

# MedeA *Interface Builder*

Connecting Materials

## At-a-Glance

The *MedeA*<sup>®1</sup> *Interface Builder* creates interfaces 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

- 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 generates models with twist grain boundaries, coherent, and/or semi-coherent interfaces, which may serve as a starting point for atomistic simulations. 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.

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.

<sup>1</sup> MedeA and Materials Design are registered trademarks of Materials Design, Inc.

<sup>2</sup> 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)

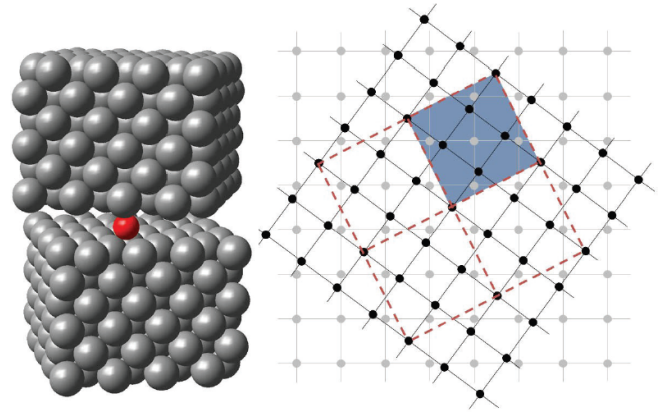


Figure 1:  $\Sigma 5(0001)$  twist grain boundary in nickel with oxygen impurity as described in<sup>2</sup>

*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. Balluffi, 'Interfaces in crystalline materials' (Clarendon, Oxford, 1995)

## Key Features

- 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  $\gamma$ -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](#)