Atomic Simulation

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Outline

Creating Atoms

```
# ---------- Create Atoms ---------------------
lattice         fcc 4
region  box block 0 1 0 1 0 1 units lattice
create_box      1 box

lattice fcc 4 orient x 1 0 0 orient y 0 1 0 orient z 0 0 1
create_atoms 1 box
replicate 1 1 1
```

Define Interatomic Potential

```
# ---------- Define Interatomic Potential ---------------------
pair_style eam/alloy
pair_coeff * * Al99.eam.alloy Al
neighbor 2.0 bin
neigh_modify delay 10 check yes
```

Output

eunsil@eunsil-ThinkPad-T430s: ~/Documents/lammps

```
  orthogonal box = (0 0 0) to (4 4 4)
  1 by 1 by 1 MPI processor grid
  4 atoms
WARNING: Resetting reneighboring criteria during minimization (min.cpp:173)
Setting up minimization ...
Memory usage per processor = 2.50375 Mbytes
Step PotEng Lx Ly Lz Press Pxx Pyy Pzz eatoms
       0   -13.417787            4            4            4     29590.11     29
590.11     29590.11     29590.11   -13.417787
      10   -13.439104         4.04         4.04         4.04    5853.9553    585
3.9553    5853.9553    5853.9553   -13.439104
      14       -13.44         4.05         4.05         4.05     2.726913     2.
726913     2.726913     2.726913       -13.44
Loop time of 0.000586987 on 1 procs (1 MPI x 1 OpenMP) for 14 steps with 4 atoms

Minimization stats:
  Stopping criterion = linesearch alpha is zero
  Energy initial, next-to-last, final =
        -13.4177872966     -13.4399999525     -13.4399999525
  Force two-norm initial, final = 3.54599 0.000335006
  Force max component initial, final = 3.54599 0.000335006
  Final line search alpha, max atom move = 0.0625 2.09379e-05
  Iterations, force evaluations = 14 19

Pair  time (%) = 0.00028348 (48.2941)
Neigh time (%) = 0 (0)
Comm  time (%) = 7.70092e-05 (13.1194)
Outpt time (%) = 1.90735e-05 (3.24939)
Other time (%) = 0.000207424 (35.3371)
```

Output

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Nlocal:    4 ave 4 max 4 min
Histogram: 1 0 0 0 0 0 0 0 0 0
Nghost:    662 ave 662 max 662 min
Histogram: 1 0 0 0 0 0 0 0 0 0
Neighs:    280 ave 280 max 280 min
Histogram: 1 0 0 0 0 0 0 0 0 0

Total # of neighbors = 280
Ave neighs/atom = 70
Neighbor list builds = 0
Dangerous builds = 0
Total energy (eV) = -13.439999952539938732;
Number of atoms = 4;
Lattice constant (Angstoms) = 4.0499999999998046;
Cohesive energy (eV) = -3.3599999881349846831;
All done!
eunsil@eunsil-ThinkPad-T430s:~/Documents/lammps$
```

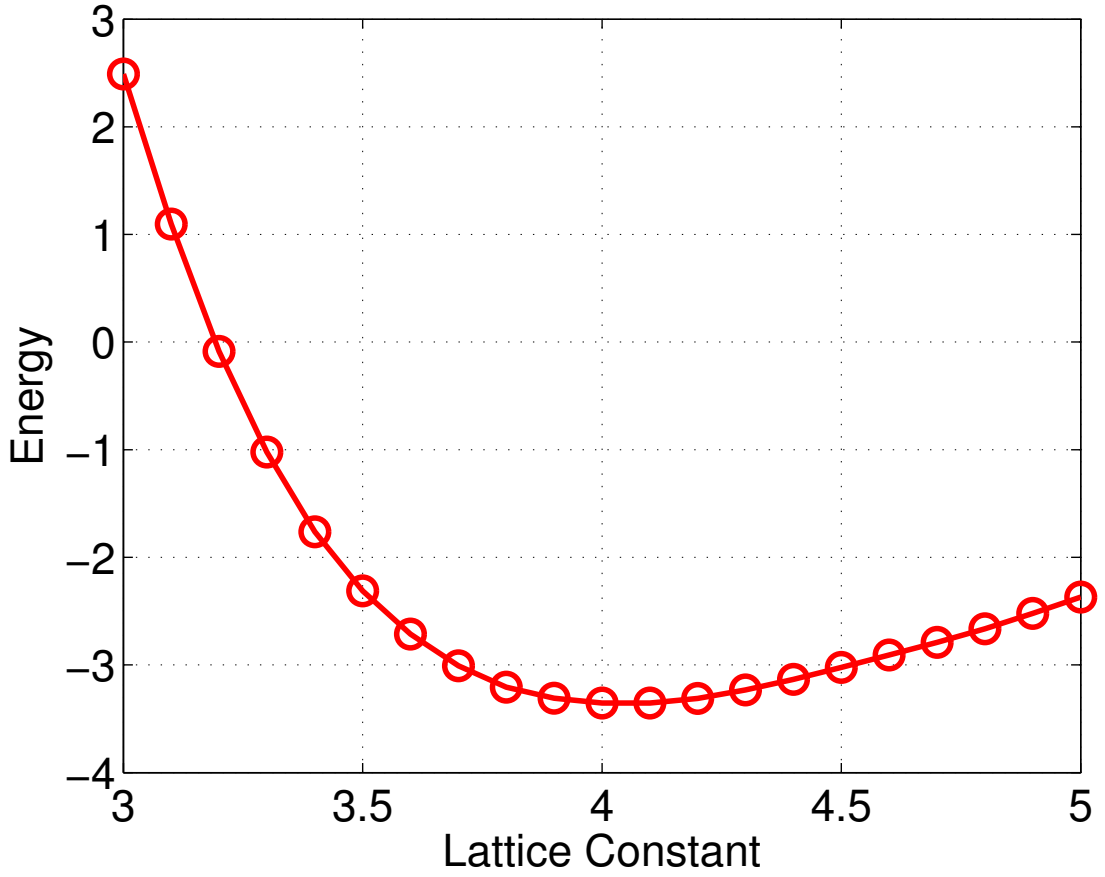
Run on Multiple Processors

"mpirun -np 4 lammps-daily < input.script"

Run with Variables

"mpirun -np 4 lammps-daily -var latconst 4 < input.script"

Energy vs. Lattice Constant

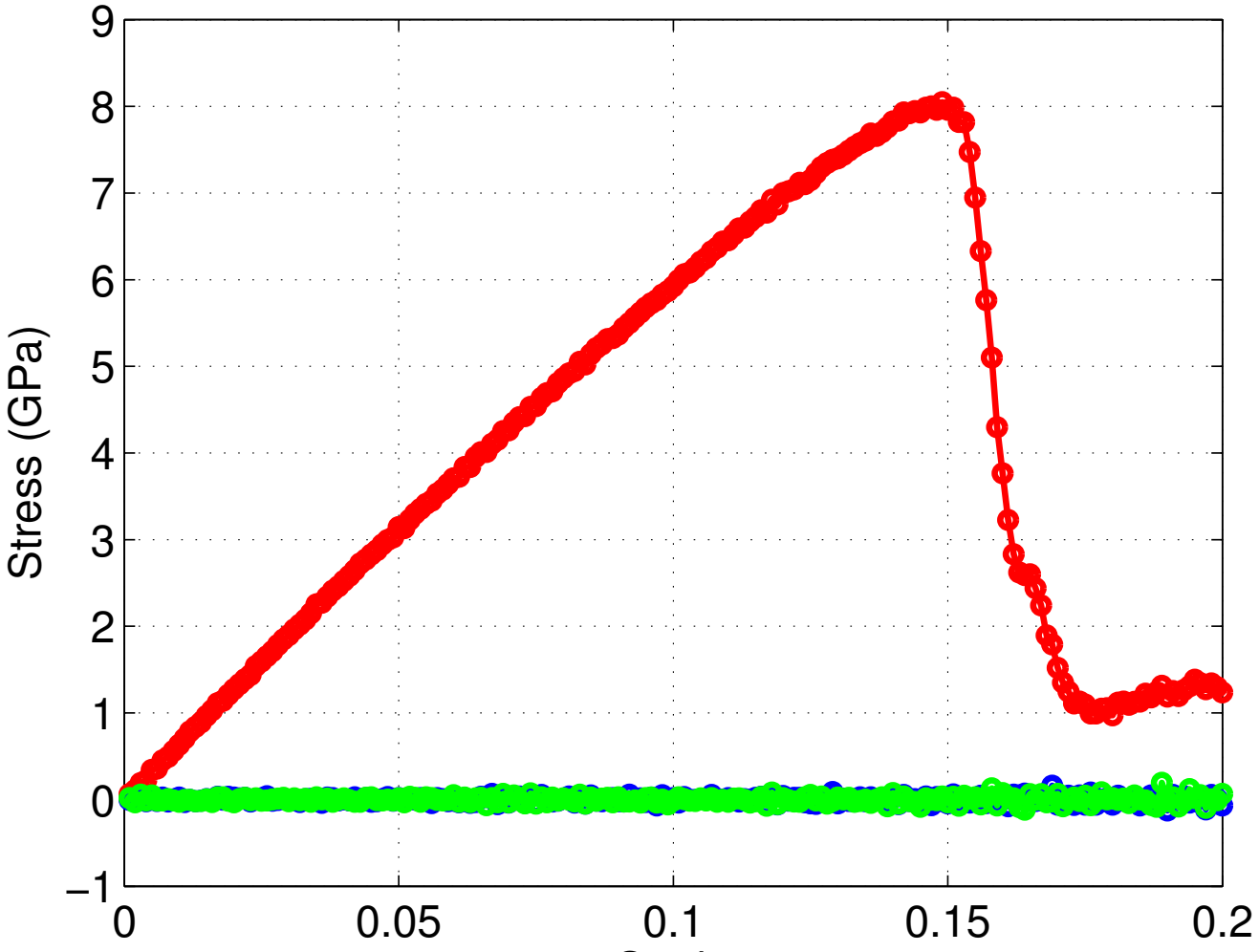


aluminum single crystal oriented in the <100> direction

Animation: (tensile.avi)

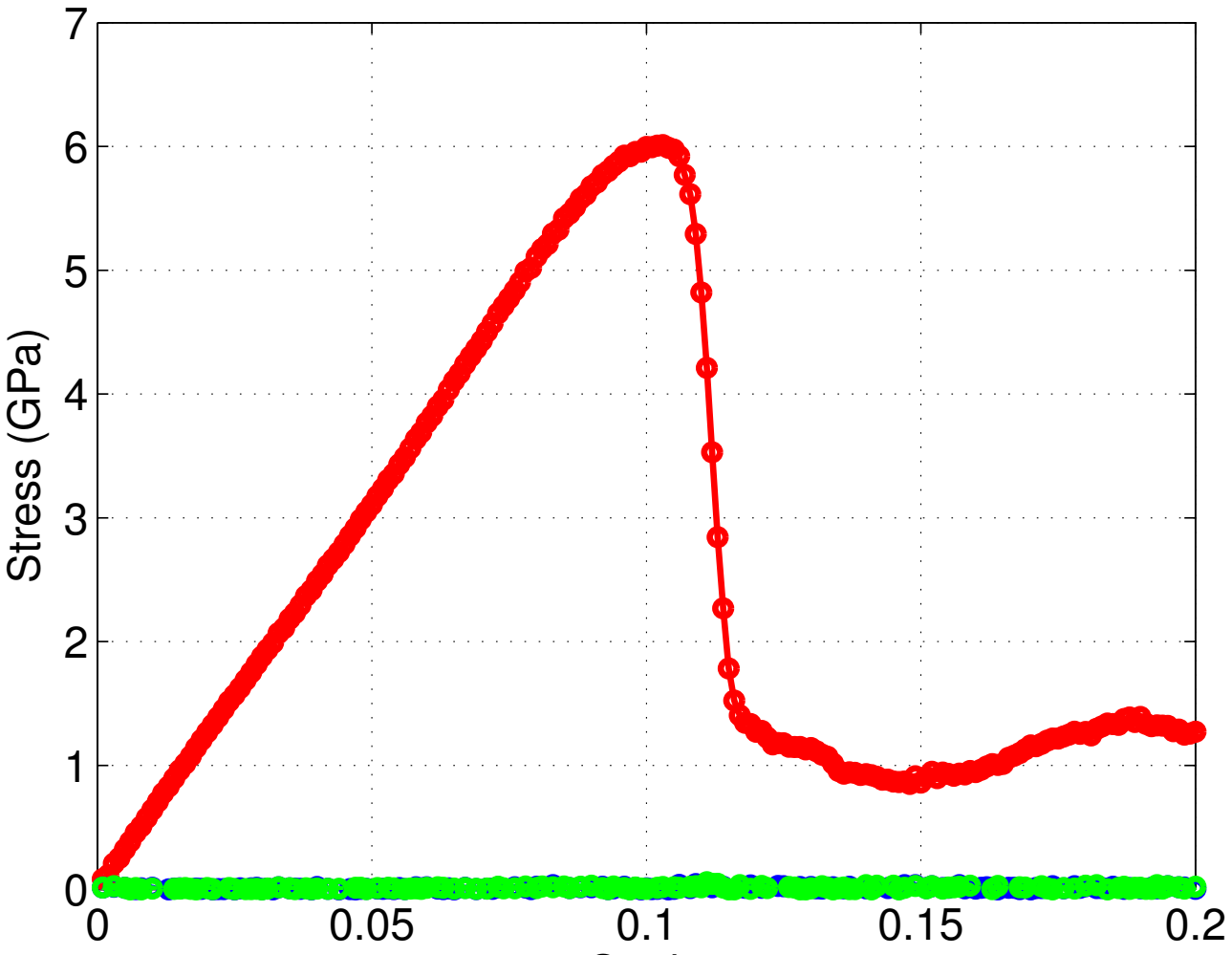
Tensile Loading

Strain-Stress Curve: 4,000 atoms



Compressive Loading

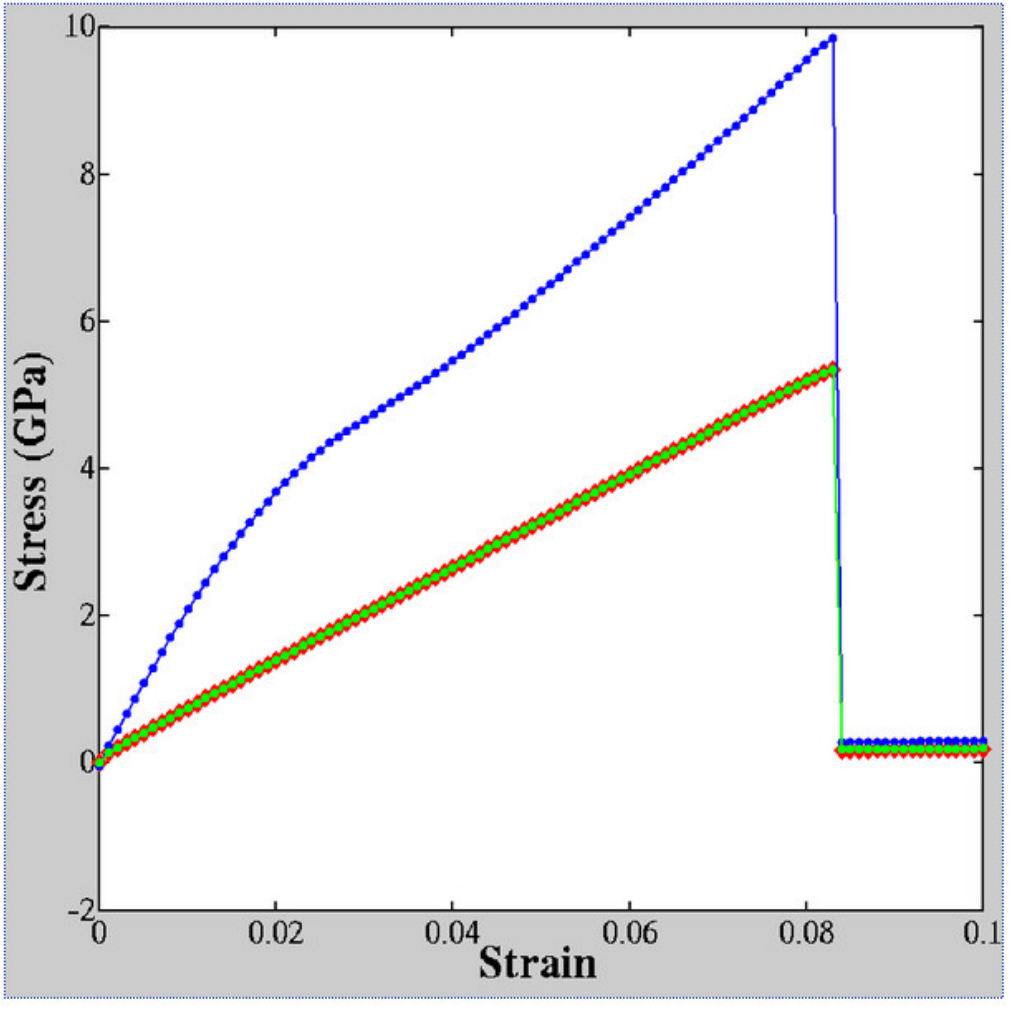
Strain-Stress Curve: 32,000 atoms



Atom Deletion

Animation: (grain.avi)

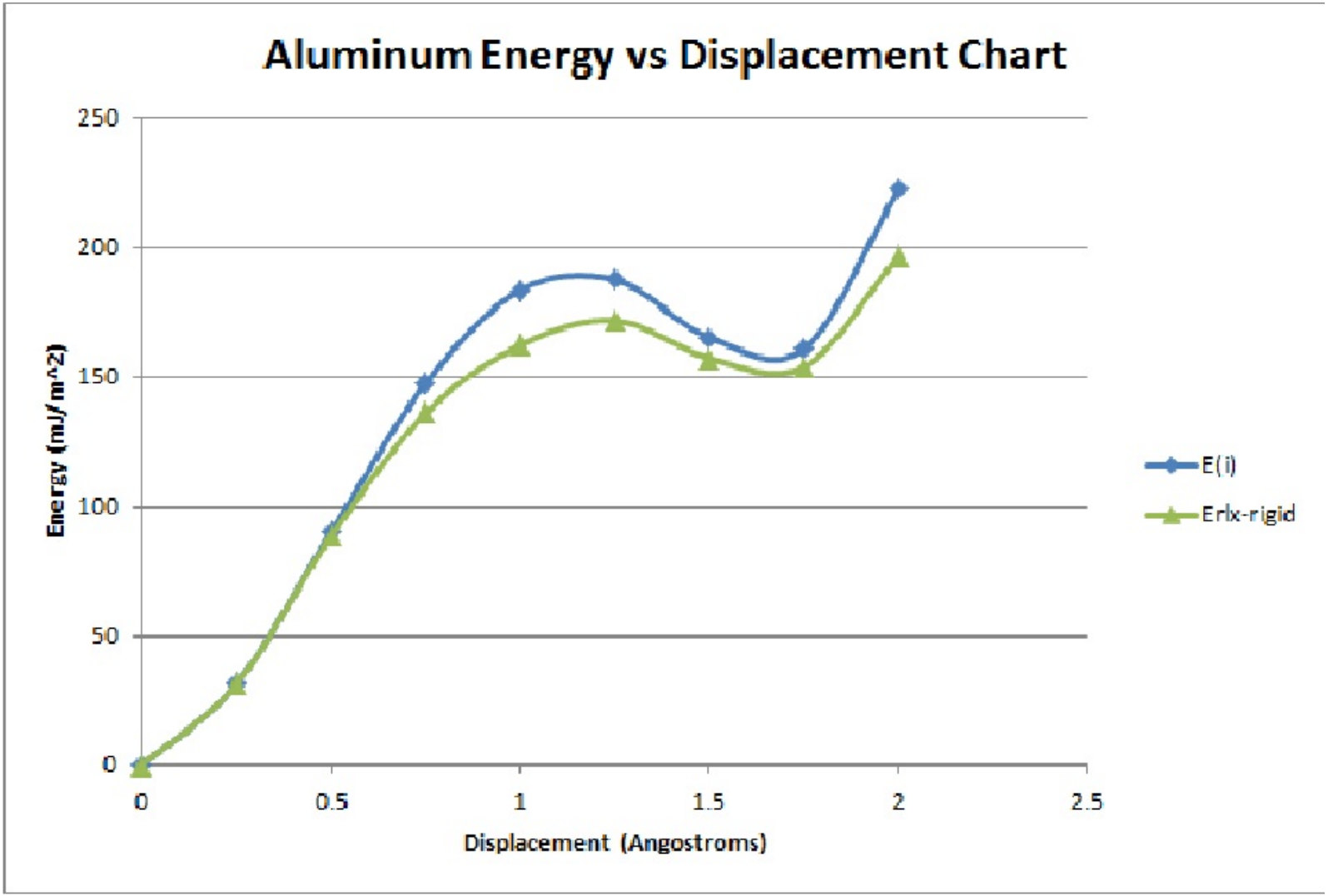
Iron-Tilt



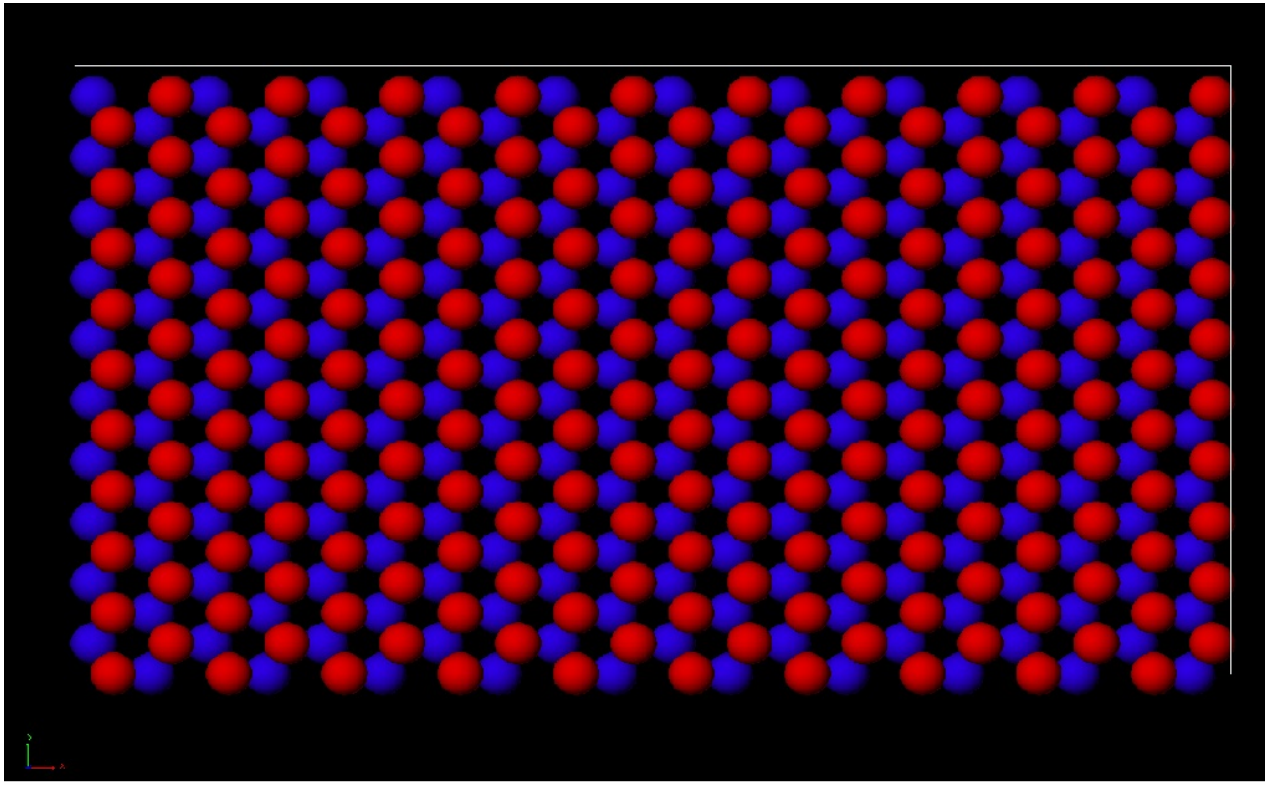
Iron-Tilt

Animation: (Fe-100-sig3-fracture.gif)

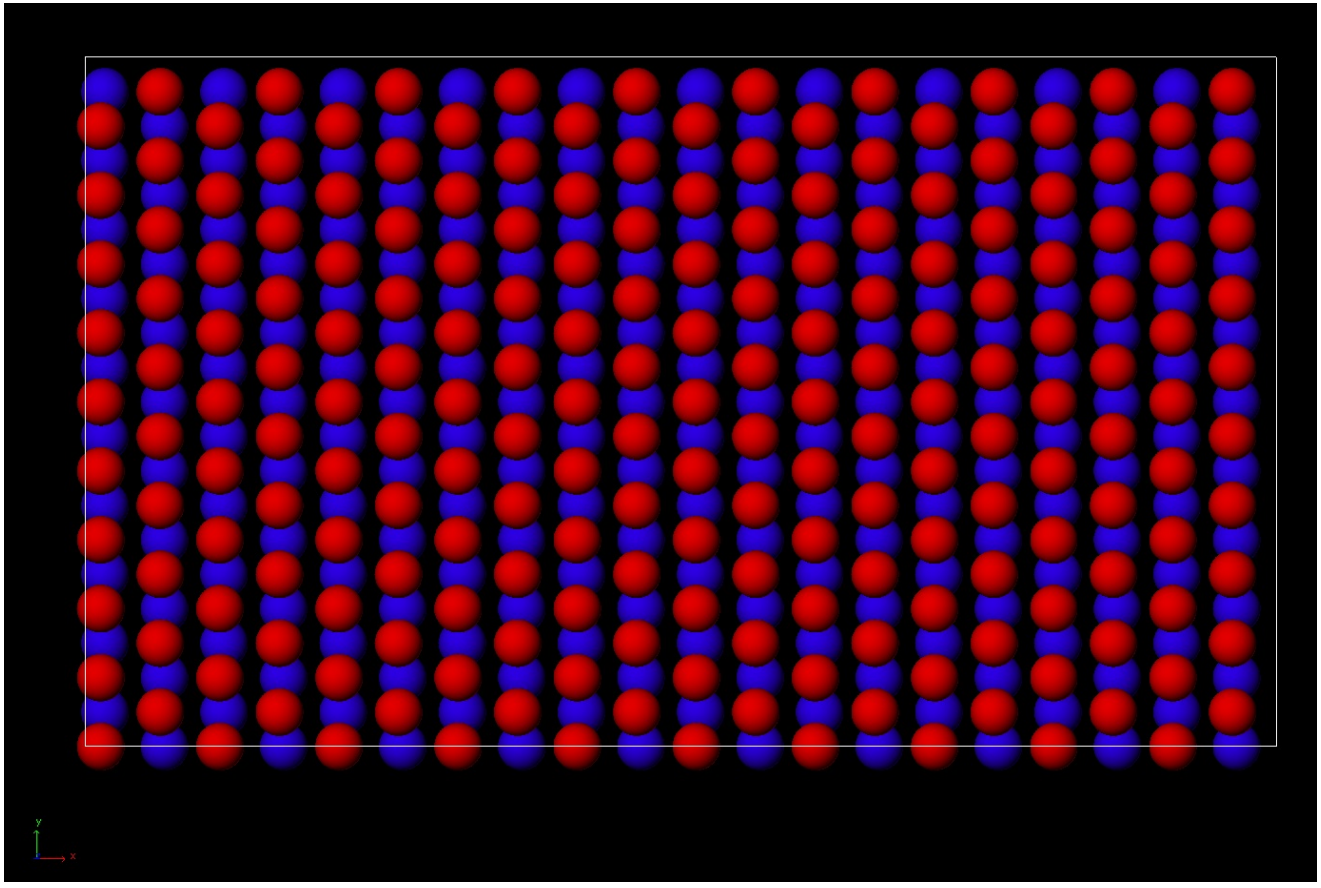
Al Energy vs. Displacement



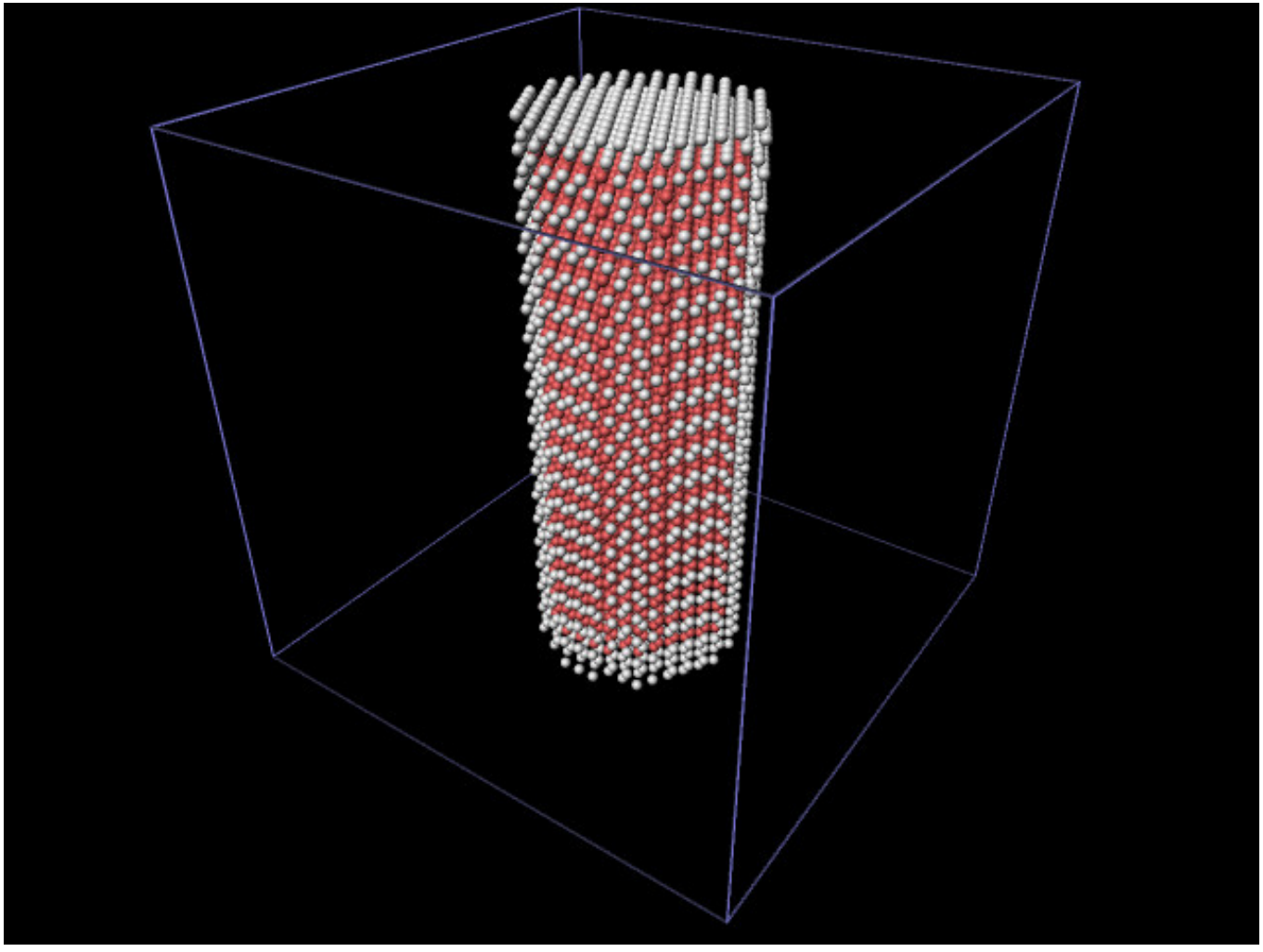
Before Displacement



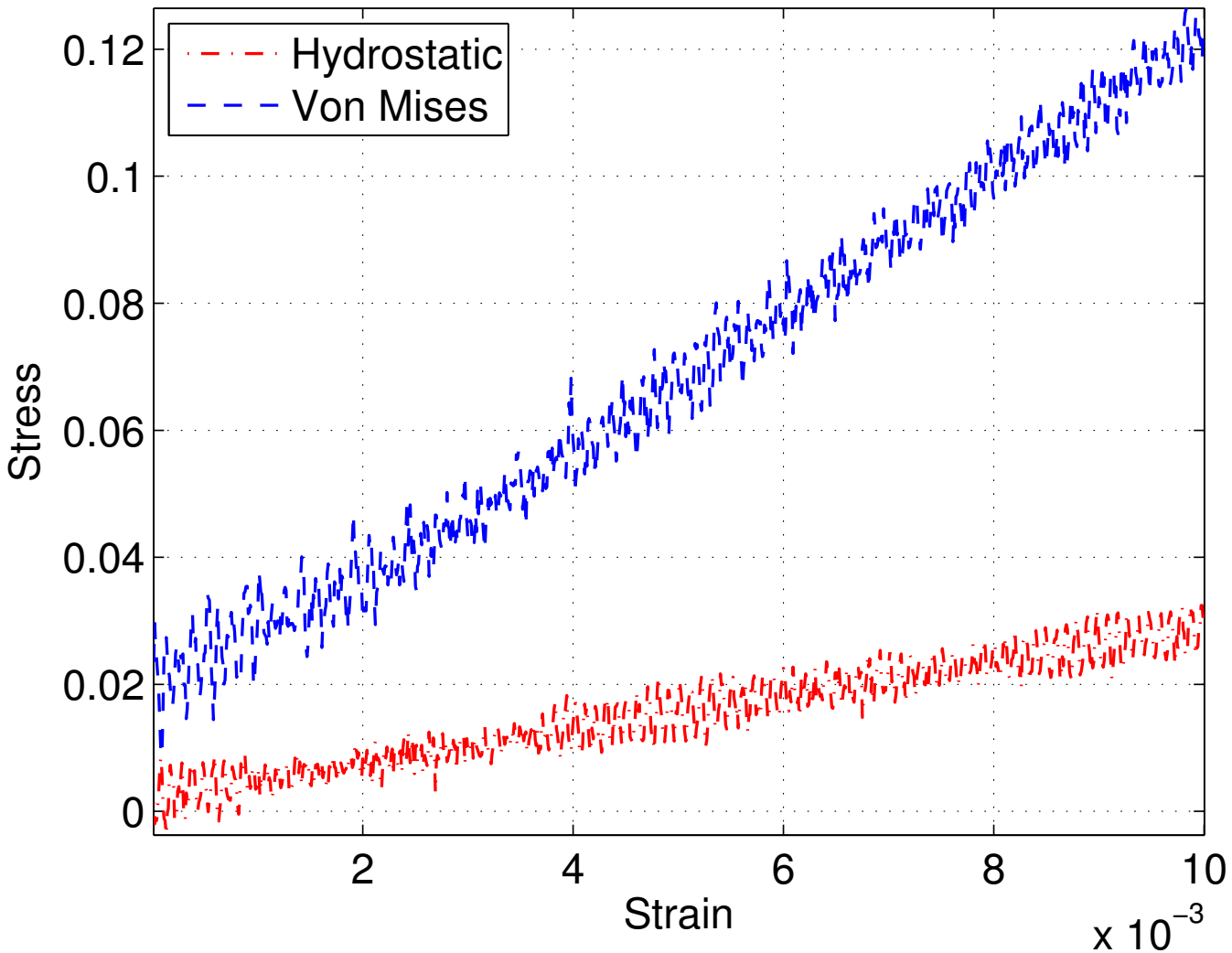
Displacement of 1



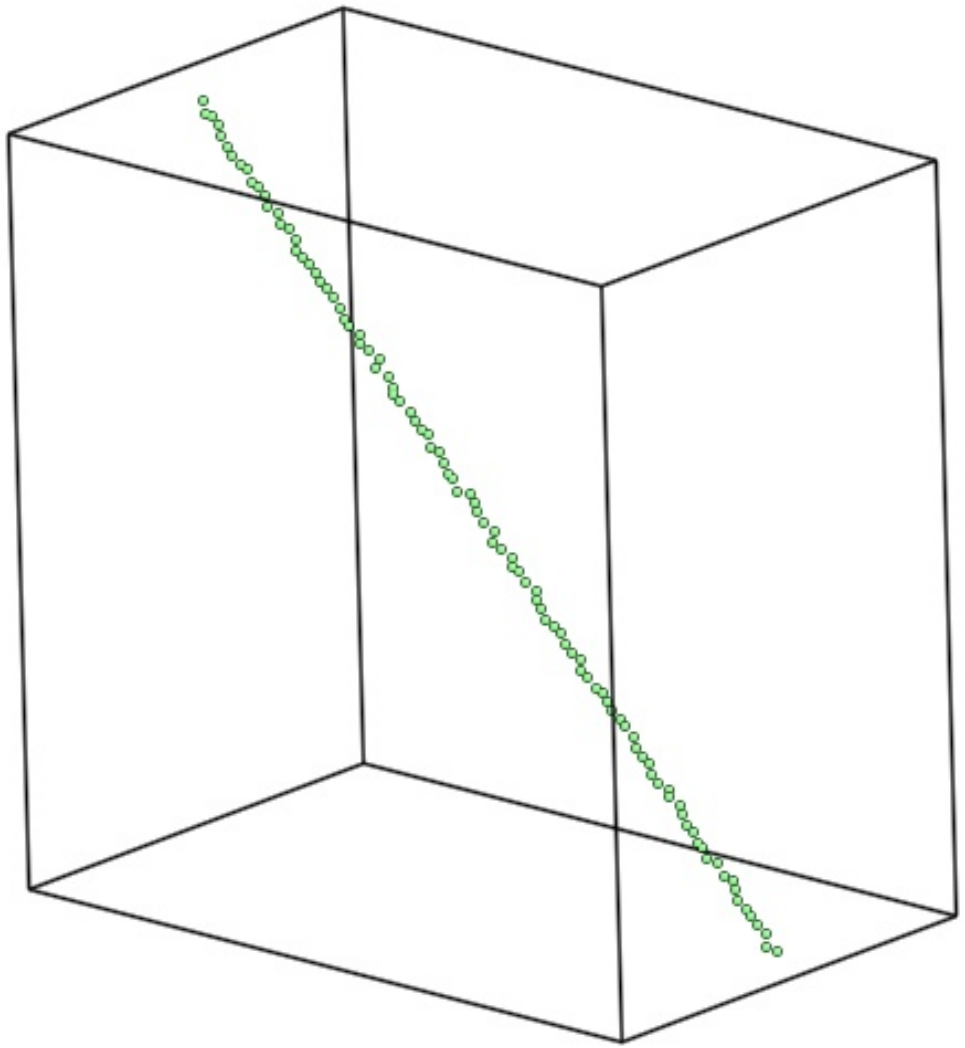
Magnesium Single Crystal Nanowire



Stress vs. Strain



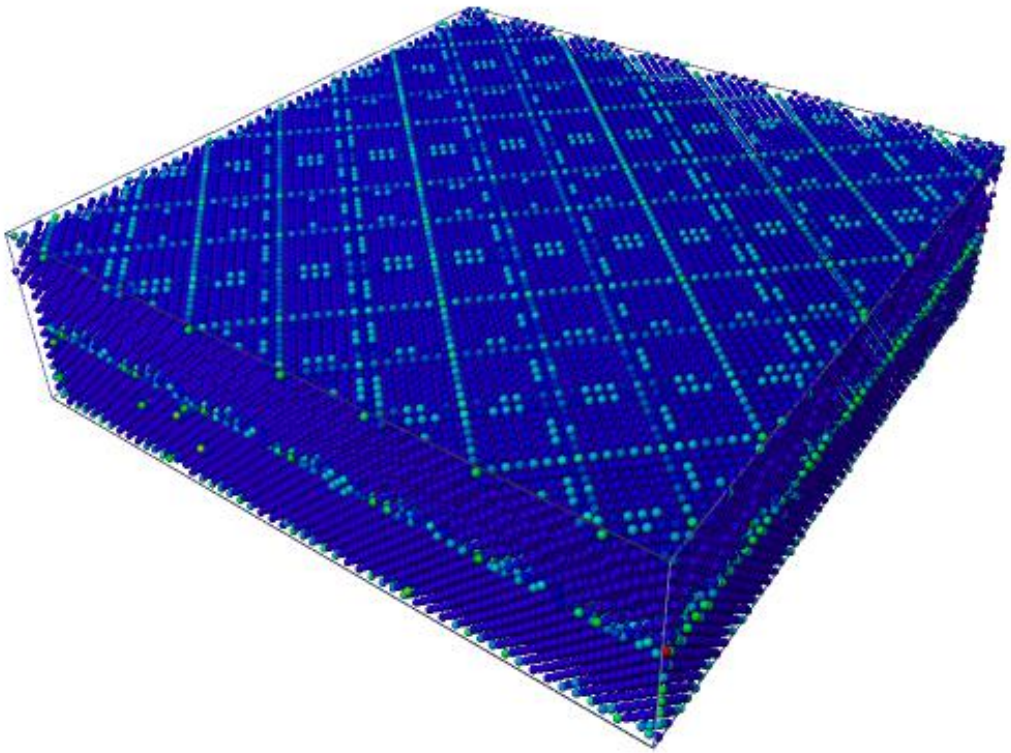
Not-deformed polymer chain



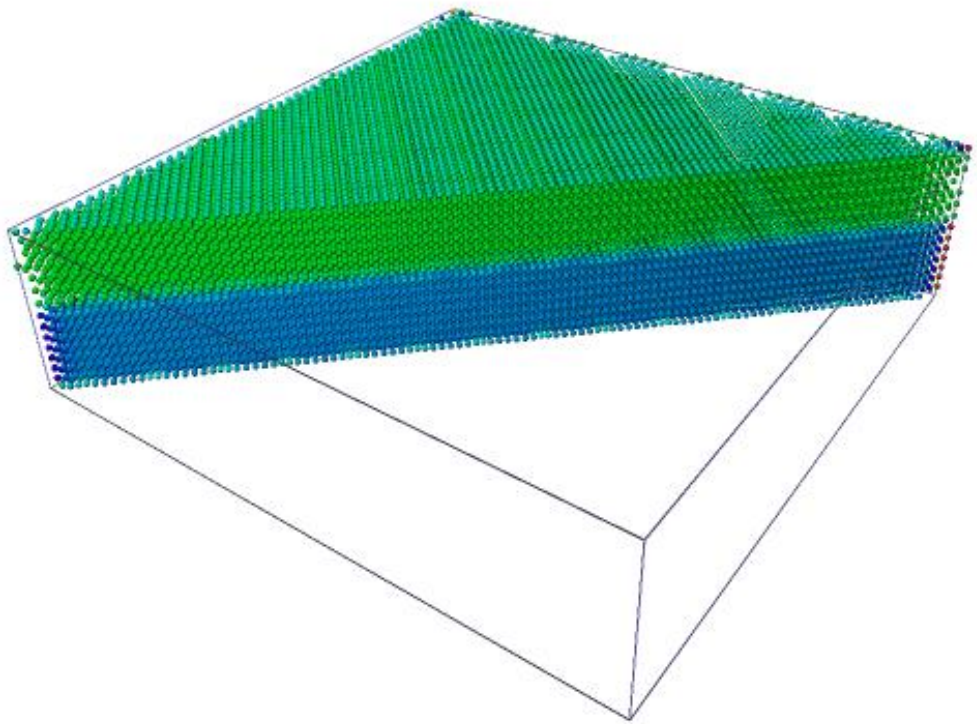
Polymer Chain Deformation

Animation: (Equ-plus-min.gif)

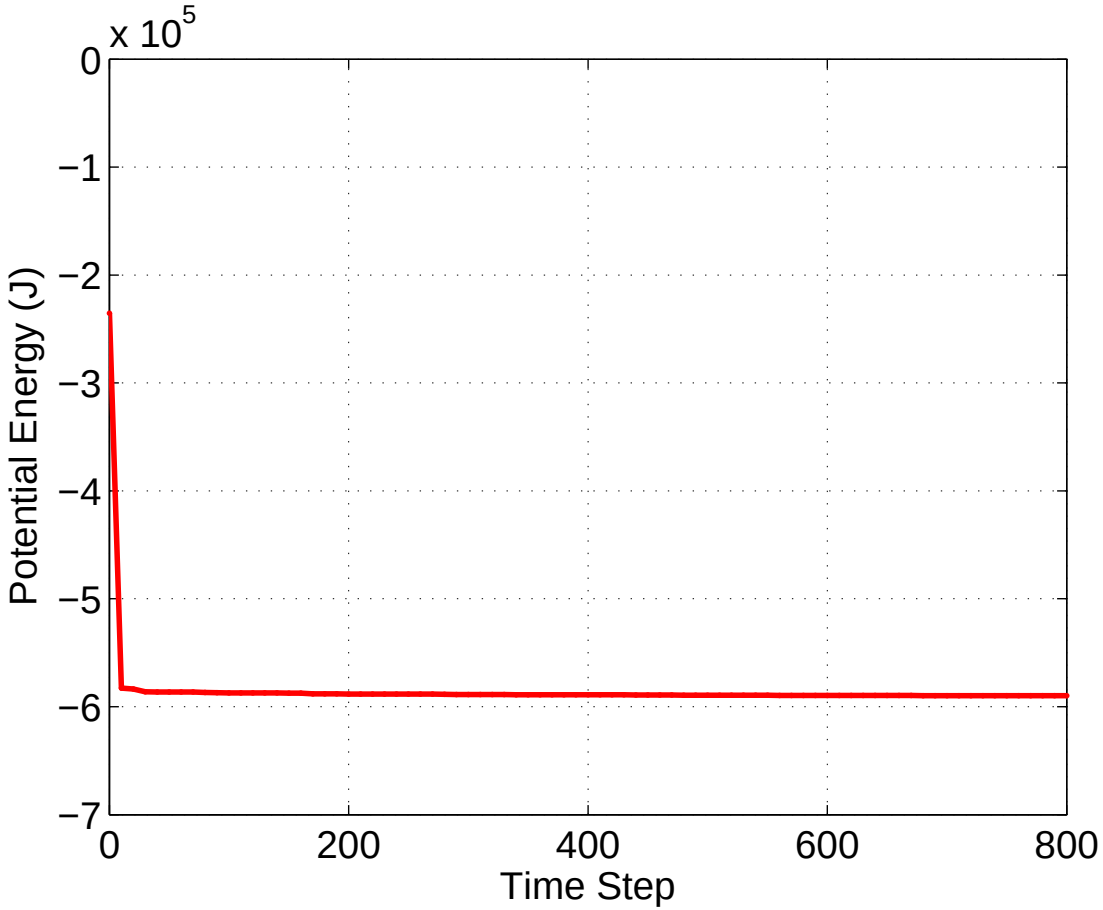
Relaxed NiAl



Misfit dislocation generated



Ni-Al Energy



Useful Commands

- fix: minimization:
  - *cg*: Polak-Ribiere version of conjugate gradient (CG) algorithm
  - *hftn*: Hessian-free truncated Newton algorithm
  - *sd*: steepest descent algorithm
  - *quickmin*: damped dynamics method
  - *fire*: damped dynamics method (adds a variable time step)

Useful Commands

- atom style:
  - *angle*: bonds and angles
  - *atomic*: only the default values
  - *bond*: bonds
  - *charge*: charge
  - *dipole*: charge and dipole moment
  - *electron*: charge and spin and eradius

Useful Commands

- change box
- displace atom
- compute
  - *ke*
  - *ke/atom*
  - *pe*
  - *pe/atom*
  - *pressure*
  - *temp*

Outline

NWChem

Examples:

- Water Single Point SCF (self-consistent field method, aka Hartree-Fock) Energy
- Restarting and Perform a Geometry Optimization
- Compute the Atomic Energy (polarizability of Ne using finite Field)
- The Energy with Applied Field
- SCF Energy of H_2CO using ECPs (Electronic Conducting Polymers) for C and O
- MP2 (second order Møller-Plesset perturbation theory) Optimizatino and CCSD(T) (coupled-cluster linearized triples approximation) on Nitrogen

NWChem

Quantum Mechanical Methods:

- Hartree-Fock Theory
- Density Functional Theory
- Excited-State Calculations
- Plane-Wave Density Functional Theory
- Tensor Contraction Engine
- MP2
- Coupled Cluster Calculations
- Multiconfiguration SCF
- Selected CI (configuration interaction)

Outline

MedeA/VASP

- MedeA Bundle- includes MedeA Graphical User Interface to generate input files for VASP and to build 3-D atomistic models through various building tools: molecular, crystal, surface, polymer chain, nanotube, and nanoparticle builders. Offers full visualization and analysis of all calculations/results. Also includes access to Pearson's experimental crystal structures database with Infomatica search engine. You can import these structures into the GUI which makes building 3-D atomistic models a lot more efficient.
- VASP5.3 Module- main engine for quantum simulations (Ab-intio and DFT methods) to handle the application and compute the properties you described. With VASP one can also do a periodic [PdX-H2-] chain.
- Embedded Atom Method Module- uses Zhou/Francis forcefield to handle larger Pd clusters.

MedeA/VASP

For an Annual License (1 simultaneous user)-

MedeA Bundle = $\$15,000.00$ VASP5.3 Module = $\$25,000.00$
LAMMPS Module = At no additional cost Embedded Atom Method Module = $\$5,000.00$

TOTAL = $\$45,000.00$ USD

For a Perpetual License (1 simultaneous user)-

MedeA Bundle = $\$37,500.00$ VASP5.3 Module = $\$62,500.00$
LAMMPS Module = At no additional cost Embedded Atom Method Module = $\$12,500.00$

TOTAL = $\$112,500.00$ USD

Other tools

- Accelrys: waiting for response
- Smeagol: no reply yet