MedeA EAM

Easy Access to Powerful Simulations of Metallic Systems

At-a-Glance

Embedded Atom Method (EAM) forcefield based simulations provide computationally efficient descriptions of structural, mechanical, and thermal properties of metallic systems. The *MedeA*®[1] *EAM* module provides straightforward access to EAM simulations in the *MedeA Environment*.

Key Benefits

- **Productivity** - Fully utilizes the powerful LAMMPS simulation workflows within the *MedeA Environment*
- **Coverage** - Supports a wide range of properties for meteallic systems:
  - Structures
  - Energetics and structural properties of defects
  - Mechanical properties
  - Dynamical properties, such as melting points
- **Flexibility** - Incorporates an extensive set of models:
  - Load models from *MedeA InfoMaticA*
  - Use the *MedeA Amorphous Materials Builder* to create models
  - Modify models with the powerful, yet intuitive simulation protocols of *MedeA Flowcharts*

Perform large scale simulations of metallic systems, spanning significant time scales using MedeA EAM

Key Features

- 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 constructions for LAMMPS simulations
- Support for the Zhou et al 2004[2] EAM parameterization supporting mixed alloys of: Cu, Ag, Au, Ni, Pd, Pt, Al, Pb, Fe, Mo, Ta, W, Mg, Co, Ti, and Zr

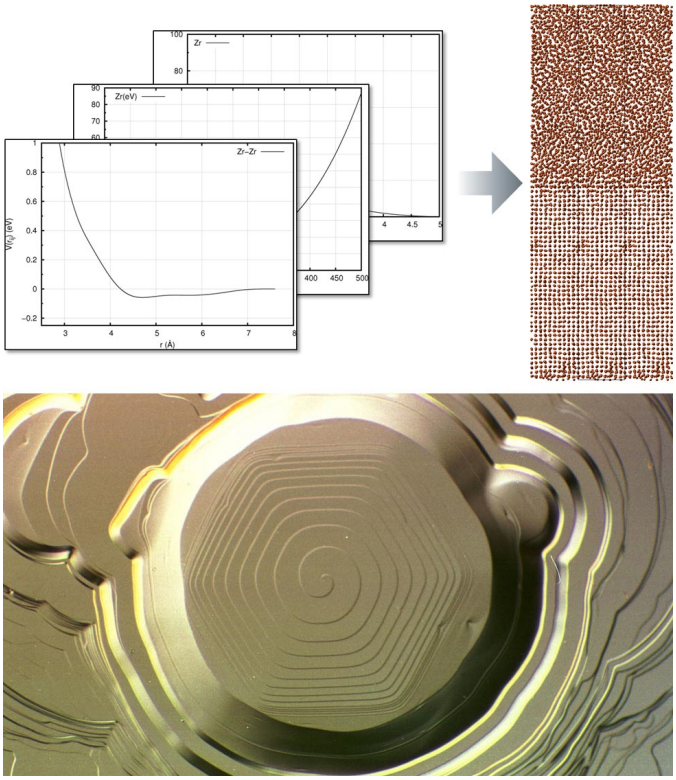

Fig. 1: The upper section shows the simulation of the melting point of a metallic system using a two region model, and described by an EAM forcefield with component functions in the inset graphs. The lower section shows screw dislocations and other defects on a metal surface.

Required Modules

- *MedeA Environment*

Related Modules

- *MedeA LAMMPS*

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.

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

- *MedeA Diffusion*
- *MedeA Surface Tension*

Find Out More

Visit the Materials Design Application Notes page to learn more about *MedeA EAM* from the following Application Note:

- *Embedded Atom Method (EAM) Simulations with MedeA*

Watch the Materials Design online tutorial and learn How to Calculate Elastic Constants with LAMMPS

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