Supporting Information

Synergistic Behavior of Tubes, Junctions and Sheets Imparts Mechano-Mutable Functionality in 3D Porous Boron Nitride Nanostructures

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Comparison of DFT versus MD results on the stress-strain response

Figure S1. Comparison of our DFT versus MD results to obtain the stress-strain plot of a (6,6) BNNT.
Elastic Constant Tensors of PBN_I to PBN_IV

\[ C_{\text{PBN}_I} = \begin{bmatrix} 123.51 & -14.17 & 16.65 & -0.54 & 1.19 & 3.79 \\ 153.14 & 17.89 & 1.56 & -0.18 & 3.45 \\ 18.81 & 0.58 & 0.67 & -1.97 & \end{bmatrix} \]

\[ C_{\text{PBN}_II} = \begin{bmatrix} 154.96 & -20.82 & 8.57 & 0.06 & 0.59 & 10.51 \\ 177.49 & 9.02 & 0.57 & -0.07 & 1.56 \\ 6.23 & 0.14 & 0.13 & -0.98 & \end{bmatrix} \]

\[ C_{\text{PBN}_III} = \begin{bmatrix} 52.06 & -7.60 & 14.21 & -0.04 & 0.70 & 1.55 \\ 63.55 & 15.11 & 0.66 & -0.01 & 0.23 \\ 43.21 & 1.14 & 1.20 & -1.49 & \end{bmatrix} \]

\[ C_{\text{PBN}_IV} = \begin{bmatrix} 66.43 & -10.25 & 7.27 & 0.05 & 0.29 & 3.37 \\ 76.13 & 8.27 & 0.32 & 0.02 & 0.27 \\ 10.41 & 0.50 & 0.47 & -0.91 \end{bmatrix} \]
S3 Effective versus Equivalent Elastic moduli of PBN

In view of the relative in-plane symmetry of the PBNs (see Figure 3 in the main manuscript) and small off-diagonal terms in equation (S1-S4), we can approximate the elastic constants tensor of a PBN with that of an orthotropic material\(^1\)

\[
\begin{bmatrix}
C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\
C_{12} & C_{22} & C_{23} & 0 & 0 & 0 \\
C_{13} & C_{23} & C_{33} & 0 & 0 & 0 \\
 & C_{44} & 0 & 0 \\
Sym & & C_{55} & 0 \\
 & & & C_{66}
\end{bmatrix}
\]  

(S5)

Then, the orthogonal shear moduli of PBN can be obtained from

\[
G_{12} = \frac{1}{\tilde{s}_{66}}, \quad G_{13} = \frac{1}{\tilde{s}_{55}}, \quad G_{23} = \frac{1}{\tilde{s}_{44}}
\]  

(S6a-c)

Here, the \(G_{12}, G_{13}\) and \(G_{23}\) refer to \(G_{XY}, G_{XZ}\) and \(G_{YZ}\), respectively. Figure S2 shows two sets of elastic moduli calculated based on effective and equivalent areas of PBN_I to PBN_IV.
Figure S2. a) Effective Young’s moduli and shear moduli of four PBN structures in GPa. The total gross cross-section of the unit-cell is used to calculate the effective moduli. b) Equivalent Young’s moduli and shear moduli of four PBN structures in GPa. The atomic area is used to calculate the equivalent moduli. In a) and b) the bars visually show the differences in elastic moduli of PBN_I to PBN_IV.
Figure S3 shows the results of specific elastic moduli that are calculated by diving the elastic moduli in Figure S2 by the apparent density of the structures.

Figure S3. a) Specific effective Young’s moduli and specific shear moduli (effective moduli divided by apparent density) of four PBN structures in GPa. The total gross cross-section of the unit-cell is used to calculate the effective moduli. b) Specific equivalent Young’s moduli and specific shear moduli (equivalent moduli divided by apparent density) of four PBN structures in GPa. The atomic area is used to calculate the equivalent moduli. In a) and b) the bars visually show the differences in specific elastic moduli of PBN_I to PBN_IV.
S4 Relation Between the Location of Octagon Rings and Stress concentration Points

Figure S4 shows a schematic picture of a BN sheet with an idealized circular hole under tensile load in X and Y directions. The triangular-shape junction and three octagons of PBN are also schematically superimposed in this Figure. In each X and Y direction, the locations of minimum and maximum stress points are marked by $C_{\text{max}}$ and $C_{\text{min}}$ using basic mechanics of materials.\(^2\)

From Figure S4, it is observed that when the tensile load is along the Y-direction (Zigzag), one out of three octagons coincides with the best possible position to bear the minimum stress ($C_{\text{min}}$). However, when the applied load is in the X (armchair) direction, the same octagon is exactly coincided with the stress concentration points ($C_{\text{max}}$) to sustain maximum stress. The other two octagons bear somewhat similar stresses regardless of the direction of applied load.

![Schematic picture of stress concentration points](image)

Figure S4. Schematic picture of stress concentration points in a typical PBN junction. The black squares represent the locations of maximum and minimum stresses in an idealized circular hole under tensile loads.\(^2\) The small red circles denote the location of three octagons of PBN, which are superimposed to the circular hole. a) When the tensile load is along the Y-direction, one out of three octagons coincides with the best possible position to bear minimum stress, $C_{\text{min}}$. b) When the tensile load is along the X-direction, the same octagon in (a) bear maximum stress, $C_{\text{max}}$. The other two octagons bear somewhat similar stresses regardless of the direction of applied load.
S5 A movie of In-Plane Deformation of PBN_IV in Armchair Direction along with Stress Contours ($\sigma_X$)

A side view of deformation of PBN_IV along the X (armchair) direction. The flattening of PBN wrinkles and junctions are clear in this movie. The blue and red colors denote respectively low and high atomic stresses along the X direction obtained from virial theorem.

S6 A movie of In-Plane Deformation of PBN_IV in Zigzag Direction along with Stress Contours ($\sigma_Y$)

A view of deformation of PBN_IV along the Zigzag (Y) direction. The blue and red colors denote respectively low and high atomic stresses along the Y direction obtained from virial theorem.

S7 A movie of Out-of-Plane Deformation of PBN_IV along with Stress Contours ($\sigma_Z$)

Initially, the out-of-plane displacement of the sheets (Regime 1) is mainly contributing to the overall deformation along the tube axis. Then, at a later stage, the actual backbone stretching of the tubes (Regime 2) contribute to the deformation. The blue and red colors denote respectively low and high atomic stresses along the out-of-plane direction obtained from virial theorem.

References

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