MedeA Deformation: Deformation and Fracture beyond the Elastic Regime

Contents

1 Introduction

Plastic deformation and fracture occur outside the elastic regime and are not easily simulated. The *MedeA 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 the utmost efficiency for computing the mechanical properties beyond the elastic regime
- Automated stress–strain curves for results validation
- Supports VASP and LAMMPS as the force compute engines

2 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.
- All deformed structures are saved in a structure list for easy retrieval.
- *MedeA Deformation* uses VASP or LAMMPS for performant force computations on computers from scalar workstations to massively parallel supercomputers.
- Creates stress–strain plots automatically for extraction of Young's modulus, yield strength, ultimate strength, fracture strength, and shear strength.

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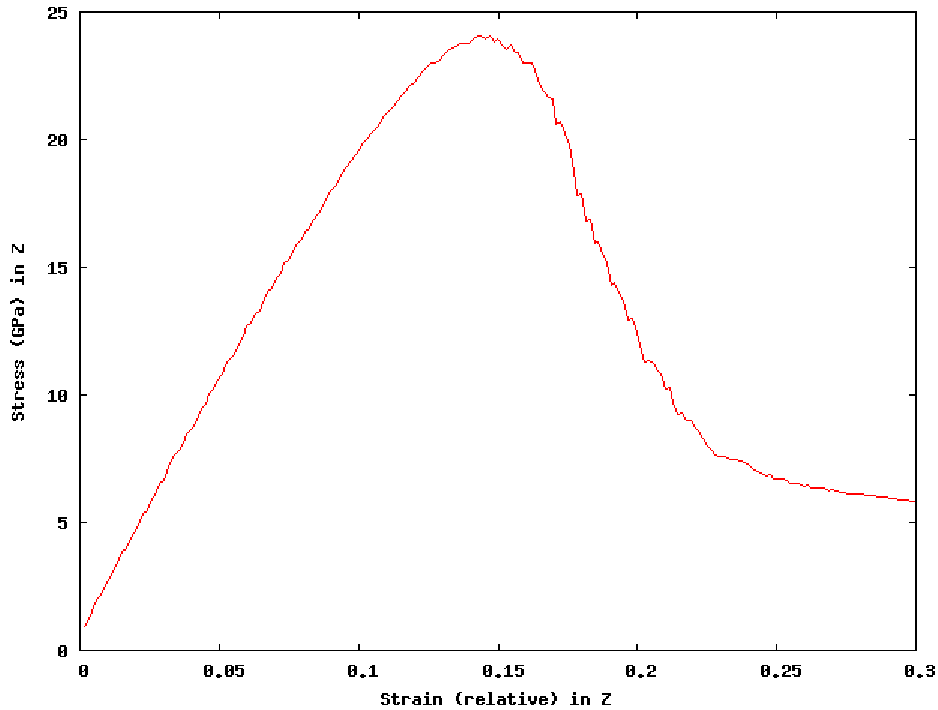

- Works with all potentials in *MedeA* when using LAMMPS as the force computation engine.

Hint: The *MedeA Deformation* module works with VASP and LAMMPS. For more information on VASP within *MedeA*, see section MedeA VASP. For more information on LAMMPS within *MedeA*, see section MedeA LAMMPS.

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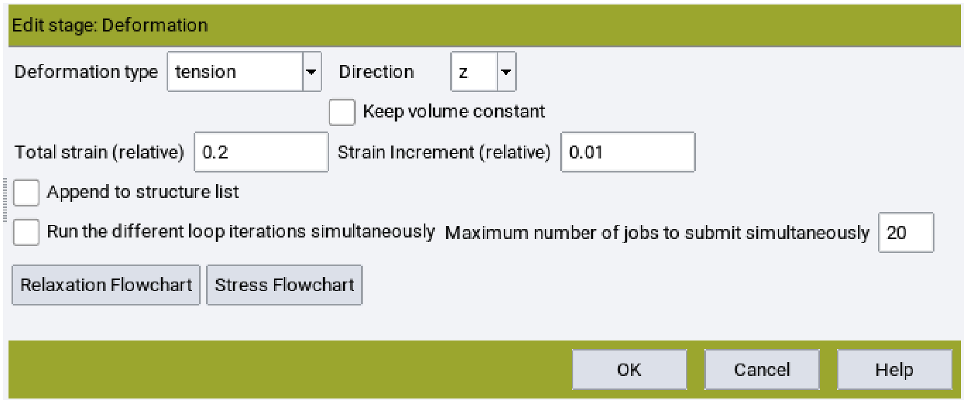
3 The *MedeA Deformation* Module

The *MedeA Deformation* module can be accessed within the flowchart interface with the **Deformation** stage under the *General Properties* section. This is a screenshot of the **Deformation** stage GUI:



Input parameters are:

- *Deformation type*: Choose from `tension`, `compression`, or `shear` types.
- *Direction*: Choose from `x`, `y`, or `z` for `tension` and `compression` deformation types, and `alpha`, `beta`, or `gamma` for the `shear` deformation type.
- ☑ *Keep volume constant*: Check this box to keep the volume constant during deformation by shrinking the lateral dimensions for tension deformations and by expanding them for compression deformations.

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This option does not apply to shear deformations.

Hint: This option is particularly useful for VASP simulations since VASP cannot relax lateral dimensions while keeping the tensile/compression direction dimension fixed. For LAMMPS simulations, one can choose to fix the tension/compression direction while allowing only the lateral dimensions to relax.

- *Total strain (relative)* or *Total strain (deg)*: Maximum strain applied to the structure.
- *Strain Increment (relative)* or *Strain Increment (deg)*: Incremental strain applied to the structure. The total strain divided by the strain increment equals the total number of compute tasks for this deformation job.
- ☑ *Append to structure list*: Append all deformed structure to a registered structure list which can be created by the **New List** stage.
- ☑ *Run the different loop iterations simultaneously*: Check this box to run multiple deformation tasks simultaneously.
- *Maximum number of jobs to submit simultaneously*: Sets the maximum number of compute tasks to submit simultaneously.

The Relaxation Flowchart button opens the flowchart used for the initial relaxation. This can be a **LAMMPS**, **VASP 5.4: Plane Wave DFT**, **VASP 5.4: High Throughput** stage, **VASP 6: Plane Wave DFT**, or **VASP 6: High Throughput** stage. Stages in this flowchart are only executed once.

The Stress Flowchart button opens the flowchart used for stress computation for each iteration. This can be a **LAMMPS**, **VASP 5.4: Plane Wave DFT**, **VASP 5.4: High Throughput** stage, **VASP 6: Plane Wave DFT**, or **VASP 6: High Throughput** stage. Stages in this flowchart are executed for each strain increment.

Note: The *Deformation* module applies strain in an instantaneous fashion. This means that the simulated strain rate is effectively many orders of magnitude higher than that typically applied in laboratory experiments. Consequently, certain types of materials, such as polymers, will not relax to thermodynamic equilibrium over the duration of the simulation performed in the Stress Flowchart. This will result in behavior that fails to accurately reflect experimental behavior, in which chain conformations change significantly to accommodate an applied deformation (in practice any such material will effectively behave as a glass).

4 Results

Deformation simulation results are included in Job.out, Deformation_{stage_id}.out, deformation_{stage_id}.png, and deformation_{stage_id}.gdt.

4.1 Job.out

Job.out contains the simulation setup, initial cell dimensions, strains, and stresses along the deformation direction.

```
Starting structure relaxation
Relaxation completed
Relaxed cell parameters: 15.0 15.0 17.039999999999999 90.0 90.0 90.0

Completed 50 tension deformation steps        flag_list: '0'

Iteration     Strain (relative) in Z Stress (GPa) in Z    Variation
1             0.01                   7.35324              ---
2             0.02                   10.90799             3.55475
3             0.03                   14.27992             3.37193
4             0.04                   17.38214             3.10222
```

```
5             0.05              20.37705             2.99491
6             0.06              23.24582             2.86877
7             0.07              25.79025             2.54443
8             0.08              28.23635             2.4461
9             0.09              30.51204             2.27569
10            0.1               32.83263             2.32059
.
.
.
49            0.49              39.73512             -0.77789
50            0.5               39.00348             -0.73164
```

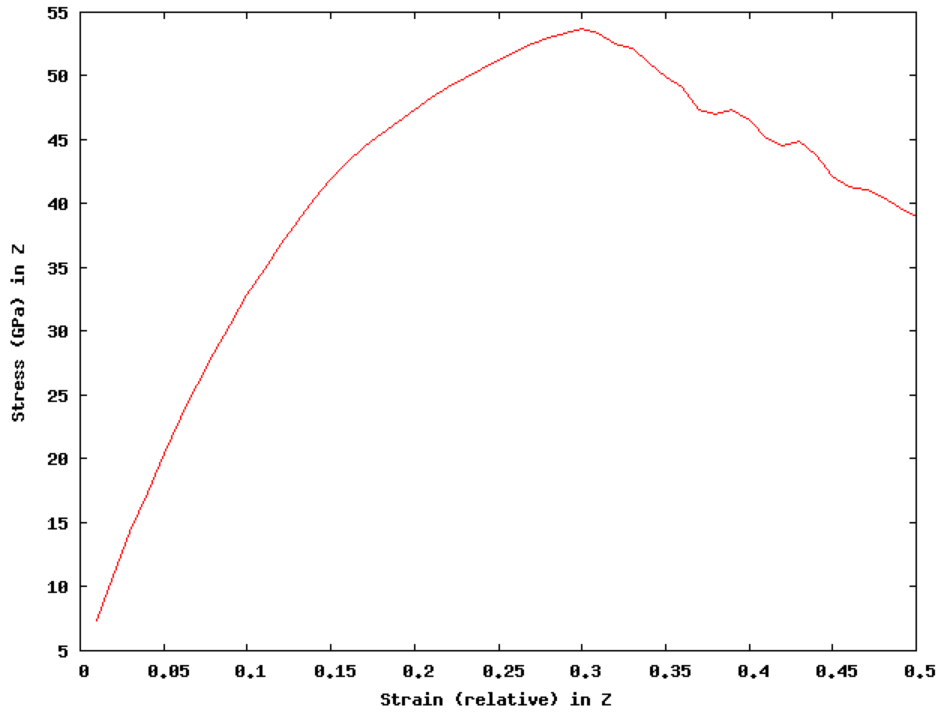
4.2 Deformation_{stage_id}.out

If the *Deformation* stage is the second stage in the flowchart, then *Deformation_{stage_id}.out* is named *Deformation_2.out*. This file contains the strains and stresses along all six directions.

```
Iteration     Strain (relative) in Z Stress (GPa) in Z     Full stress (GPa)
1             0.01              7.35324              {6.54204 6.54204 7.35324 0 -
↪0 0}
2             0.02              10.90799             {6.65784 6.65784 10.90799 0␣
↪-0 -0}
3             0.03              14.27992             {6.75655 6.75655 14.27992 -0␣
↪-0 -0}
4             0.04              17.38214             {6.97077 6.97077 17.38214 -0␣
↪-0 -0}
5             0.05              20.37705             {7.10256 7.10256 20.37705 0␣
↪-0 -0}
6             0.06              23.24582             {7.17606 7.17606 23.24582 0␣
↪-0 0}
7             0.07              25.79025             {7.25834 7.25834 25.79025 -0␣
↪0 -0}
8             0.08              28.23635             {7.33868 7.33868 28.23635 -0␣
↪0 0}
9             0.09              30.51204             {7.39272 7.39272 30.51204 -0␣
↪0 -0}
10            0.1               32.83263             {7.47937 7.47937 32.83263 -0␣
↪-0 -0}
.
.
.
49            0.49              39.73512             {7.47723 7.47723 39.73512 -0␣
↪0 -0}
50            0.5               39.00348             {7.43198 7.43198 39.00348 -0␣
↪0 0}
```

4.3 deformation_{deformation}.png

This figure plots the stress–strain curve along the deformation direction. If one wishes to plot the stress–strain curves along other directions, one should extract data from *Deformation_{stage_id).out*.



4.4 deformation_{stage_id}.gdt

This file is the raw data used to plot *deformation_{stage_id}.png*.

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