

For a full Analysis as I performed, one needs to follow this flow:

Chose NL = 50

step	Folder name	Main script/code	Input file	Output file	description	Remarks
1	gidis_codes	hcpnnn.f/l argehcpnn n.f	-----	hcpnnn.out/lar gehcpnnn.out	Calculate the surface tension of an HCP crystal in next near neighbors approximation	
2	wulff const codes	constructin g_wulff_sh ape.m	hcpnnn.out/lar gehcpnnn.out	Wulff shape NL= 50.txt	Calculate the Wulff shape when given a surface tension surface	
3	create_hcp_model	create_hcp _crystal_in _wulff_shape.m	Wulff shape NL= 50.txt	Wulff HCP crystal NL = 50.txt	Creating a HCP crystal in Wulff shape	
4	cutting_rot_and_connecting_crystals_GUI	cutting_rot _and_cone cting_cryst als.m	Wulff shape NL= 50.txt	crystal1_x.txt crystal2_x.txt crystal1_x.xyz crystal2_x.xyz both crystals_x.xyz  where x is a ceriacle number of files	Allow to cut, rotate, move and connect 2 crystals	For using the files later on to calculate the twisted and tilted grain boundary, one need to follow the instructions given in the twisted and tilted grain boundary read me files.
5	GUI_TWISTED	GUI_TWIST ED.m	crystal1_x.txt crystal2_x.txt	-----	Calculate surface energy for the twisted grain boundary in HCP crystal for infinite and finite boundary conditions. Suitable to specific files.	For the calculate the twisted, one needs to follow the instructions given in the twisted in the 4 step of cutting the crystal
5	tilted_energy	GUI_TILTE D.m	crystal1_x.txt crystal2_x.txt	-----	Calculate surface energy for the tilted grain boundary in HCP crystal for infinite conditions. Suitable to specific files.	For the calculate the tilted, one needs to follow the instructing given in the twisted in the 4 step of cutting the crystal

- For more information please read the readme files attached to each code and the project report.