materials design

APPLICATION NOTE

Stress-Strain Behavior of a Cu Nanowire Simulated with MedeA®-LAMMPS

The stress-strain behavior of a Cu nanowire is simulated with the MedeA® environment using a quasi-classical embedded atom potential and the LAMMPS molecular dynamics code. The monocrystalline wire has a diameter of 3.3 nm and is stretched in the [100] direction. The simulations show an initial elastic region with a linear increase in stress, which reaches a maximum just before the onset of slip in (111) planes. Upon further strain the model reveals the formation of more slip planes and necking until the break point is reached.

Keywords: Nanowire, stress-strain, necking, slip, fracture, MedeA®, LAMMPS, embedded atom method

Purpose

This application note illustrates the capability of the MedeA® software environment with LAMMPS [1] to simulate the deformation of metals under strain and to compute the stress-strain behavior of a material. A monocrystalline nanowire of Cu with a diameter of 3.3 nm oriented in the [100] direction of this face-centered cubic material is chosen as specific example.

Model Construction

Starting from the unit cell of elemental Cu, which is readily retrieved from the databases available within MedeA®, a model of a nanowire is constructed using the standard building tools of MedeA®. To initiate the desired break point, a few atoms near the middle of the slab are deleted, thereby creating a little notch. The resulting model is shown in Fig. 1.

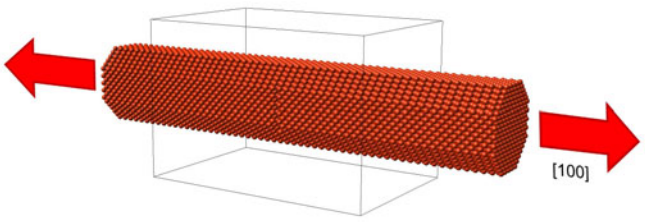

Figure 1. Model of a Cu nanowire containing 10,189 atoms oriented along the [100] direction of this face-centered cubic material. The direction of strain is indicated by red arrows. A small notch near the middle of the model is used to initiate the separation.

From the library of potentials for the embedded atom method (EAM), the form of Adams *et al.* [2] is chosen and the parameters are assigned to the atoms by a few mouse clicks. These simple steps lead to a model with assigned forcefield parameters.

Stress-Strain Calculation

The nanowire is now subject to the following computational protocol: the cell dimension in the x-direction is set to a series of increasing values. For each value, the cell is stretched using the structure from the previous step, then a short molecular dynamics simulation is carried out (in this example the temperature is 150 K and the dynamics is run for 10 ps) and the last structure of the dynamics run is relaxed by energy minimization. The Flowchart capability of MedeA® with its loop structure makes it very easy to create such a computational protocol.

Fig. 2 displays the result of this simulation. As expected, near equilibrium the total energy of the system depends parabolically on the strain and the stress increases linearly in this elastic regime. As soon as slip occurs, the stress of the system decreases in an oscillatory behavior, which is also seen in the total energy of the system. As more slip planes develop and the displacements increase, the wire forms a neck, which becomes thinner upon further stretching until the breakpoint is reached. At this point the stress drops to zero. Due to the blunting of the tips, the total energy decreases after separation.

In this model, the maximum stress is 1170 MPa. This refers to a monocrystalline nanowire with a cross section of 11.2 nm^2 in a box, which has a cross section of 52.3 nm^2. Since the computed stress refers to the box, one obtains a maximum stress of 5464 MPa for the wire itself. This is, of course, much higher than values reported for polycrystalline copper, namely 220 MPa for the ultimate tensile strength. Furthermore, the present simulations are performed at a temperature of 150 K where one expects brittle behavior.

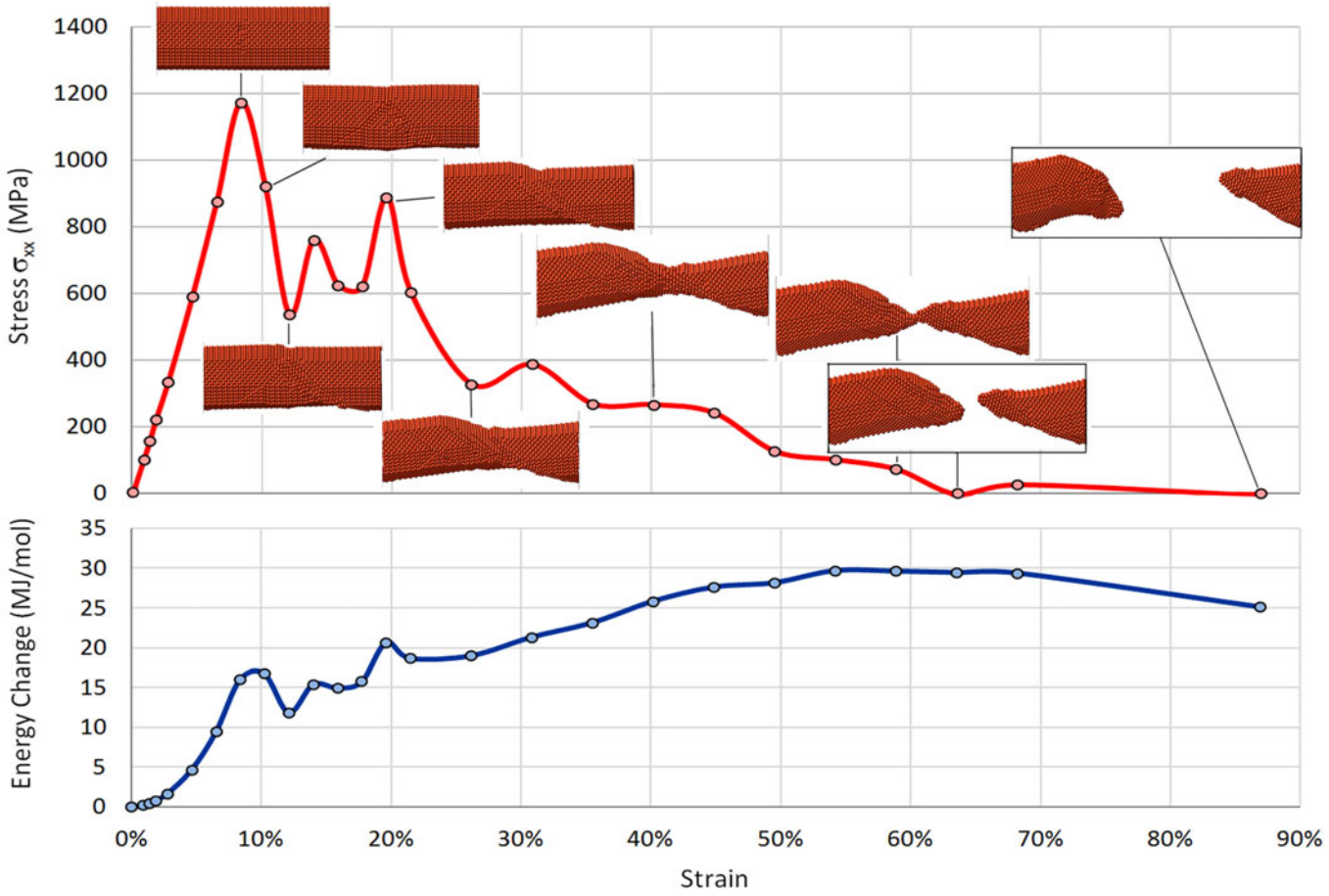

Figure 2. Stress-strain behavior of a Cu nanowire computed with an embedded atom potential using MedeA®-LAMMPS. After each step straining the material, the system is subject to a short molecular dynamics run followed by an energy minimization. Note the elastic behavior up to the point of highest stress, where slip in the (111) plans sets in. The tip blunting after fracture leads to a small lowering of the total energy of the system. The stress refers to a simulation box with a cross section of 52.27 nm^2; the cross section of the nanowire itself is 11.16 nm^2.

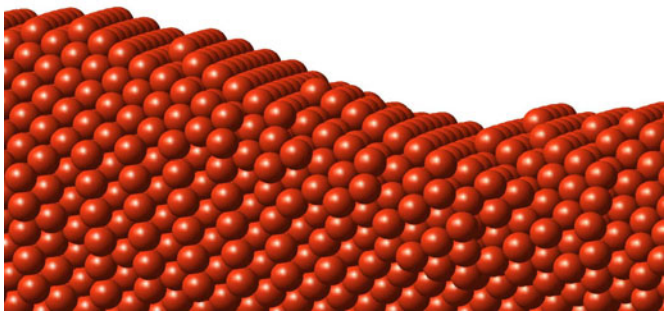

Figure 3. Detail of (111) slip planes forming in the neck region.

Significance

The MedeA® environment makes the exploration of system variables straightforward. For example, in the present case, the dimensions of the wire, the crystallographic orientation, and the size and location of the notch could be varied, the temperature and duration of the simulation could be explored, and the effect of alloy composition on stress strain behavior could be investigated. Grain boundaries could be built into the initial model and their effect on the stress-strain curve could be investigated. MedeA® Flowcharts make such systematic analyses straightforward. In the present case for example, the nanoscale impact of dopant species at different concentrations can be explored making use of the forcefield by Zhou *et al.* [3] which permits the simulation of Cu and 15 common metallic alloying elements. The insights obtained by such simulations can be invaluable in analyzing and targeting experimental investigation.

Analogous simulations could be performed for brittle ionic materials using Buckingham-type potentials, which are also available within the MedeA® environment. In principle, this type of simulations may

also be performed using the quantum mechanical VASP program to compute energies, forces, and the stress tensor. VASP can be invoked as one of the stages within MedeA® Flowcharts. Such simulations may require a careful choice of the structural models and substantial computing resources.

It should be made clear that the present example is intended as an illustration of the capability of MedeA® with LAMMPS rather than a detailed investigation of the stress-strain behavior of metallic nanowires. In fact, such studies have been performed, for example by Liang *et al.* [4] who have investigated the role of surface effects on the elastic behavior of Cu nanowires.

MedeA® Modules Employed in this Example

The present calculations were performed with the MedeA® platform using the following integrated features and modules:

- The standard MedeA® framework including crystal structure builders and geometric analysis tools
- The MedeA®-LAMMPS interface with Flowcharts
- The MedeA®-Embedded Atom Method
- The MedeA® JobServer and TaskServers
- The standard MedeA® visualization tools.

References

1. S. Plimpton *J. Comp. Phys.* **117**, 1 (1995)
2. J. B. Adams, S. M. Foiles, and W. G. Wolfer, J. Mater. Res. **4**, 102-112 (1989)
3. X. W. Zhou, R. A. Johnson, and H. N. G. Wadley, Phys. Rev. B **69**, 144113 (2004)
4. H. Liang, M. Upmanyu, and H. Huang, Phys. Rev. B **71**, 241403 (2005)

For additional information please contact

Materials Design, Inc.
PO Box 31325
Santa Fe, NM 87594, USA
T +1 760 495-4924
F +1 760 897-2179
info@materialsdesign.com
www.materialsdesign.com