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Supplementary Information for

Role of tilt grain boundaries on the structural integrity of WSe_2 monolayers

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1. Stress-strain response of pristine WSe_2:

Stress-strain curves for pristine WSe_2 at 300K temperature are plotted. The strain rate used for the simulation was 10^9/s.

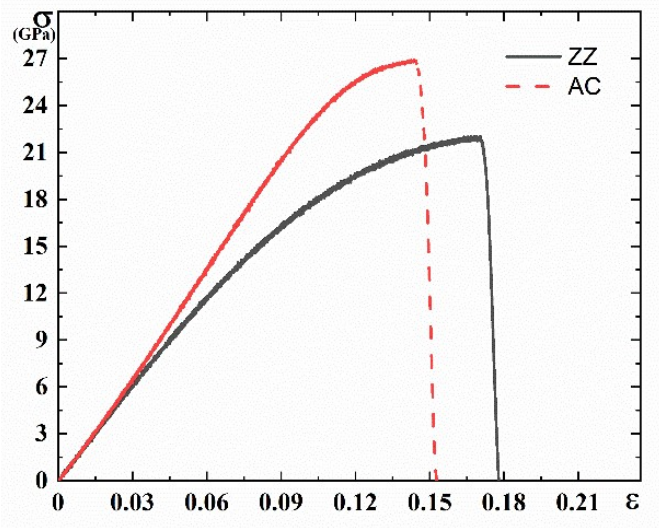

Figure S1. Variation of stress with strain for pristine WSe_2 in the Zigzag and Armchair loading direction at 300K temperature. $10^9 s^{-1}$ strain rate was used for the tensile test.

2. Structure Dimension:

Table S1. Molecular structure information for AC tilt Se5|7 and W5|7 GBs.

Misorientation Angle	No. of Atoms			Dimension (Å)	
Degree	Total	W	Se	x	y
9.4°	24612	8204	16408	280.97	275.49
13.2°	19176	6392	12784	244.60	246.74

21.8°	24000	8000	16000	279.48	270.55

Table S2. Molecular structure information for ZZ tilt W5|7+ Se5|7 GBs.

Misorientation Angle	No. of Atoms			Dimension (Å)	
Degree	Total	W	Se	x	y
39.4°	24192	8064	16128	279.80	272.29
44.6°	28644	9548	19096	297.35	303.03
48.4°	25980	8660	17320	289.65	281.95

3. Stress-strain response of tilt GBs:

Stress-strain curves for all the structures at different temperatures are presented in Figs. S3-S5.

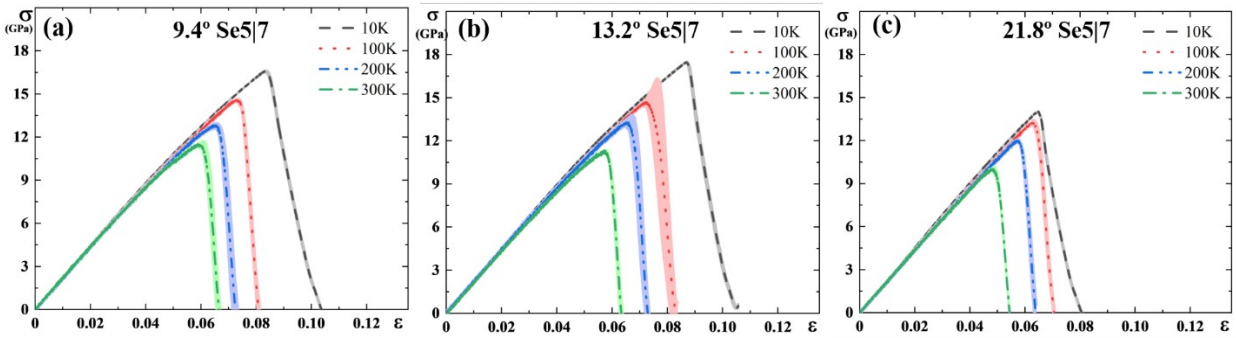

Figure S2. Variation of stress with strain at different temperatures. Stress-strain curves for (a) 9.4° Se5|7, (b) 13.2° Se5|7, and (c) 21.8° Se5|7 structures at 10K,100K,200K and 300K. The strain rate was 10^9 s^{-1}.

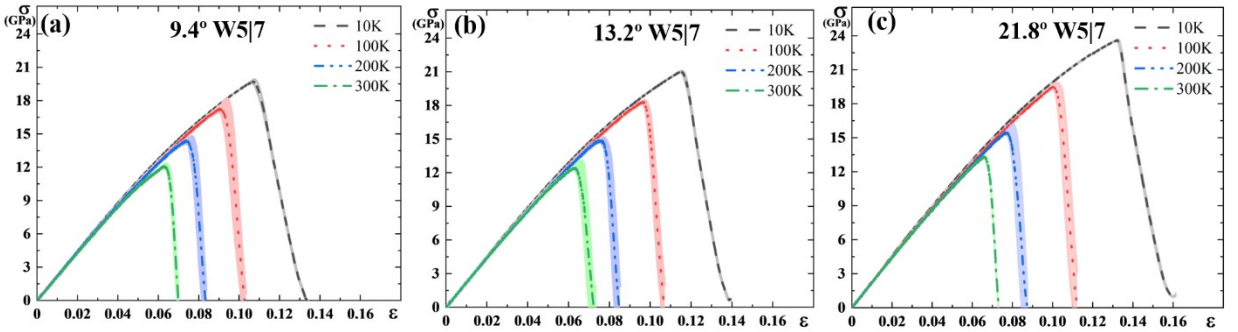

Figure S3. Variation of stress with strain at different temperatures. Stress-strain curves for (a) 9.4° W5|7, (b)13.2° W5|7, and (c) 21.8° W5|7 structures at 10K,100K,200K, and 300K. The strain rate was 10^9 s^{-1}.

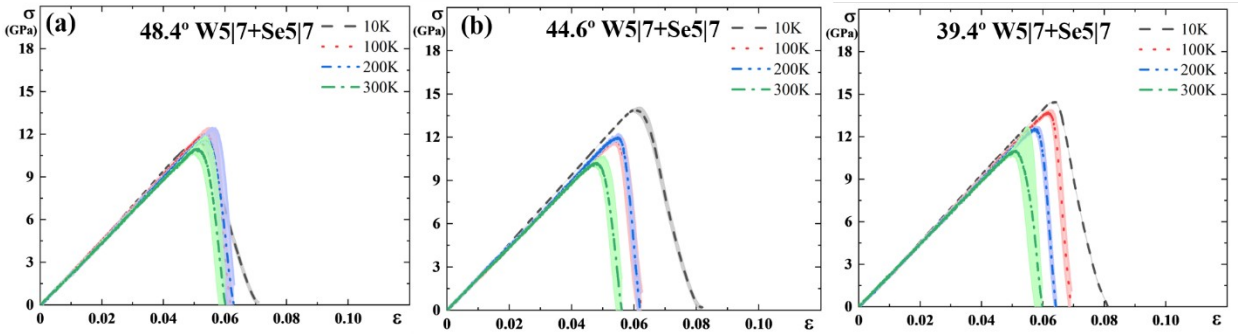

Figure S4. Variation of stress with strain at different temperatures. Stress-strain curves for (a) 48.4° W5|7+Se5|7, (b) 44.6°

W5|7+Se5|7, and (c) 39.4° W5|7+Se5|7 structures at 10K,100K,200K and 300K. The strain rate was 10^9 s^{-1}.

4. Bond Rotation of Heptagon:

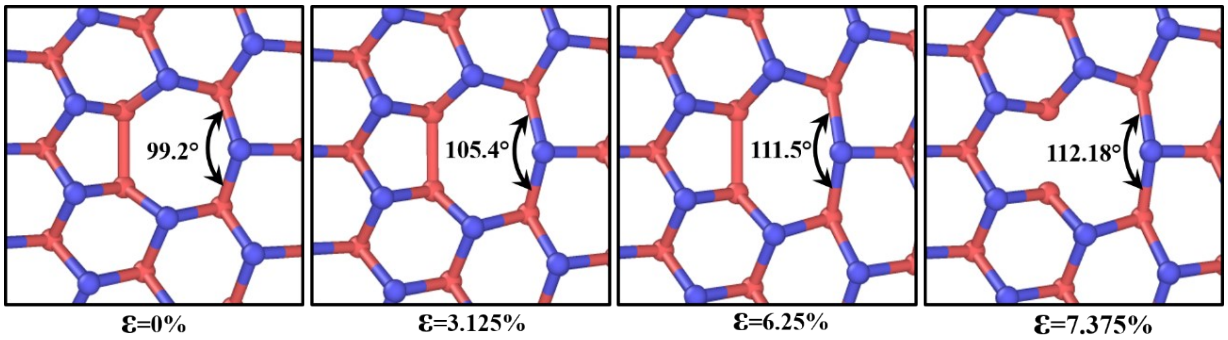

Figure S5. Rotation of bond to accommodate strain for 13.2° AC tilt W5|7 GB. Red circles represent W atoms, and Blue circles represent Se atoms.

5. Fracture:

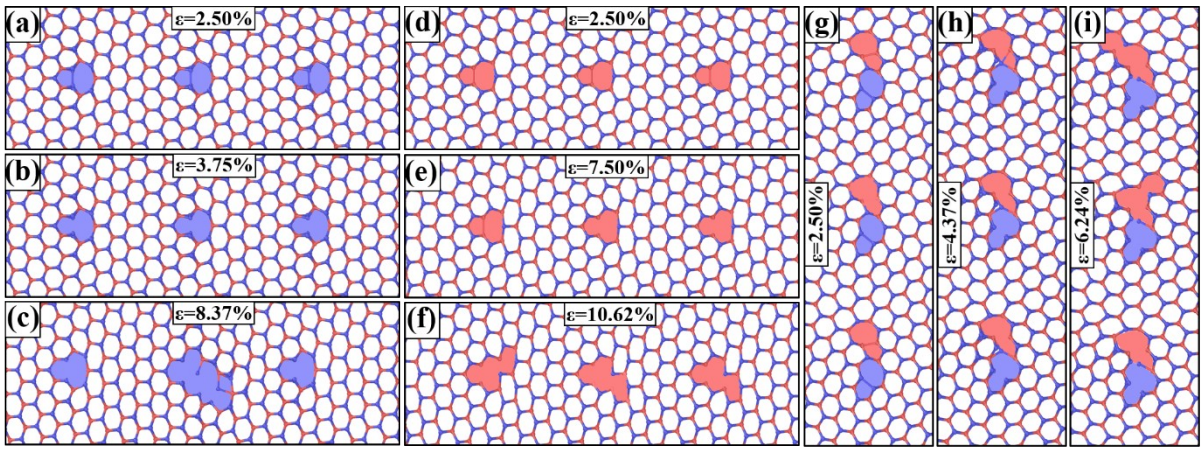

Figure S6. Kinetics of fracture in different WSe_2 GBs. The bond that cannot accommodate strains via rotation breaks first, followed by propagation of the cracks within the ZZ direction with max shear.

6. Transformation of ZZ tilt GB during relaxation:

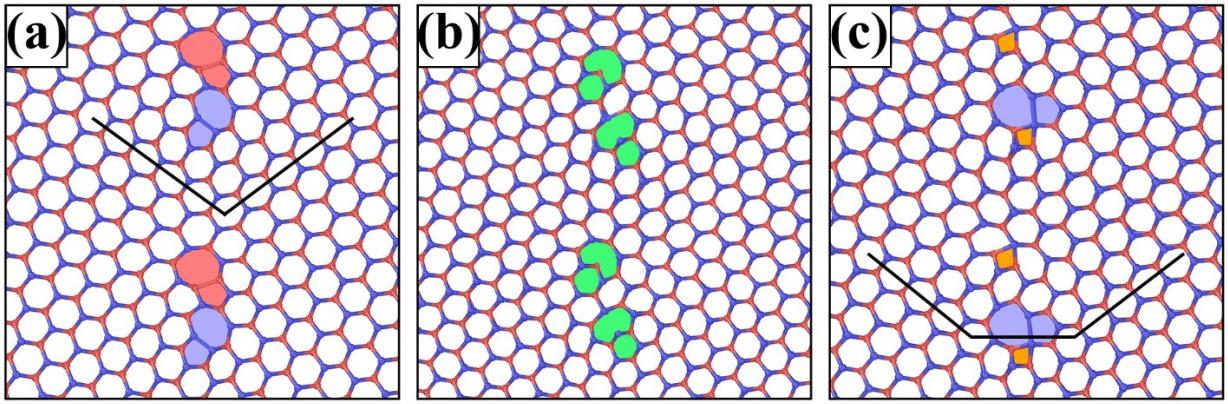

Figure S7. Transformation of GB during relaxation at temperatures above 100K. (a) The initial structure of GB with 44.6° misorientation angle after energy minimization using conjugate gradient method; (b) Intermediate structure during relation at T≥100K where the 5|7 dislocations dissociate to 6|8 dislocation pair; and (c) Final GB structure at T≥100K, after relaxation where horizontal 5|7 dislocations formed that relax the internal stresses. W5|7 and Se5|7 defects are colored red and blue, respectively, 8|6 defects are colored green, and tetragons are colored orange. The black line indicates the high GB transformed into two low angles upon relaxation.