Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Grain-size Dependence of Mechanical Properties in Polycrystalline Boron-Nitride: A Computational Study

Matthew Becton and Xianqiao Wang*

College of Engineering and NanoSEC, University of Georgia, Athens, GA 30620 United States

Tersoff potential

The Tersoff potential used in this paper takes the form

$$E = \frac{1}{2}\sum_{i}\sum_{j\neq i} f_C(r_{ij})[f_R(r_{ij}) + b_{ij} f_A(r_{ij})]$$

where f_R is a repulsive two-body term while f_A is an attractive three-body term managed by the b_{ij} bond function. The details of each component are

$$f_C(r) = \begin{cases} 1 : r < R - D \\ \frac{1}{2} - \frac{1}{2}\sin\left(\frac{\pi(r-R)}{2D}\right) : R - D < r < R + D \\ 0 : r > R + D \end{cases} \quad \text{(S1)}$$

$$f_R(r) = A^{-\lambda_1 r} \quad \text{(S2)}$$

$$f_A(r) = -B^{-\lambda_2 r} \quad \text{(S3)}$$

$$b_{ij} = (1 + \beta^n \zeta_{ij}^{\,n})^{-\frac{1}{2n}} \quad \text{(S4)}$$

$$\zeta_{ij} = \sum_{k\neq i,j} f_C(r_{ik}) g(\theta_{ijk})^{\lambda_3^m (r_{ij} - r_{ik})^m} \quad \text{(S5)}$$

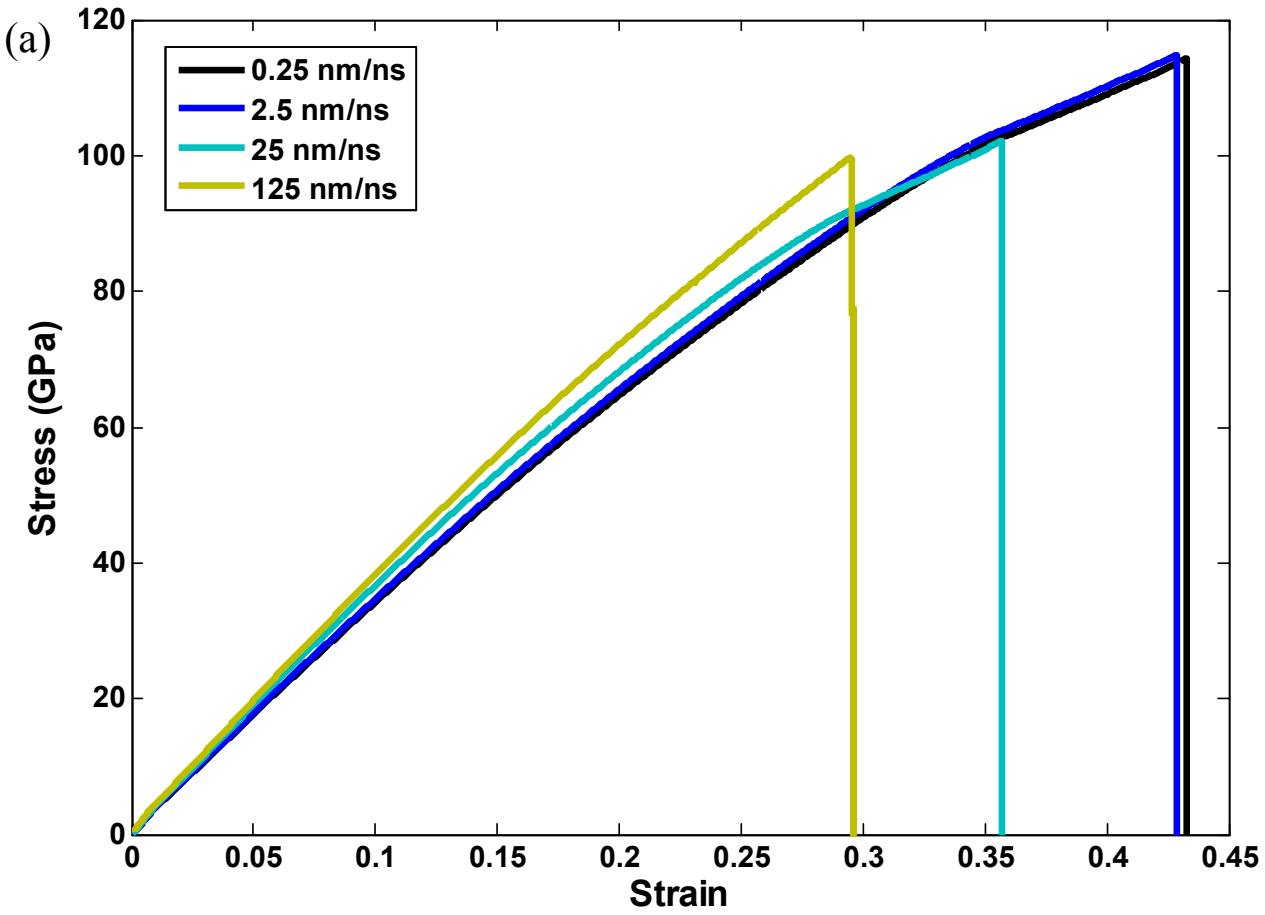
$$g(\theta) = \gamma_{ijk}\left(1 + \frac{c^2}{d^2} - \frac{c^2}{\left[d^2 + (\cos\theta - \cos\theta_0)^2\right]}\right) \quad \text{(S6)}$$

Table S1: The Tersoff potential parameters used in the current work (from Matsunaga, Fisher; 2000).

Elements	B	N
A (eV)	2.7702×10^{2}	1.1000×10^{4}
B (eV)	1.8349×10^{2}	2.1945×10^{2}
λ (Å^{-1})	1.9922	5.7708
μ (Å^{-1})	1.5856	2.5115
β	1.6000×10^{-6}	1.0562×10^{-1}
n	3.9929	12.4498
c	5.2629×10^{-1}	7.9934×10^{4}
d	1.5870×10^{-3}	1.3432×10^{2}
h	0.5000	−0.9973
R (Å)	1.8	2.0
S (Å)	2.1	2.3

Effects of pulling speed and grain orientation

(a)


0.25 nm/ns
2.5 nm/ns
25 nm/ns
125 nm/ns
Stress (GPa)
Strain
0
20
40
60
80
100
120
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.45

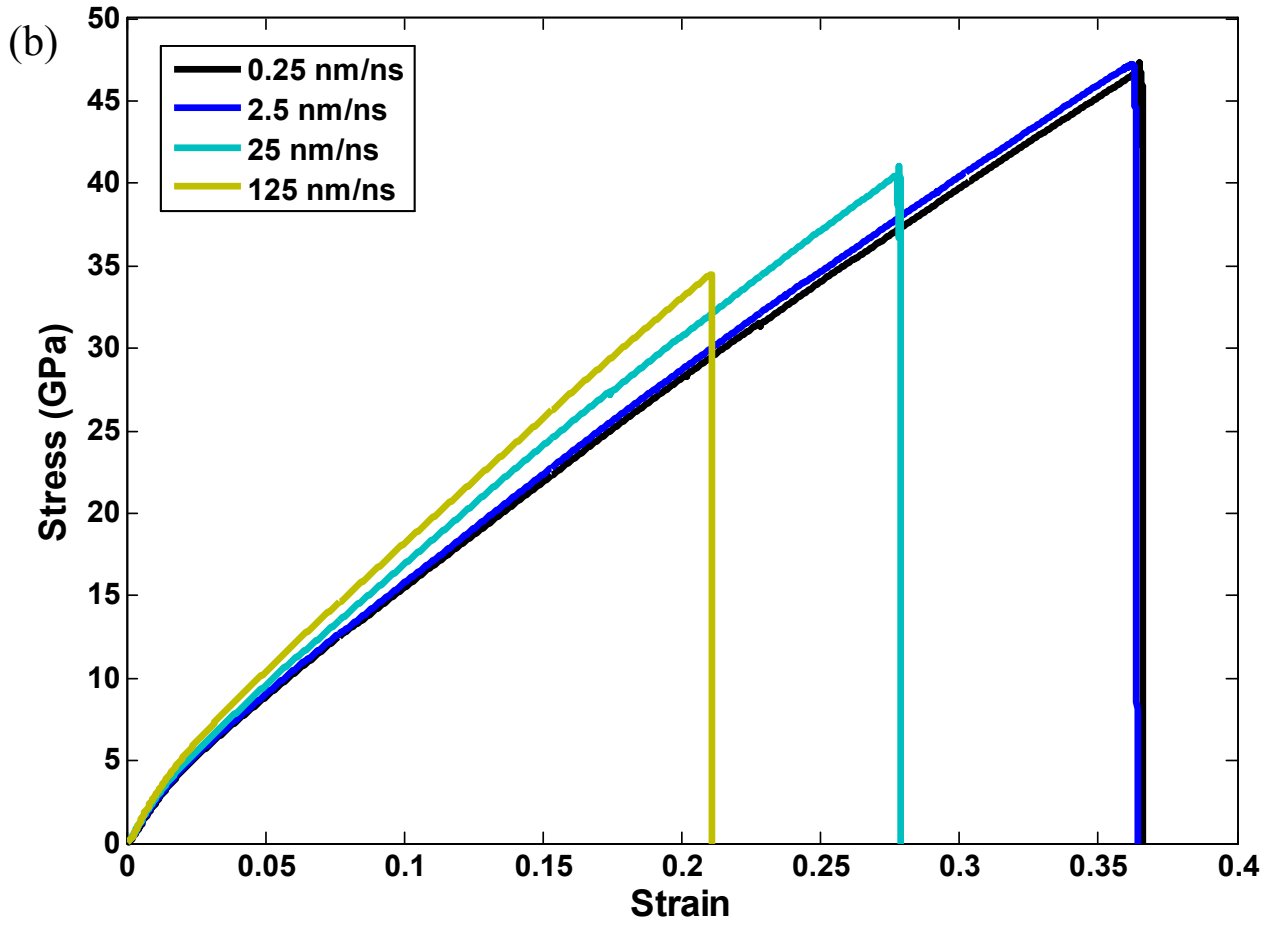
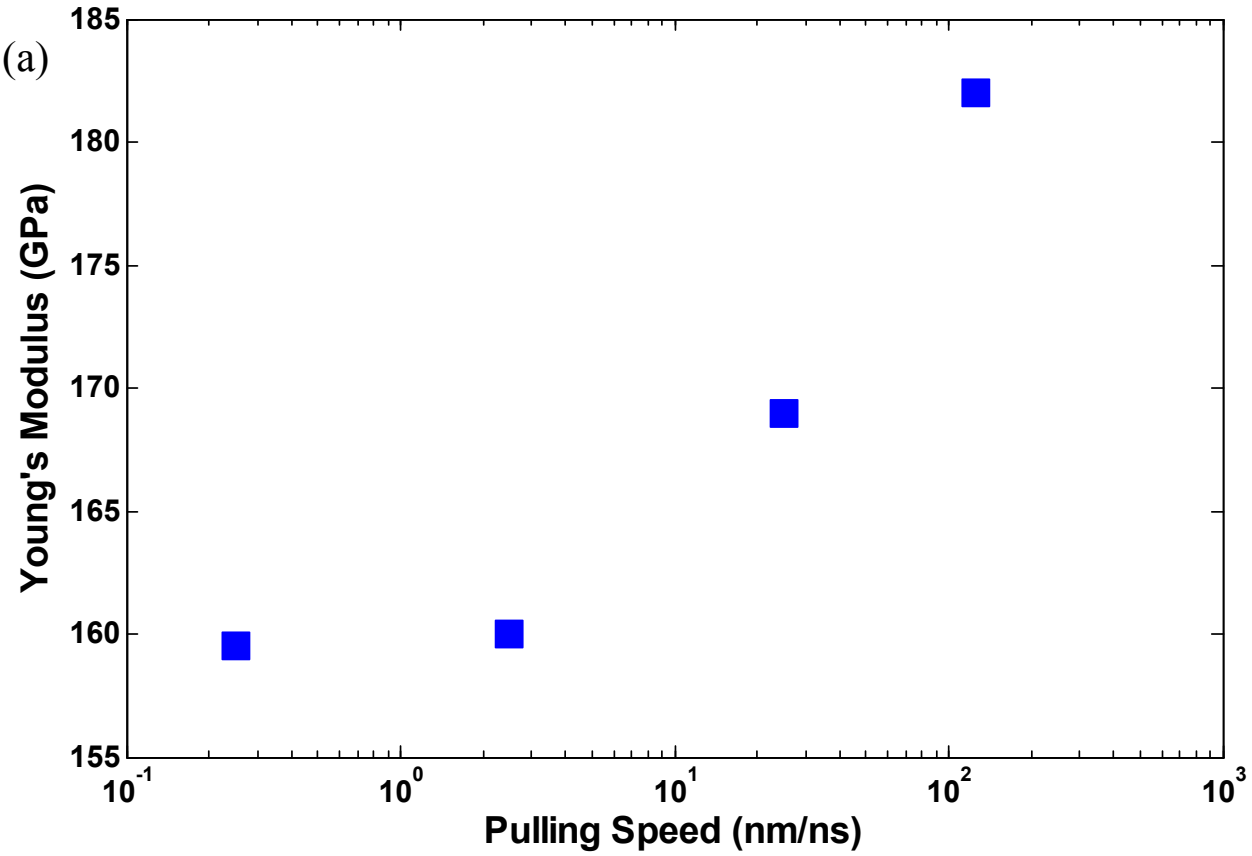
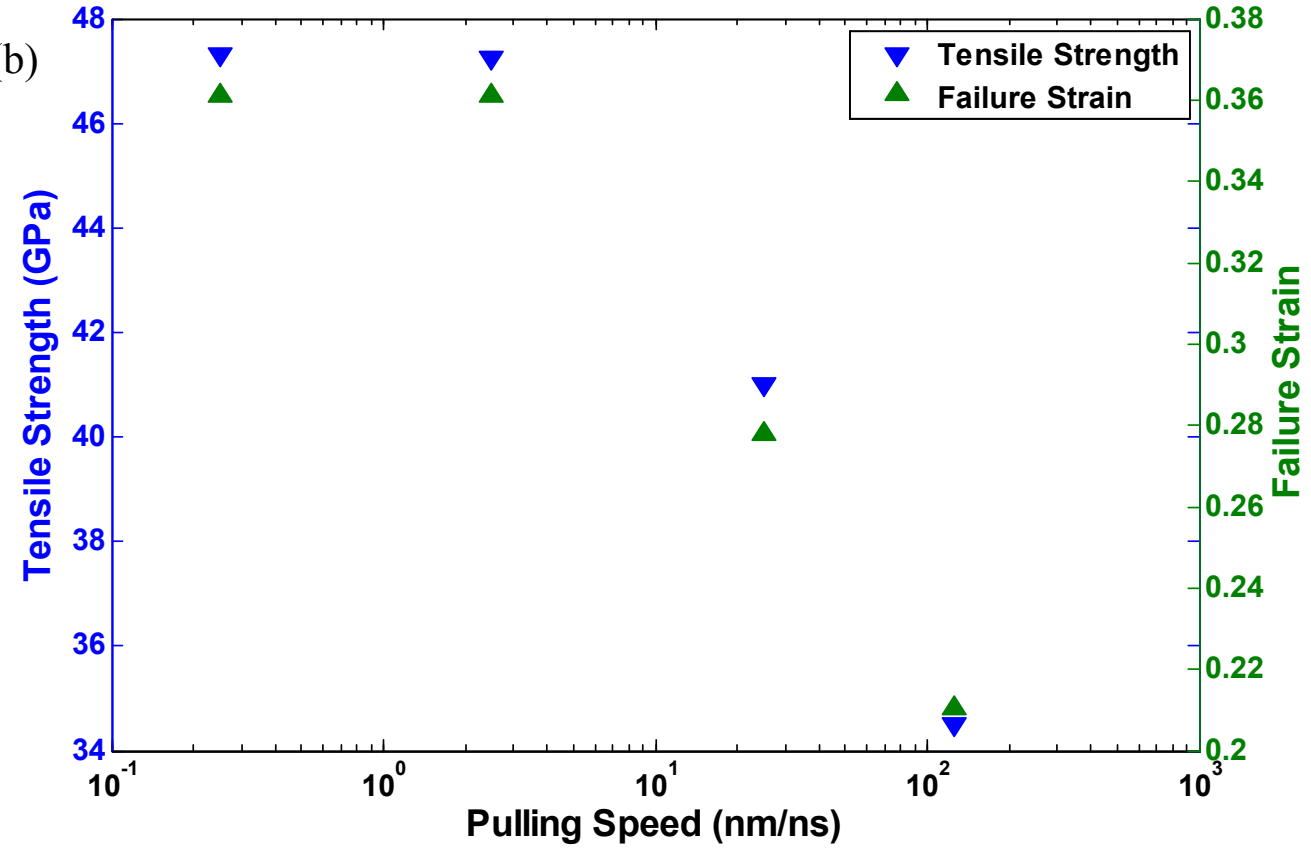


Figure S1: Effects of pulling speeds on stress-strain relationship: (a) Pristine BN; (b) 4 nm grain PBN.

(a)


185
180
175
170
165
160
155
Young's Modulus (GPa)
10^-1
10^0
10^1
10^2
10^3
Pulling Speed (nm/ns)

(b)


Tensile Strength
Failure Strain
Tensile Strength (GPa)
Failure Strain
Pulling Speed (nm/ns)
48
46
44
42
40
38
36
34
0.38
0.36
0.34
0.32
0.3
0.28
0.26
0.24
0.22
0.2
10^-1
10^0
10^1
10^2
10^3

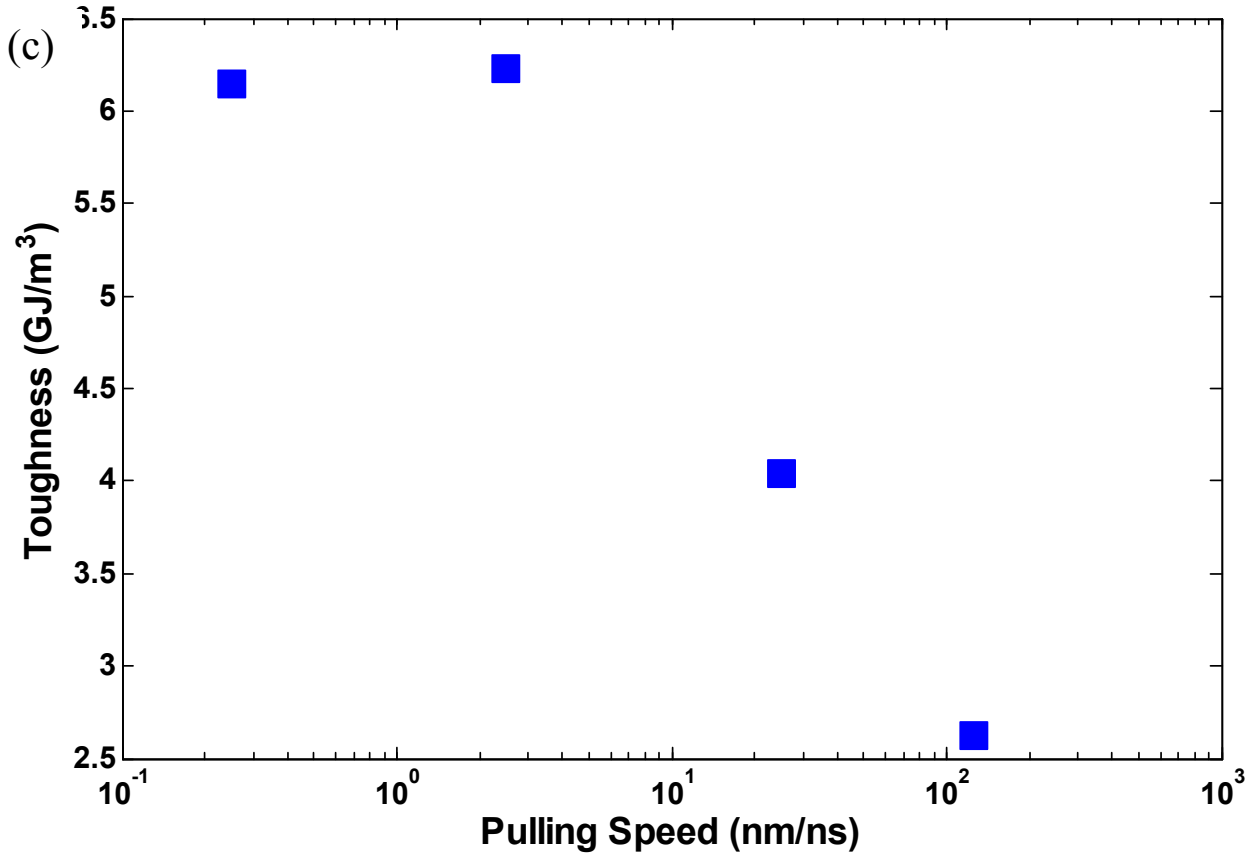


Figure S2: Effects of pulling speed on the mechanical properties of PBN with 4 nm sized grains: (a) Young's Modulus, (b) failure stress/strain, and (c) toughness.

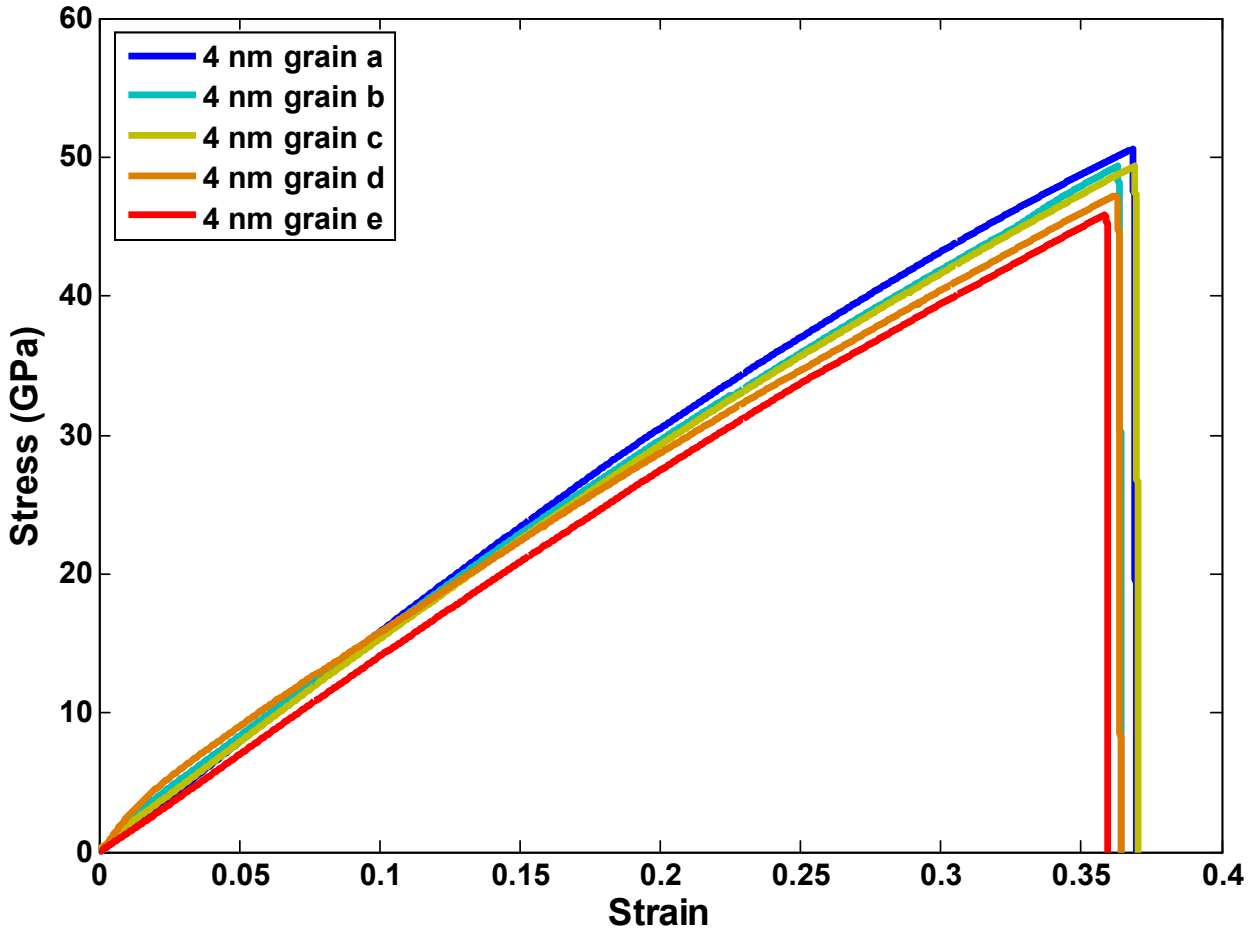
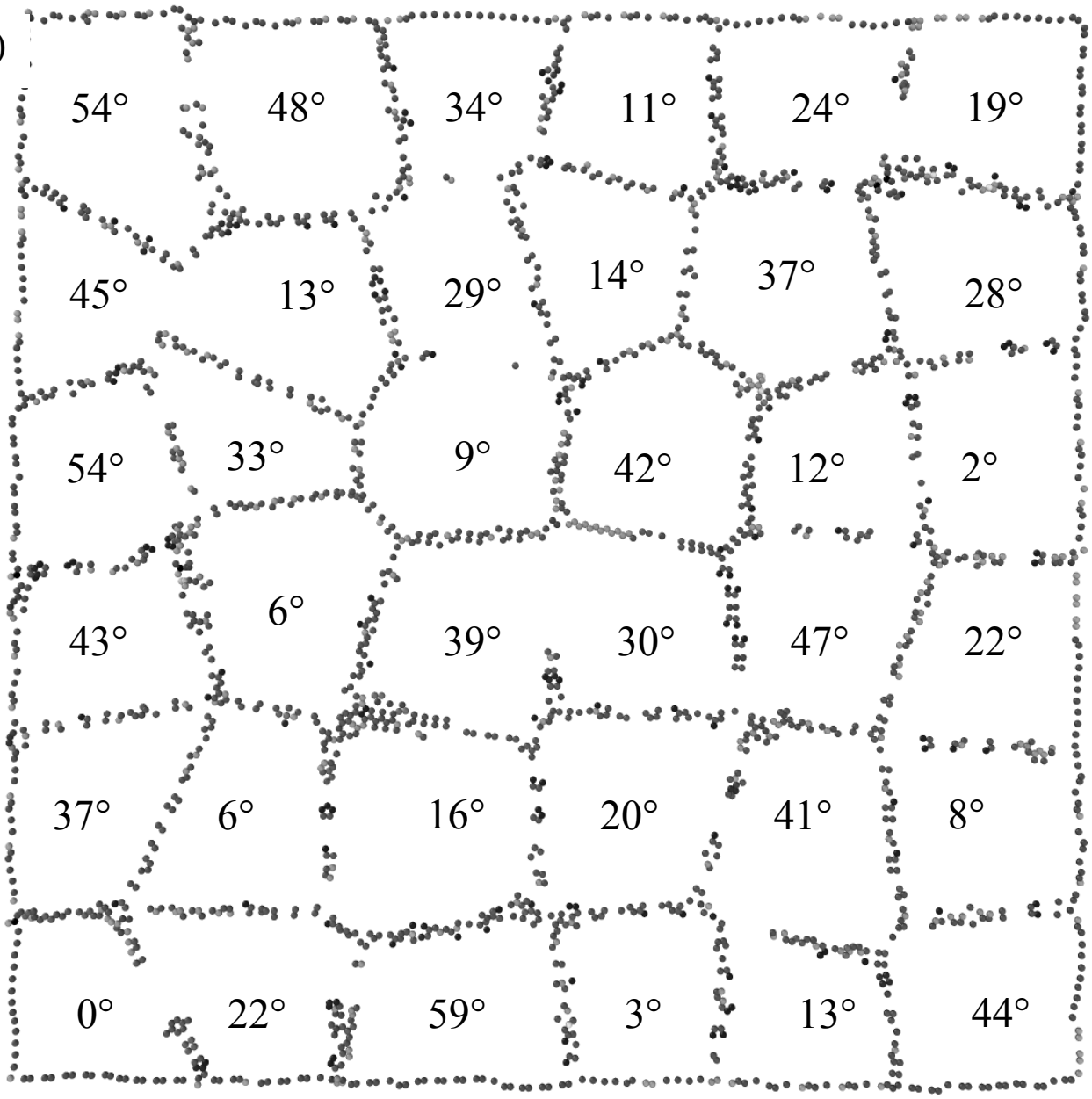


Figure S3: Effect of grain orientations on stress-strain relationship of PBN with 4 nm sized grains. Here four different grain orientations are considered. A comparison of several differently oriented grain structures for 4 nm grain size PBN. Note the similarity for each.

(a)


54° 48° 34° 11° 24° 19°
45° 13° 29° 14° 37° 28°
54° 33° 9° 42° 12° 2°
6°
43° 39° 30° 47° 22°
37° 6° 16° 20° 41° 8°
0° 22° 59° 3° 13° 44°

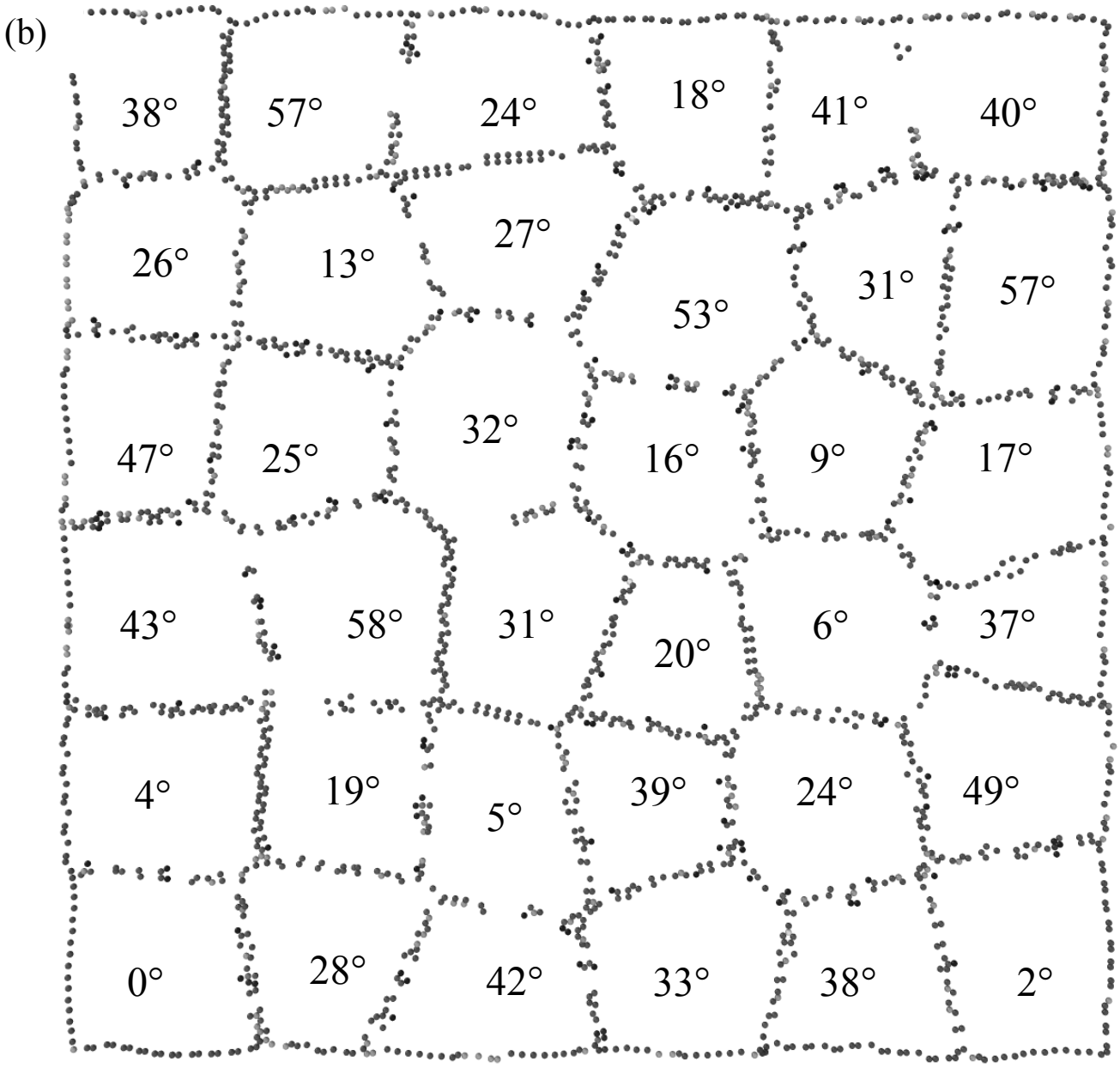


Figure S4: A representation of the randomly oriented grains for 2 cases of 4 nm PBN (cases 'a' and 'b'), with only the atoms in the grain boundaries shown for clarity. The grains are given an orientation randomly chosen between 0° and 60°, as BN has hexagonal rotational symmetry. The first (bottom left) grain is always oriented in the 'armchair' direction (0°). In this case 30° would be the 'zigzag' direction.