

Katpiza conductance of 5 most significant GBs in Si

S-No	θ	GB	Type	Plane	Axis	$E_{gb}(mJ/m^2)$	$\Delta T(K)$	$J(GW/m^2)$	$\sigma_K(GW/m^2 K)$
1	60.00	$\Sigma 3$	Twist	(111)	$\langle 1\ 1\ 1 \rangle$	0.003	-	15.36	-
2	36.87	$\Sigma 3$	Symmetric tilt	$(0\bar{2}1)$	$\langle 1\ 0\ 0 \rangle$	1.329	18.22	15.36	0.8430
3	38.94	$\Sigma 9$	Symmetric tilt	$(\bar{2}21)$	$\langle 1\ 1\ 0 \rangle$	1.097	17.47	15.36	0.8792
4	50.48	$\Sigma 11$	Asymmetric tilt	$(\bar{2}23)$	$\langle 1\ 1\ 0 \rangle$	16.507	12.83	15.36	1.1972
5	46.40	$\Sigma 29$	Mixed	(112)	$\langle 1\ 0\ 0 \rangle$	26.066	14.13	15.36	1.0870

Notes

- simulation of exp-1 is running
- Need to understand *how to find the average KC from the GB Charecter distribution*

Observations

- GBE of *Asymmetric* and *Mixed* GBs are deviating far from the expected limits.
- $L_z > 2000$ Angstroms for all the GB-models, and atoms in each bin is sufficiently larger for calculating the temperature of each bins.

Tasks

- planning for few set of experiments to understand GBE(1/1.5 day)