Simulation and visualization of crystal shapes and interfaces - Supplementary Material

Joan Adler, Lilach Saltoun[1] and Emil Polturak

Physics Department, Technion-Israel Institute of Technology, Haifa, Israel.

E-mail: `phr7ja@tx.technion.ac.il`

Abstract. Nature often arranges atoms in the shape of perfect crystals, but sometimes she creates defects and multiple domains. The optimal crystal shape at zero kelvin can be found via the Wulff construction, which can be only be carried out analytically for those trivial cases where next nearest neighbour interactions can be neglected. For our system of interest - videlicit the HCP non-Bravais case, numerical simulation is needed. This system is of relevance because we are modeling Helium crystals. We have modeled two adjacent crystallites with different orientations in contact creating twist or tilt grain boundaries, and calculated the surface energy of the interface. Experience gained from several aspects of this project have a wider applications, including the condensed matter simulation application to sample construction for multi-domain crystals, and a visualization one for representation in the presence of grain boundaries. The optimization of sample shapes into their groundstates is also related to wavefront optimization in multimirror telescopes. This is additional material for our paper; including figures and a table.

1. Experiments
In Fig. 1 the evolution of a Helium crystal on heating is shown. These images are from the laboratory of S.G. Lipson at the Technion and were collated by JA and published in [5] Each image is in a cryostat, the crystal is at lower left and the "eyes" are an optical illusion. The edges become round and facets become rough as the temperature increases. The change from flat facets with sharp edges to rough and rounded is known as the roughening transition. All crystals exhibit such behaviour, but due to equilibration times in metals it is harder to observe there.

2. Simulation and visualization of roughening transitions and their visualization
Crystal interfaces and their roughening can be studied numerically with SOS (Solid-On-Solid) models, or as interfaces in Ising models, either by direct simulation or for simple cases by series expansions. The SOS models have also been applied to telescope phasing, discussed here only in the visualization context. For the simulations, visualization is very important. An early example was by Adler and Arian, using TOPDRAW, see the left hand frame of Fig. 2. Adler, Lipson, Baum, Gemintern and Hashibon [5] made Simulations along the facets requires attention to

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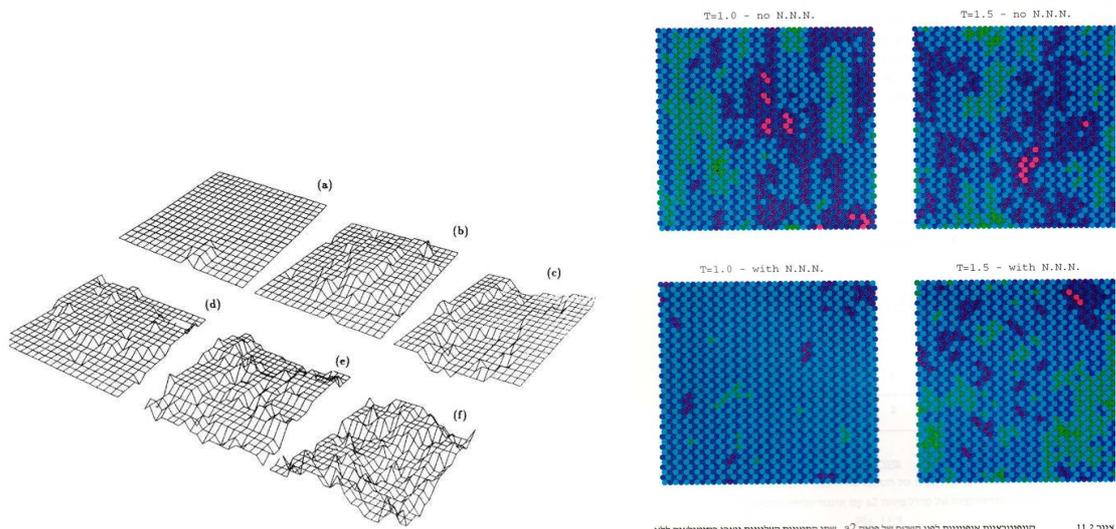
[1] Present address: Hebrew University, Jerusalem, Israel.
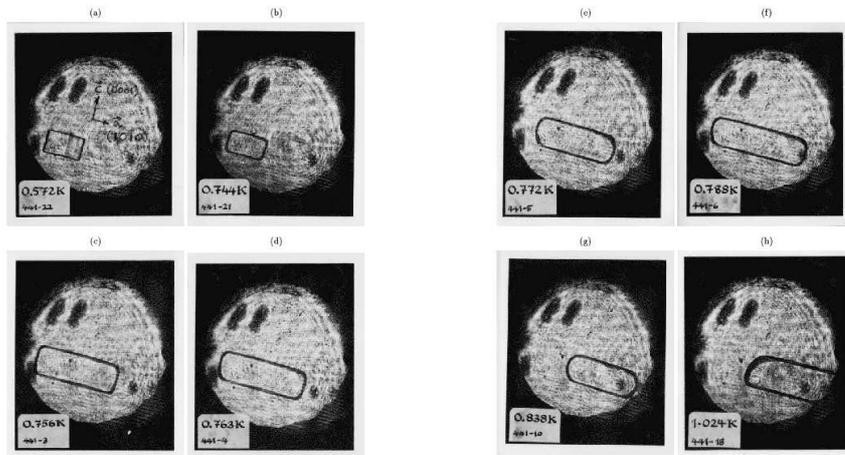
Figure 1. Roughening of a helium crystal in a cryostat.

boundary conditions and equilibration, and various types of visualizations were used to check these. On the right of Fig. 2 we show images where color i sused to indicate height from the MSc. thesis of G. Baum, 1994.

Figure 2. At left early roughening simulation by Adler and Arian with TOPDRAW and at right color images of HCP with and without next-nearest-neighbours from thesis of G. Baum.
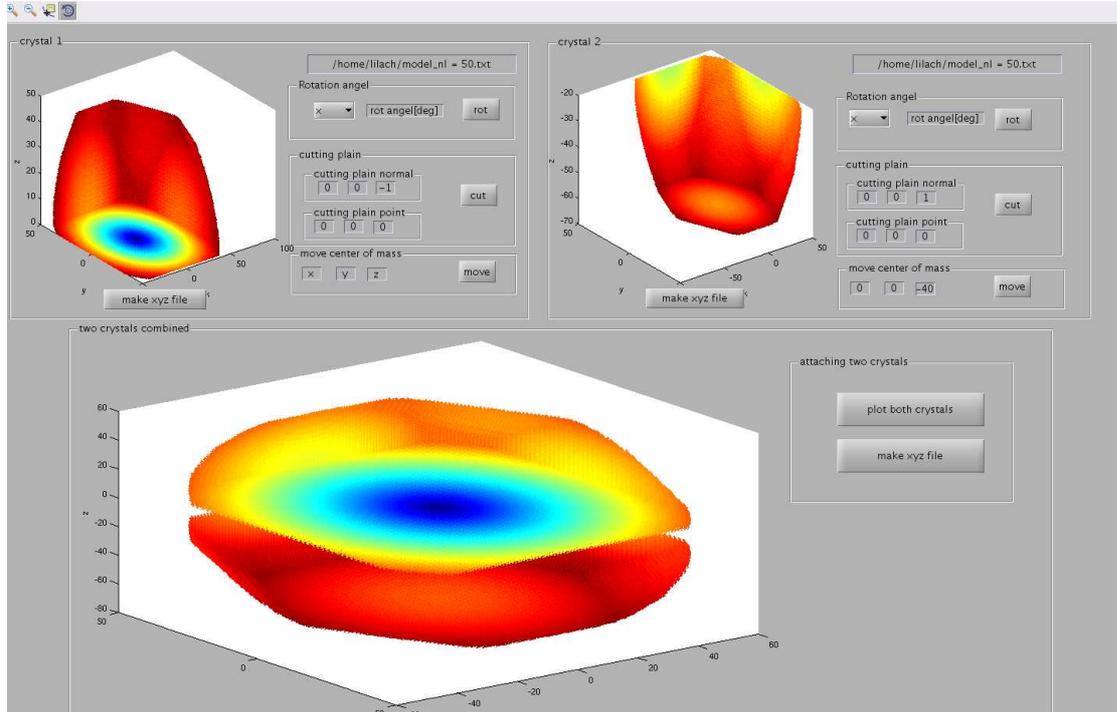
Figure 3. Interface of the cutting_rot_and_conecting_crystals.m routine.

Table 1. Codes and files.

	Code	Input	Output	Description
(i)	-	-	L value (e.g. L=50)	sample size
(ii)	hcpnn.f	L value	hcpnnn.out	surface tension
(iii)	constracting_wulff_	hcpnnn.out	Wulff shapeNL=50.txt	Wulff shape
	shape.m			from surface tension
(iv)	create_hcp_crystal_	Wulff shape	Wulff HCP crystal	create HCP crystal
	in_wulff_shape.m	NL=50.txt	NL=50.txt	in Wulff shape
(v)	cutting_rot_and_	see Fig. 3	crystal1_x.txt	x is a serial index
	conecting_crystals.m		crystal2_x.txt	also files with 2 crystals
(vi)	GUI_TWISTED.m	see Fig. 4	surface energy	twist angles
(vii)	GUI_TILTED.m		surface energy	tilt angles
(viii)	AViz	crystal*.xyz	show interface bonds	images

3. Codes and Instructions

The codes and their instructions can be downloaded from the project website [3]. In Table 1 a detailed list of names and inputs is given for the different stages. The file lilach.tar, linked from [3] has subdirectories with sample files for each stage, that can be placed in the matlab windows when paths of files are requested. More istructions are given in the readme files of each directory and in the pdf report linked from [3] many details are provided.

In Fig. 3 an enlarged image of the GUI of the main code is shown. The values in the windows there will reproduce the displayed images and can, of course, be altered as desired. There are also buttons to prepare .xyz files for AViz when desired. In Figs. 4 and 5 repectively, the interfaces of the routine that calculates the energy of the twisted interface is shown. Default
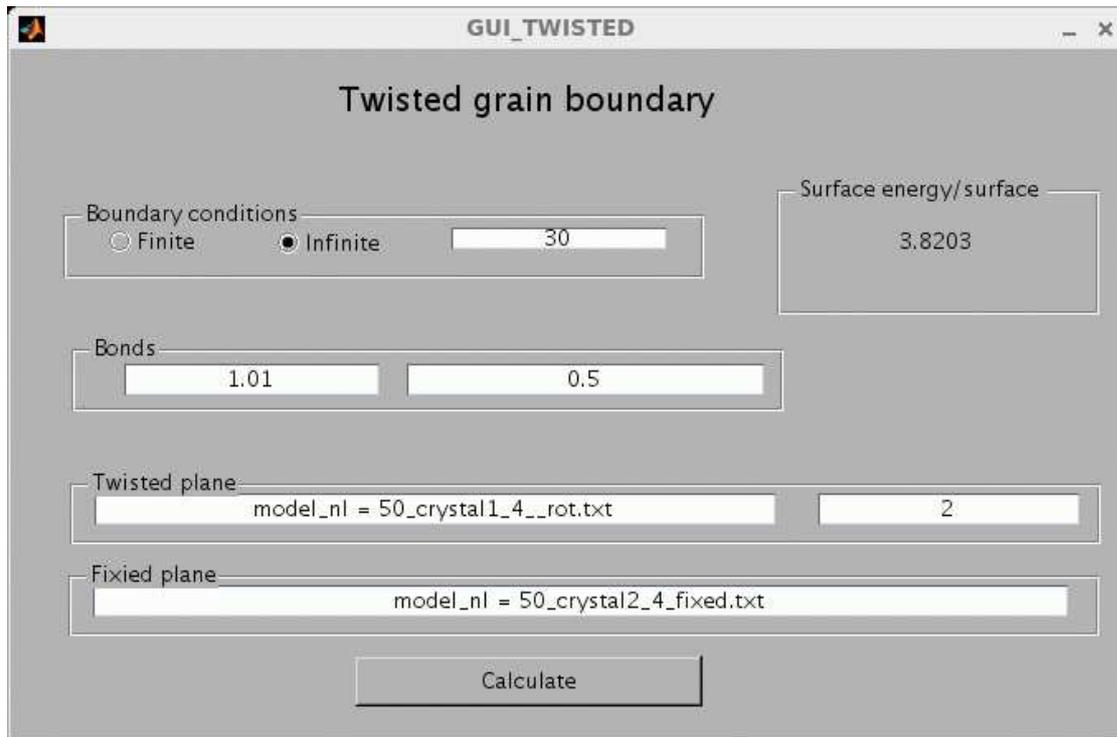
Figure 4. Interface of the GUI_TWISTED.m routine.
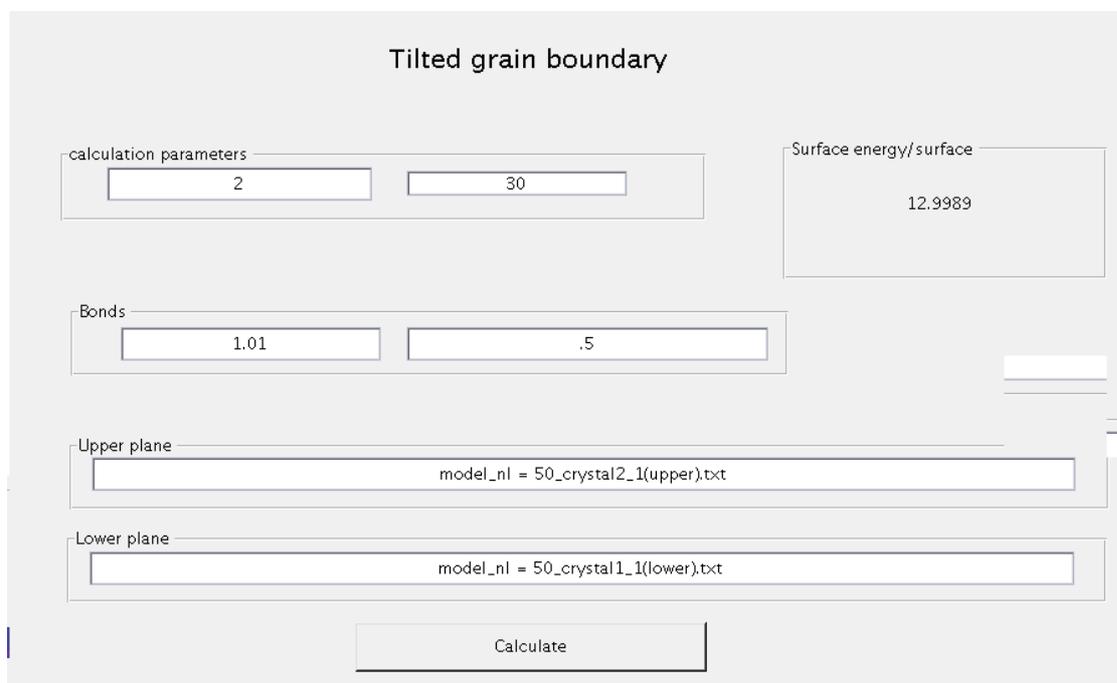

Figure 5. Interface of the GUI_TILTED.m routine.

values for the various variables can again be read off the image, and details found in our paper and in the report file in [3].

We note that the GUIs reproduced here were run on a Red Hat server, with a 2014 version of MATLAB. It may be necessary to adjust the GUI parameters for windows or newer versions of MATLAB.

References

[1] http://www.simphony-project.eu

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[5] Hashibon A, Adler J, Baum G, and Lipson S. G. 1998 Roughening transitions and surface tension in an hcp lattice with higher neighbor interactions *Phys. Rev. B* **58** 4120

[6] Herring C 1951 Some Theorems on the Free Energies of Crystal Surfaces *Phys. Rev.* **82** 87

[7] Bavli P, Polturak E. and Adler J 2001 Molecular dynamics study of melting in the hcp metal Mg *Phys. Rev. B* **84** 235442

[8] Peled D, Silverman A and Adler J 2013 3D visualization of atomistic simulations on every desktop *IOP Conference Series* **454** 012076