

# 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)

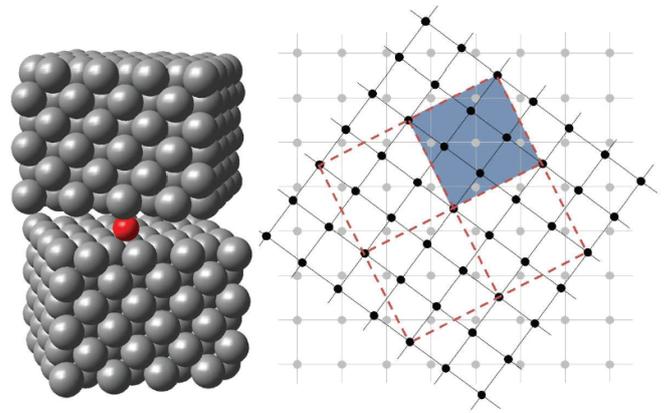


Figure 1:  $\Sigma 5(0001)$  twist grain boundary in nickel with oxygen impurity as described in<sup>2</sup>

*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](#)