in *MedeA* when using *LAMMPS* as the force computation engine.
- Works with all exchange-correlations and functionals with *MedeA VASP*.

Required Modules

- *MedeA Environment*
- *MedeA Deformation*
- *MedeA VASP* or *MedeA LAMMPS*

Recommended Modules

- *MedeA ReaxFF*
- *MedeA COMB3*
- *MedeA EAM*

Find Out More

Learn more about *MedeA Deformation* by watching this webinar recording:

- Elasticity and Beyond: Predicting Mechanical Properties with MedeA

Check out this tutorial for additional information:

- Introduction to MedeA Deformation: Plastic Deformation and Fracture of Single-walled Carbon Nanotube