MPC Calibration

3/3/2022

Heechen E. Cho, Ph.D.

Computing Environment (need update & include linux version)

- Computing environment
  - ✓Windows 7, 64-bit
  - ✓MPCv4_pkg.exe (a self extracting archive)
  - ✓MATLAB Compiler Runtime (MCR) 8.1, may be downloaded from http://www.mathworks.com/supportfiles/MCR_Runtime/R2013a/MCR_R2013a_win64_installer.exe

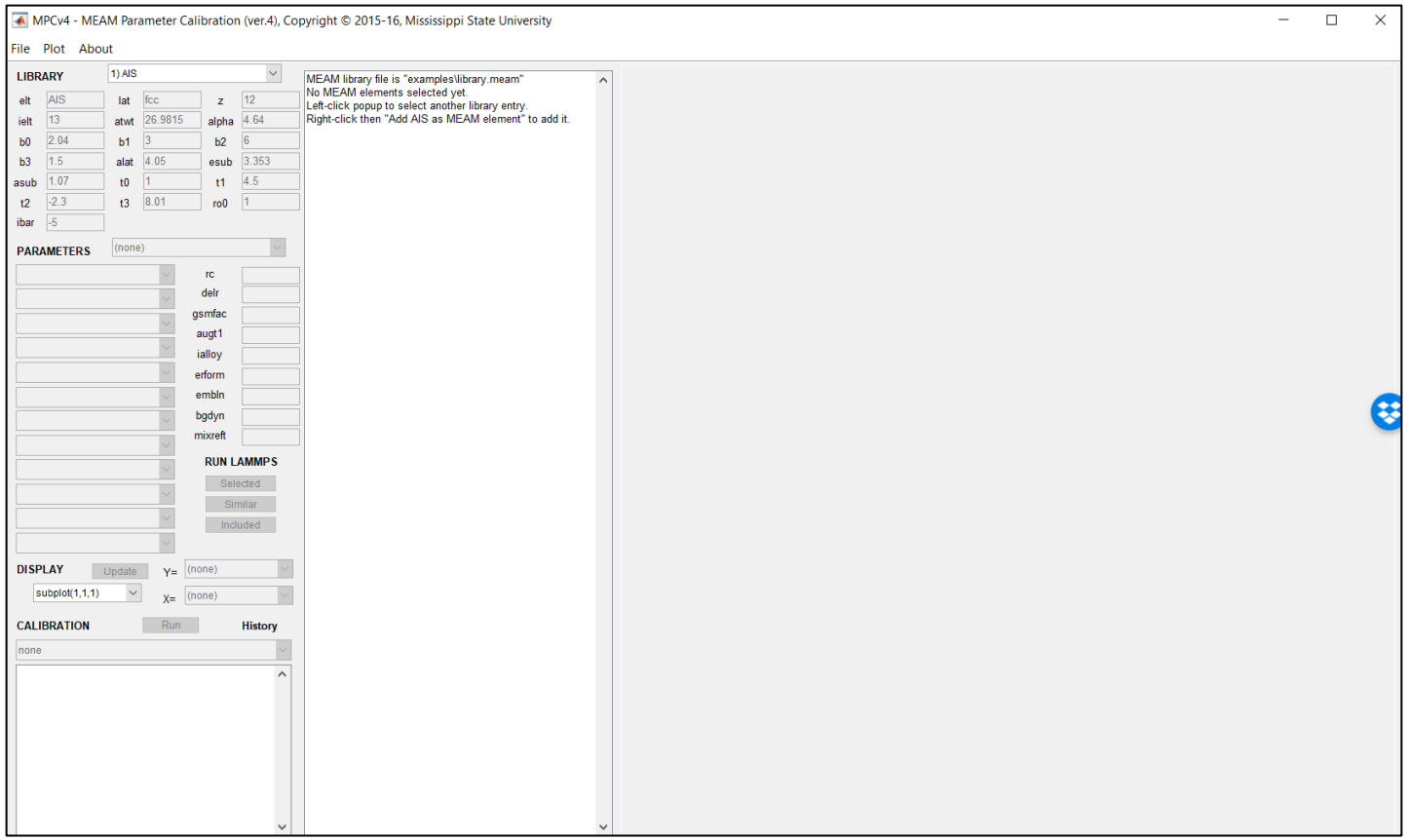
- If MPCv4_pkg.exe is 400+MB in size, the MCR installer should be included in the package.

Installation

- Make directory C:\MPCv4, copy MPCv4_pkg.exe to new directory, then run MPCv4_pkg.exe to extract files from the package. If the MCR installer is included in the package, the installer will automatically start.
- Run MCR_R2013a_win64_installer.exe if not already installed, or if a different version of the MCR is installed

Run

- Open a command line window (Windows Start, then type/enter "cmd.exe" in 'Search programs and files' box)
- Change directory to C:\MPCv4
- Type/enter "MPCv4.exe", wait for a few moments

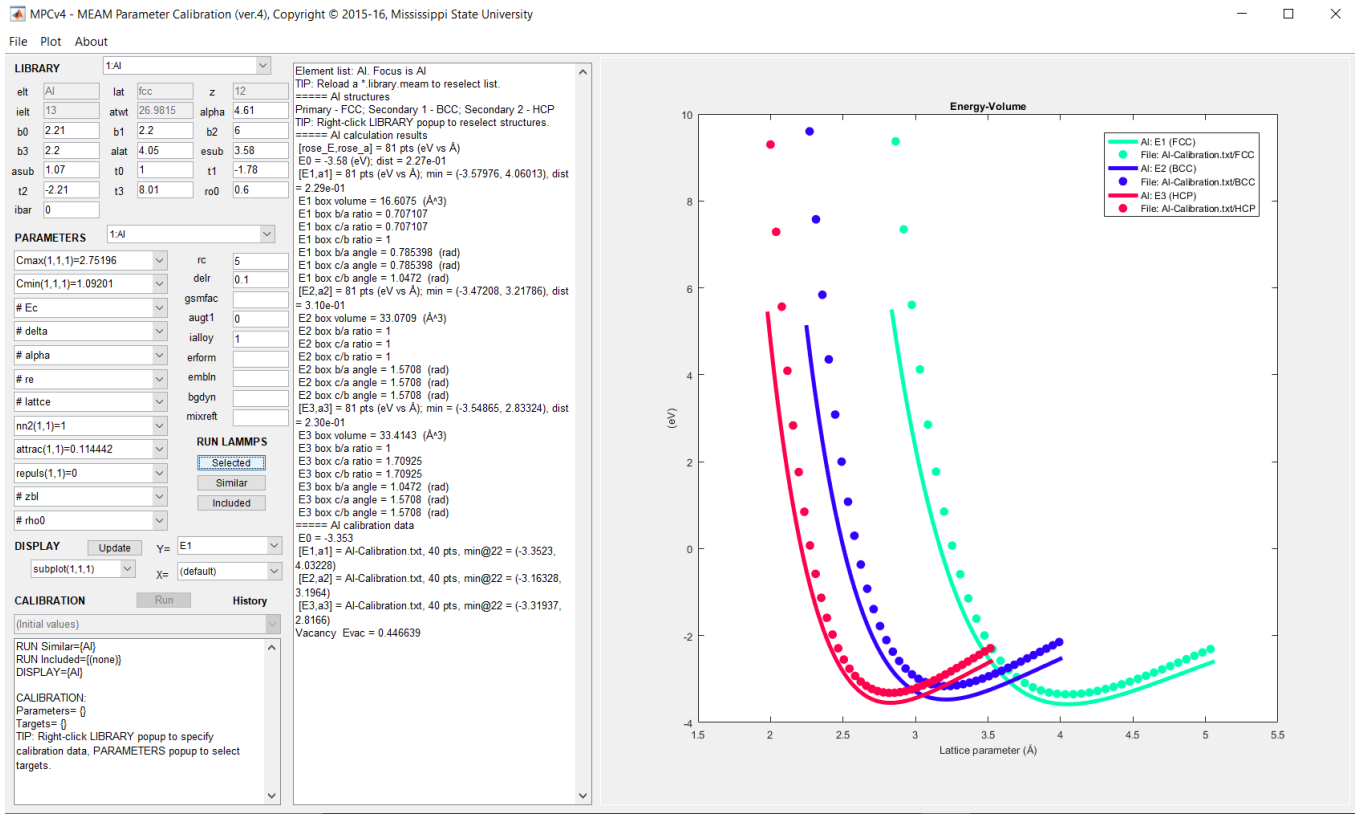


Calibration Setup

- Load “library.meam”
- In “Library”, determine a target material
- after right click, select “Add -- as MEAM element”
- after right click, select “Fix element(s) to --”
- Load MEAM parameter file in File tab
- In “Library”, determine secondary 1 and secondary 2 structures
- Click “Selected” in “RUN LAMMPS”
- In “Library”, select “Load calibration data file for --”

Calibration Setup

- In “Plot” tab, select “E1 vs. a1” under “Single elements …” to calibration the reference structure energy
- Repeat this to include the secondary 1 (E2) and secondary 2 structure (E3), then click “Selected” in “RUN LAMMPS”
- Repeat this process to include other values (E0, C, GSFE, etc.)



MPC Calibration Process

1. **Calibration to FCC energy versus lattice spacing**: load the FCC curve from DFT; calibrate alat, esub, and alpha for LAMMPS to match the minimum FCC energy; calibrate attrac and repuls to to fit points away from the minimum.
   - To fit Universal Equation of State (UEOS) and DFT results
   - We minimize error near lattice constant near equilibrium using the three parameters (these can be determined from DFT data or experimental data):
     - ✓"alat": equilibrium lattice constant
     - ✓"esub": energy per unit volume
     - ✓"alpha": bulk modulus-related constant (bulk modulus is automatically calculated based on alpha in MPC)
   - To minimize error far area from equilibrium, following two parameters are used:
     - ✓"attract"
     - ✓"repuls"

MPC Calibration Process

2. **Calibration to minimum BCC energy**: load the BCC curve from DFT or experimental BCC energy; calibrate b0 parameter for LAMMPS to match the BCC energy
   - From DFT or experimental data for BCC structure, minimize error for the energy vs. lattice spacing curve:
     ✓"b0": to determine minimum BCC energy

3. **Calibration to minimum HCP energy**: load the HCP curve from DFT or experimental HCP energy; calibrate t3 parameter for LAMMPS to match the HCP energy.
   - Minimize error for energy vs. lattice spacing curve for HCP"b0": to determine minimum BCC energy
     ✓"t3": to determine minimum HCP energy

MPC Calibration Process

4. **Calibration to elastic constants C44 and C'**: load the elastic moduli C44, C11 and C12 from DFT results or experimental results. Calibrate t2 and b2 for LAMMPS to match C44 and C' (= (C11-C12)/2).
   - t2 and b2 are calibrated against these elastic moduli

   ✓"t2"

   ✓"b2"

5. **Calibration to vacancy formation energy (VFE)**: load the VFE target from DFT or experiment; calibrate t1 for LAMMPS to match.
   - t1 to calibrate VFE

   ✓"t1"

MPC Calibration Process

5. **Calibration to generalized stacking fault energy (GSFE) curve**: load the GSFE curve from DFT; calibrate Cmin and asub for LAMMPS to match the first local maximum; calibrate b1 and b3 for LAMMPS to match the second local maximum.
   - ✓"Cmin": related to first maximum (unstable dislocations) of GSFE curve
   - ✓"asub": related to minimum (stable dislocations) of GSFE curve
   - ✓"b1" and "b3": related to second maximum (sometimes related to deformation twinning) of GSFE curve

MPC Calibration Process

Using optimization capability for calibration

- Right click any parameters that you want to optimize
- Select “Add to calibration parameter list”
- Right click “PARAMETERS”, and select the target curve or data
- Click “Run” in CALIBRATION
- When you exclude these parameters from the optimization-assisted calibration, do right click and remove each one

MPC Calibration Tutorials & Useful Info

- https://www.youtube.com/watch?v=bipKWVFX01I
- https://www.youtube.com/watch?v=1YTUQm7xY60
- https://icme.hpc.msstate.edu/mediawiki/index.php/ICME_2017_HW1.html
- https://icme.hpc.msstate.edu/mediawiki/index.php/MPC.html

Reference

- Horstemeyer MF, Hughes JM, Sukhija N, Lawrimore WB, Kim S, Carino R, Baskes MI (2015) “Hierarchical Bridging Between Ab Initio and Atomistic Level Computations: Calibrating the Modified Embedded Atom Method (MEAM) Potential (Part A).” JOM, 67(1):143–147. https://doi.org/10.1007/S11837-014-1244-0/TABLES/1