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Fracture Patterns and Energy Release Rate of Phosphorene

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Figure

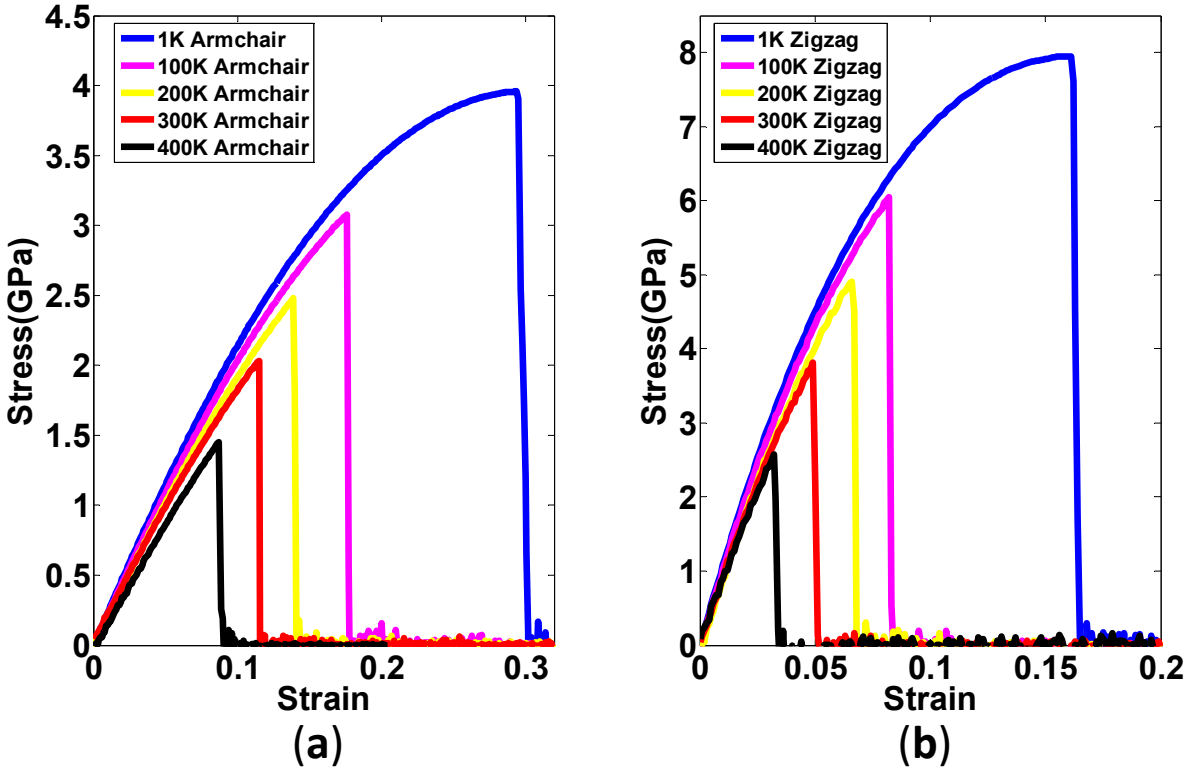

Figure S1. Stress-Strain curves under uniaxial tension at different environmental temperatures (a) Armchair direction (b) Zigzag direction

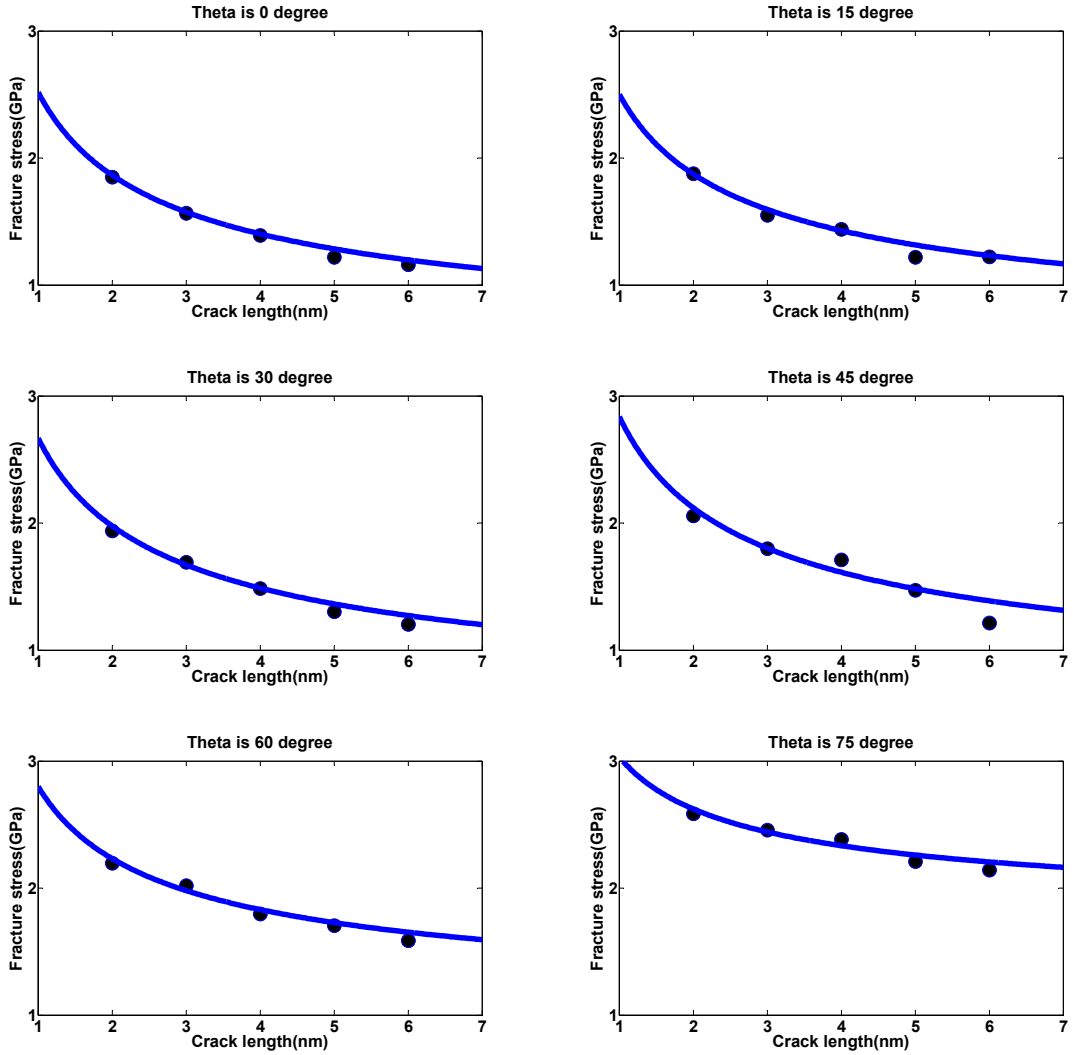

Figure S2. Fracture stress versus crack length for different crack orientations under armchair unidirectional tension (dots represent original data while curves represent fitted results according to Equation 5)

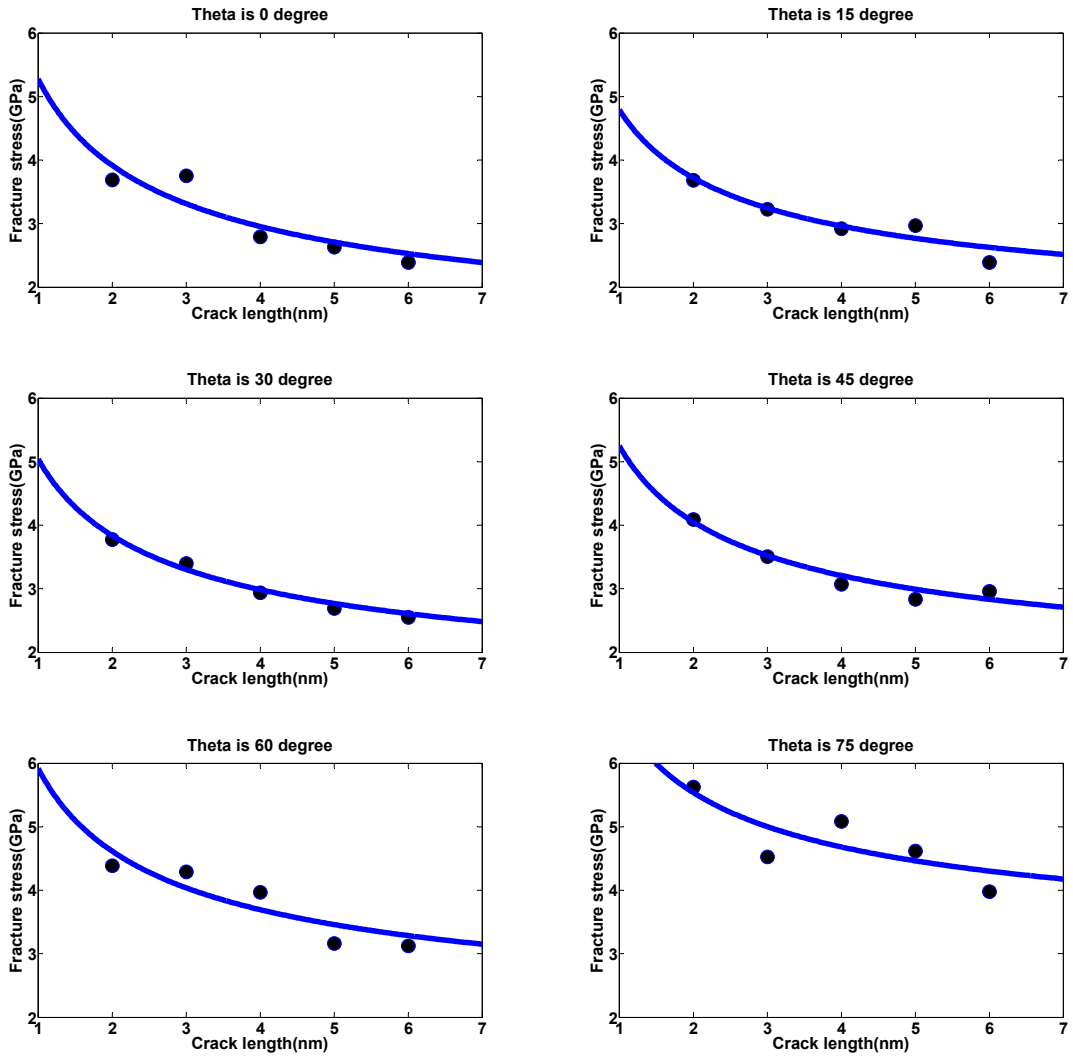

Figure S3. Fracture stress versus crack length for different crack orientations under zigzag unidirectional tension (dots represent original data while curves represent fitted results according to Equation 5.)

Table

Table S1. Mechanical properties at different temperatures for the pristine phosphorene layer

Temperature(K)	1	100	200	300	400
Young's Modulus(Armchair)(GPa)	24.3	22.4	20.6	19.1	18.6
Young's Modulus(Zigzag) (GPa)	103.8	100.8	93.1	88.8	81.5
Fracture Stress(Armchair)(GPa)	3.96	3.08	2.48	2.03	1.45
Fracture Stress(Zigzag)(GPa)	7.95	6.04	4.91	3.82	2.58

Table S2. Geometrical factors α for different crack orientation Θ under both armchair and zigzag unidirectional tension.

Degree	0	15	30	45	60	75
Armchair direction	0.2282	0.2239	0.2363	0.2214	0.1753	0.1337
Zigzag direction	0.2354	0.2179	0.2221	0.2119	0.1933	0.1549