

MedeA® Interface Builder

MedeA® Interface Builder creates interfaces from two surfaces, allowing for a certain amount of mismatch between the two layers. There is no restriction on the surface cells that you start with – they can be as complex or simple as needed. The interface models produced are twist grain boundaries, coherent, and/or semi-coherent interfaces; and serve as the starting point for atomistic simulation. The resulting models are fully periodic and can be directly used with MedeA®-VASP, MedeA®-LAMMPS or MedeA®-MOPAC. And, of course, you can further edit the structures in MedeA® to introduce impurities, vacancies and interstitial species as appropriate.

Key Benefits of MedeA® Interface Builder

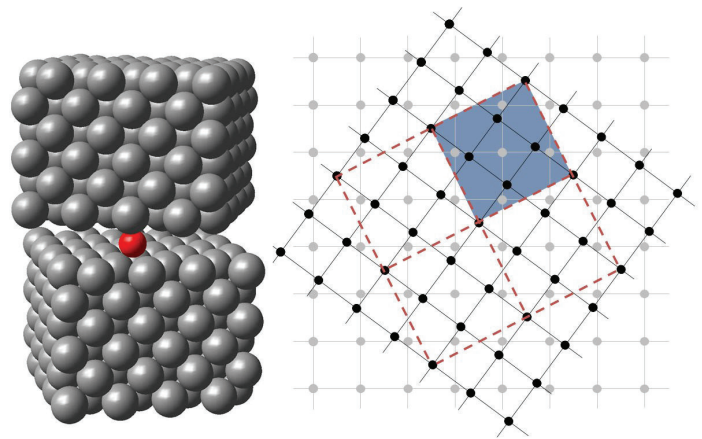
- ▶ Automated search for possible coherent interfaces
- ▶ Straightforward model construction for subsequent calculations of, for instance, interface energies, effect of impurities on strength, and interface thermal resistance (Kapitza resistance)

Capabilities of MedeA® Interface Builder

- ▶ Handles any pair of surfaces
- ▶ Control over maximum mismatch
- ▶ Adjustment of how the mismatch is distributed between layers to account for differing stiffnesses
- ▶ Adjustment of gap between layers
- ▶ Interactive adjustment of lateral offsets for full access to the gamma surface
- ▶ Separation of the two layers into distinct systems, facilitating the calculation of the interface energy
- ▶ Produces models ready for use in subsequent VASP, LAMMPS or MOPAC calculations

Computational Characteristics

- ▶ The search for interfaces is carried out in a background job handled by the JobServer
- ▶ The MedeA® graphical interface allows intuitive, interactive building and adjustments to interfaces discovered by the background job.



$\Sigma 5(001)$ twist grain boundary in nickel with oxygen impurity as described in: M. Christensen, J. Ballard, T. Angeliiu, J. Vollmer, R. Najafabadi, E. Wimmer, Proceedings of Top Fuel, 2165 (2009).

Required MedeA® Modules

- Core MedeA® Environment
- MedeA® JobServer and TaskServer

Recommended MedeA® Modules

- MedeA®-VASP
- MedeA®-LAMMPS
- MedeA®-MOPAC

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