

Electronic Supplementary Information (ESI) on the manuscript “Atomistic Structures of <0001> Tilt Grain Boundaries in a Textured Mg Thin Film”

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Table S1 List of supercell parameters and GB energy from atomistic simulations.

Σ	θ (°)	L_x (nm)	L_y (nm)	L_z (nm)	No. atoms	E_{GB} (mJ/m ²)
31	17.90	42.7	6.2	1.6	17,856	243
31	42.10	37.0	1.8	1.6	4,464	274
37	9.43	40.4	3.9	1.6	10,656	176
37	50.57	39.0	6.8	1.6	17,760	199
61	7.34	51.9	5.0	1.6	17,568	153
61	52.66	40.0	4.3	1.6	11,712	173
73	11.64	43.7	9.5	1.6	28,032	197
73	48.36	37.8	5.5	1.6	14,016	222

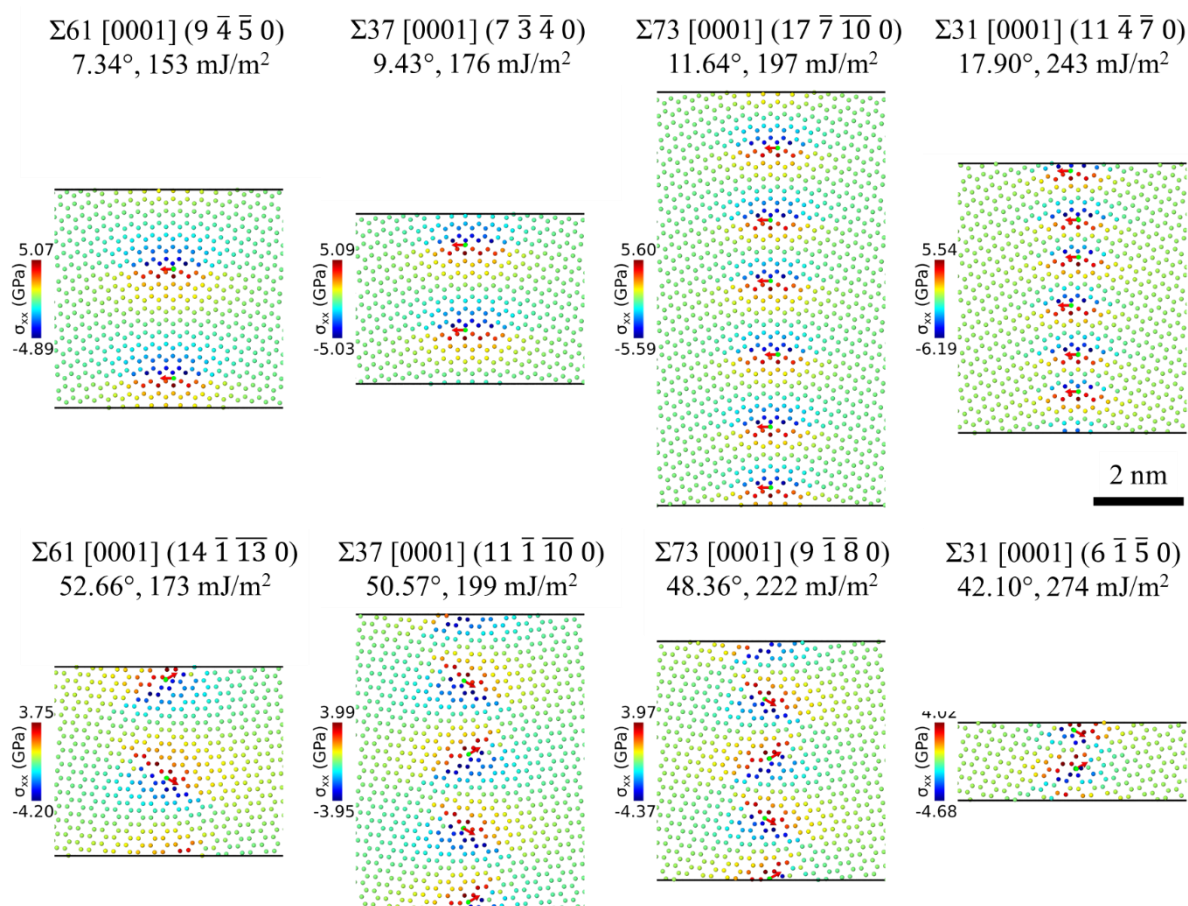


Fig. S1 Atomic configurations of relaxed simulation cells for type-1 (upper row) and type-2 (lower row) $\Sigma 61$, $\Sigma 37$, $\Sigma 73$, $\Sigma 31$ [0001] tilt GBs. Color codes denote the stress field along x . Dislocation lines parallel to the viewing direction are colored in green and overlaid Burgers vectors $\mathbf{b} = \frac{1}{3}\langle 2\bar{1}10 \rangle$ are indicated using red arrows.