materials design

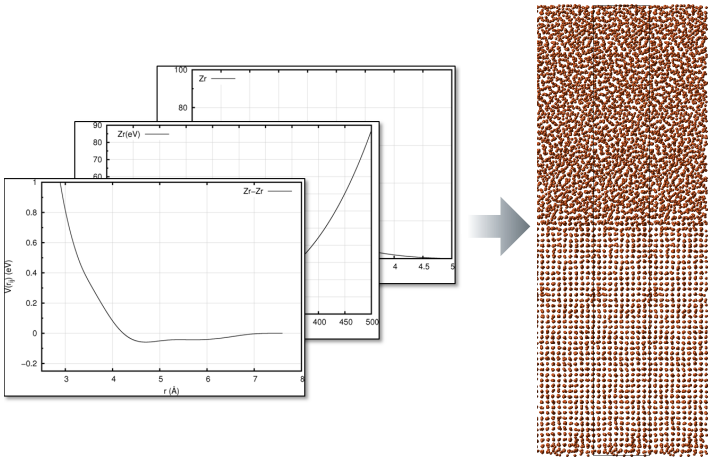
MedeA® LAMMPS-EAM

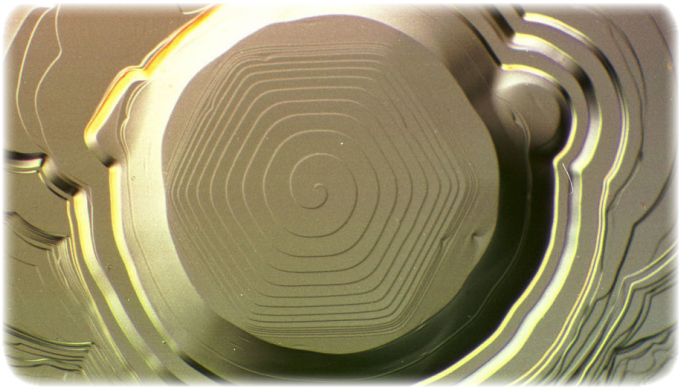
Embedded Atom Method (EAM) forcefield based simulations provide computationally efficient descriptions of structural, mechanical, and thermal properties of metallic systems.

The MedeA® LAMMPS-EAM module provides straightforward access to EAM simulations in the MedeA® environment.

Key Features of MedeA® LAMMPS-EAM:

- *Support for Finnis-Sinclair format EAM forcefield files with simple extensions for template type assignment and referencing*
- *Support for atom type assignment template rules to facilitate construct-then-type model construction for LAMMPS simulations*
- *Support for the Zhou et al 2004[1] EAM parameterization supporting mixed alloys of: Cu, Ag, Au, Ni, Pd, Pt, Al, Pb, Fe, Mo, Ta, W, Mg, Co, Ti, and Zr*





Key Benefits of MedeA® LAMMPS-EAM:

- *Fully utilizes the powerful LAMMPS simulation workflows within the MedeA® environment*
- *Supports a wide range of properties for metallic systems:*
  - *Structures*
  - *Energetics and structural properties of defects*
  - *Mechanical properties*
  - *Dynamical properties such as melting points*
- *Incorporates a wide range of models:*
  - *Load models from MedeA® InformaticA*
  - *Use the MedeA® Amorphous Materials Builder to create models*
  - *Modify models with the powerful, yet intuitive, simulation protocols of MedeA® Flowcharts*

1. X. W. Zhou, R. A. Johnson, H.N.G. Wadley, Phys. Rev. B. 69, 144113 (2004)

Required MedeA® Modules:

- *Core MedeA® Environment*
- *MedeA® JobServer & TaskServer*
- *MedeA® Forcefield*

Supported MedeA® Modules:

- *MedeA® InfoMaticA*
- *MedeA® Mechanical Properties (MT)*
- *MedeA® LAMMPS-Diffusion*

Visit our website www.materialsdesign.com or contact your local Materials Design office for further information.

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