MedeA Interface Builder

Connecting Materials

At-a-Glance

The *MedeA* ®[1] *Interface Builder* creates interfaces and grain boundaries using two different methods. The user can construct a high-symmetry Coincidence-Site Lattice (CSL) grain boundary by customizing template models. In addition, general interface models can be built from two surfaces, allowing for a certain degree of lattice mismatch between the layers. There is no restriction on the surface cells that you start with, they can be as complex or simple as needed.

Key Benefits

- *Easy access to high-symmetry CSL grain boundaries*
- *Automated search for possible coherent interfaces*
- *Straightforward model construction for subsequent calculation of, for instance, interface energies, effect of impurities on strength, interface thermal resistance (Kapitza resistance), and more*

The *MedeA* Interface Builder includes two powerful tools to generate interface and grain boundary models to be used in atomistic simulations.

1) High-symmetry grain boundary builder: CSL grain boundaries can easily be built from template models in a database. The database contain models with the following crystal lattices: fcc, bcc, hcp, sc, rocksalt, zincblende, wurtzite, nickeline, and fluorite. Both twist-, and tilt boundaries are available, with Σ values up to Σ13. The user can select atom types (elements), and specify lattice parameter and the size of the atomistic model.

2) Surface matching: Two arbitrary surfaces are matched together forming an interface (of twist-type), and rotated with respect to each other in search of low-strain structures. The search for interfaces is conveniently carried out in a background job handled by the JobServer. All found interfaces satisfying the search criteria are collected in a list with geometrical data for each interface. The *MedeA* graphical interface allows further intuitive, interactive adjustment of interface structures by specifying parameters such as the spacing between the two surfaces and their relative lateral shift.

The resulting models are fully periodic, and can be used directly with *MedeA VASP*, *MedeA LAMMPS*, or *MedeA MOPAC*. Additionally, the user can further edit the structures in *MedeA* to introduce impurities, vacancies, and interstitial species as needed.

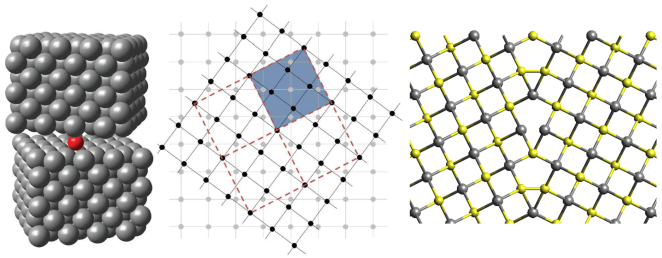

Fig. 1: Σ5(001)/[001] twist grain boundary in nickel with oxygen impurity as described in[2] *and ZnS Σ5(3-10)[001] grain boundary*

The study of the behaviour of polycrystalline materials is often reduced to the study of the behaviour of their interfaces

A.P. Sutton and R.W. Ballufi, 'Interfaces in crystalline materials' (Clarendon, Oxford, 1995)

Key Features

- High-symmetry grain boundary builder and Interface building by surface matching tool

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

[2] M. Christensen, J. Ballard, T. M. Angeliu, J. Vollmer, R. Najafabadi, and E. Wimmer, "Proceedings of the Water Reactor Fuel Performance Meeting" Top Fuel, p. 2165 (2009)

- Customizable CSL grain boundaries up to Σ13
- Surface matching handling of any pair of surfaces
- Control over maximum lattice mismatch
- Adjustment of how the lattice mismatch is distributed between the two surfaces to account for differing stiffnesses
- Adjustment of the spacing (gap) between the two surfaces
- Interactive adjustment of lateral offsets for full access to the γ-surface
- Generation of models ready for use in subsequent VASP, LAMMPS, or MOPAC calculations

Required Modules

- *MedeA Environment*

Recommended Modules

- *MedeA VASP*
- *MedeA LAMMPS*
- *MedeA MOPAC*

Find Out More

Learn more how the *MedeA Interface Builder* can be used to build interfaces in the following video tutorial:

- How to Create Interfaces

12121 Scripps Summit Drive, Suite 160 San Diego CA 92131, USA
P: +1 760 495-4924 - F: +1 760 897-2179 - E: info@materialsdesign.com