Electronic Supplementary Information for RSC Advances

Electronic Supplementary Information (ESI)

Mechanical response of bilayer silicene nanoribbons under uniaxial tension

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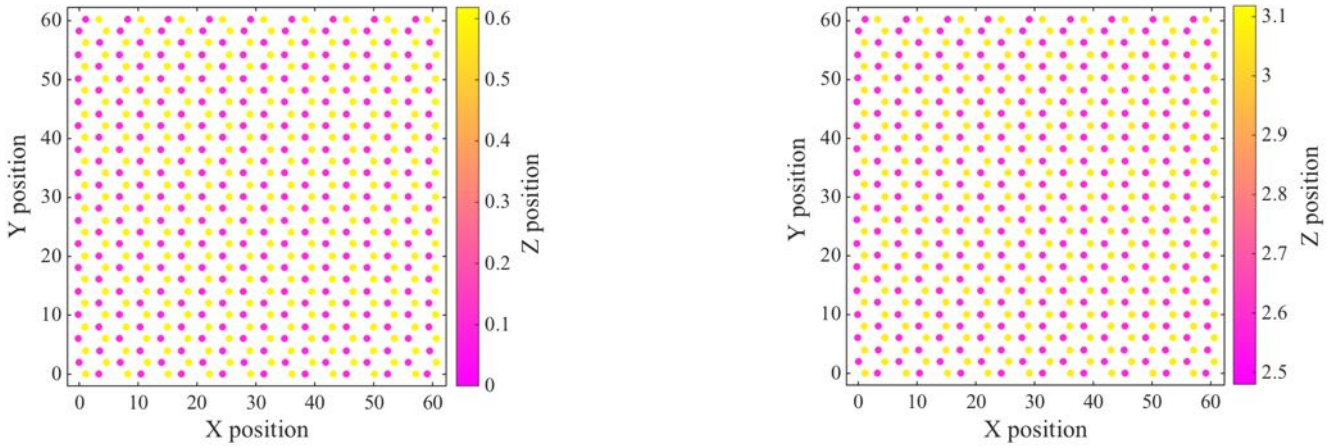

(a) Bottom layer (b) Top layer

Fig. S1 Distribution of atomic relaxed positions for B-SNR of 60 Å side (ach3). Interlayer distance z=2.48 Å.

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Fig. S1 shows atoms positions after relaxation. Positions X, Y and Z are in Å. Average buckling (h_{avg}) is defined as $|z^o_{avg} - z^i_{avg}|$, where z^o_{avg} and z^i_{avg} are the average z-positions of the outer and inner atoms of the layers, respectively. h_{avg} obtained for the ach3 B-SNRs is around 0.50 Å. All B-SNRs sizes considered in this study show similar results.

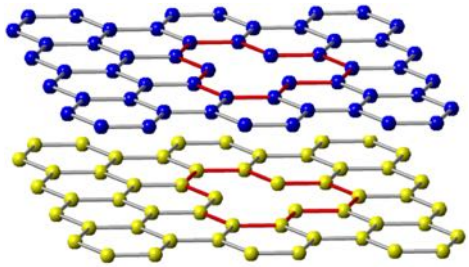

Fig. S2 Schematic representation of a central mono-vacancy defect in both layers of the B-SNRs (mv12 configuration). Yellow balls represent atoms in the 1st layer and blue ones the atoms in the 2nd layer. Red bonds are defined in order to trace the mono-vacancy defect.

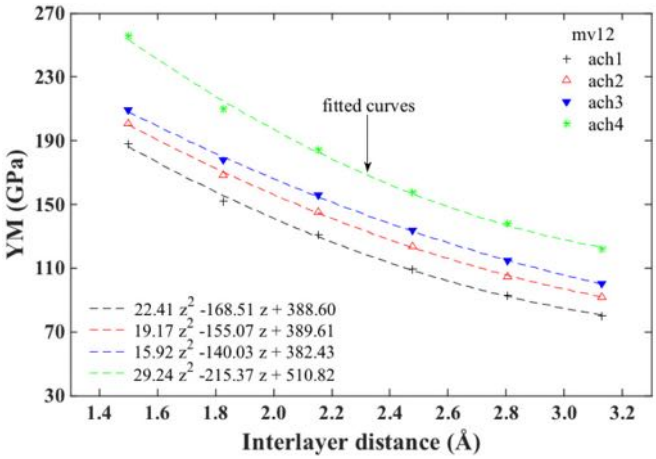

Fig. S3 Young's modulus of mv12 defective B-SNRs configuration *vs* interlayer distance. ach and number label indicate the chirality and the size of the ribbon, respectively (see Table 1). Fitted curves represent the non-linear behaviour of the Young's modulus.

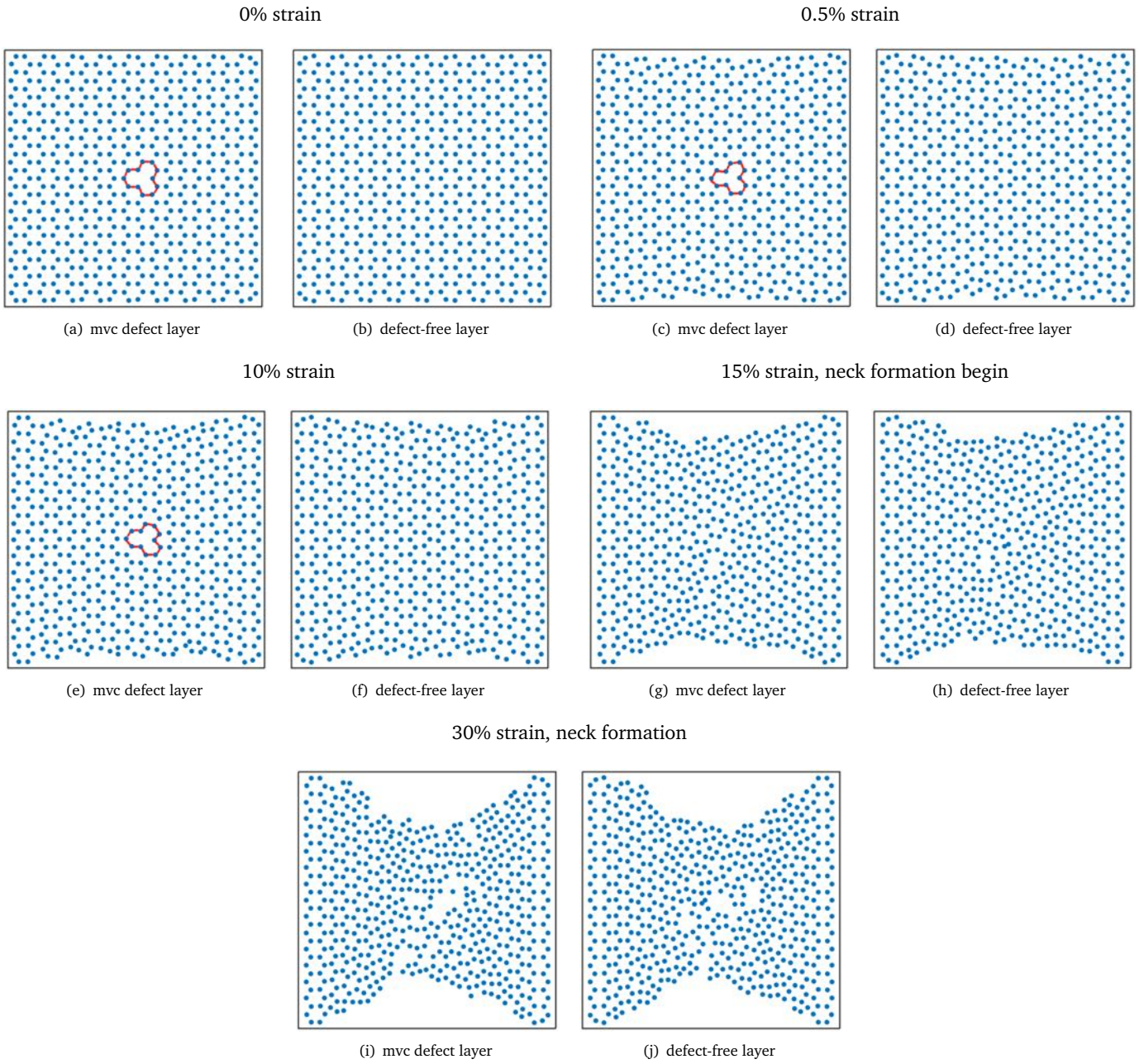

Fig. S4 Atomic configurations for the ach3 B-SNR shown in Fig. 5, at different strains. Interlayer distance z=2.48 Å. Figures on the left side correspond to the first layer and those on the right correspond to the second layer. Note that the box has been scaled along the strain direction.