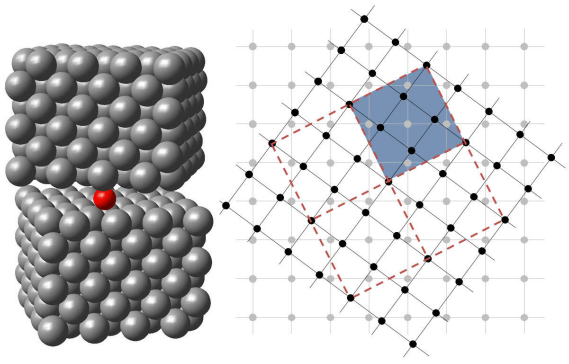
Interface Builder (IB)

This module searches for optimal matches between two interfaces, for example a Si(001) surface and a W(110) surface by exhaustive geometric searches. The IB module constructs 3D periodic models which can be used as input for subsequent VASP or other calculations. Application of the IB module to systems an interface of the same material, for example a Ni(001) surface with itself generates a family of twist grain boundaries.



5(001) twist grain boundary in nickel with oxygen impurity.

Results from Interface Builder

Interface models ready to be used in subsequent VASP calculations

- Ability to prepare models of different lateral displacements (points on gamma surface)

Computational characteristics

- The interface builder uses the geometric features of two surfaces without resorting to energy calculations

Required MedeA modules

- Core MedeA environment

More on our website:

www.materialsdesign.com

- Interface Energy of Metal-Ceramic Interface Co/WC Using ab initio Thermodynamics
- Strength of Ni Grain Boundary and the Effect of Boron

Relevant Publications

- M Christensen, J Ballard, T Angeliu, J Vollmer, R Najafabadi, E Wimmer, *Proceedings of Top Fuel 2009* p. 2165, 2009