METADISE Grain Boundary Guide

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Short step by step guide for using METADISE to generate grain boundary structures.

1. Once you have your desired surface, copy the "staco" file to a new folder taking care to ensure that there is only a single surface termination printed within this staco file. The scripts described in this guide are setup for bash so this guide will only work for bash systems.
2. Rename the staco file to input.txt and run the script st2gb. To generate a tilt boundary, when prompted input 0 for reflect, 2 for minimise, 0.2, 0 and 0.
3. Run the scan_gb.sh script. This will create a file called d1/. Navigate to the d1 folder and run the script again. You will now have potentially thousands of sub folders, each containing a different input file, corresponding to a different orientation of the two surfaces.
4. Run the ScanSetup script. This script is requires the potent.txt file to be in previous directory.
5. To run the GB scan run the RunScan script.
6. The script ScanProgress can be run to check on the progress of the scan
7. If the scan fails for some reason e.g. a power cut, you can use the meta_fix script to restart the scan
8. Once the scan finishes run the collect_grid_emin.sh script. This will collect the energies as a function of surface displacements. Then run the eng2xml script to convert this data to an exml file.
9. the file emin.txt contains info on the displacement with the lowest energy.
10. the script GB-Surface.py can be used to generate a contour plot showing the surface energies as a function of surface displacements. This requires some fiddling, the xml file will need to be opened in excel and saved as a csv file.