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Size, vacancy and temperature effects on Young's modulus of silicene nanoribbons

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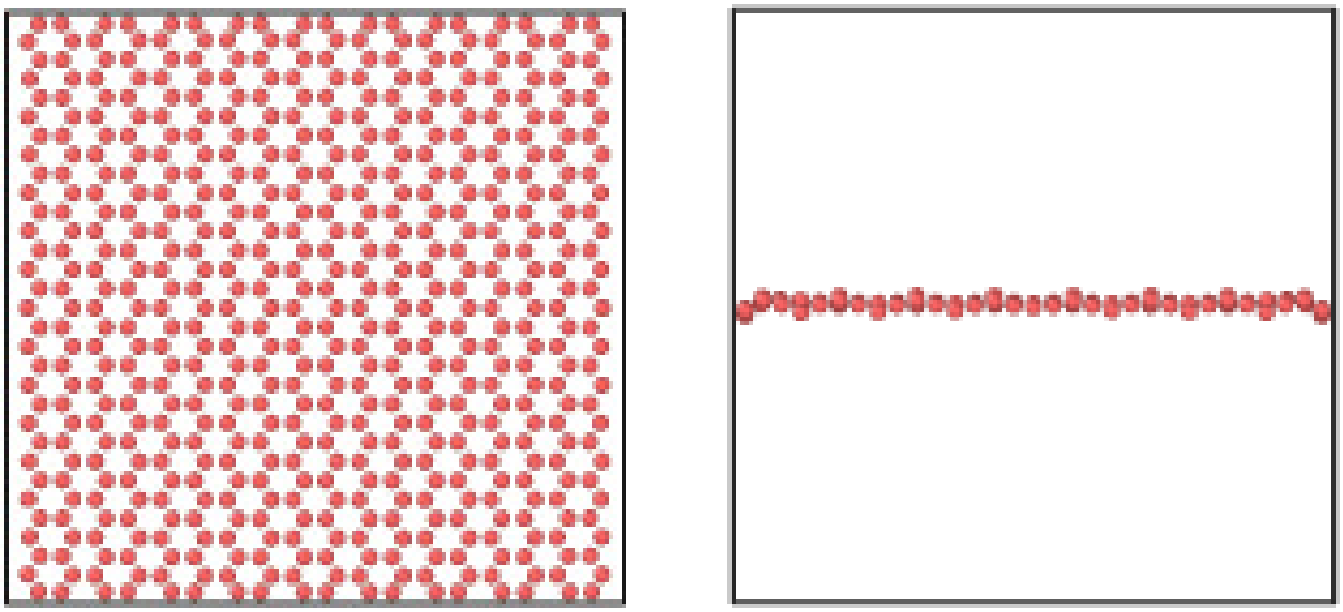
1 Methodology



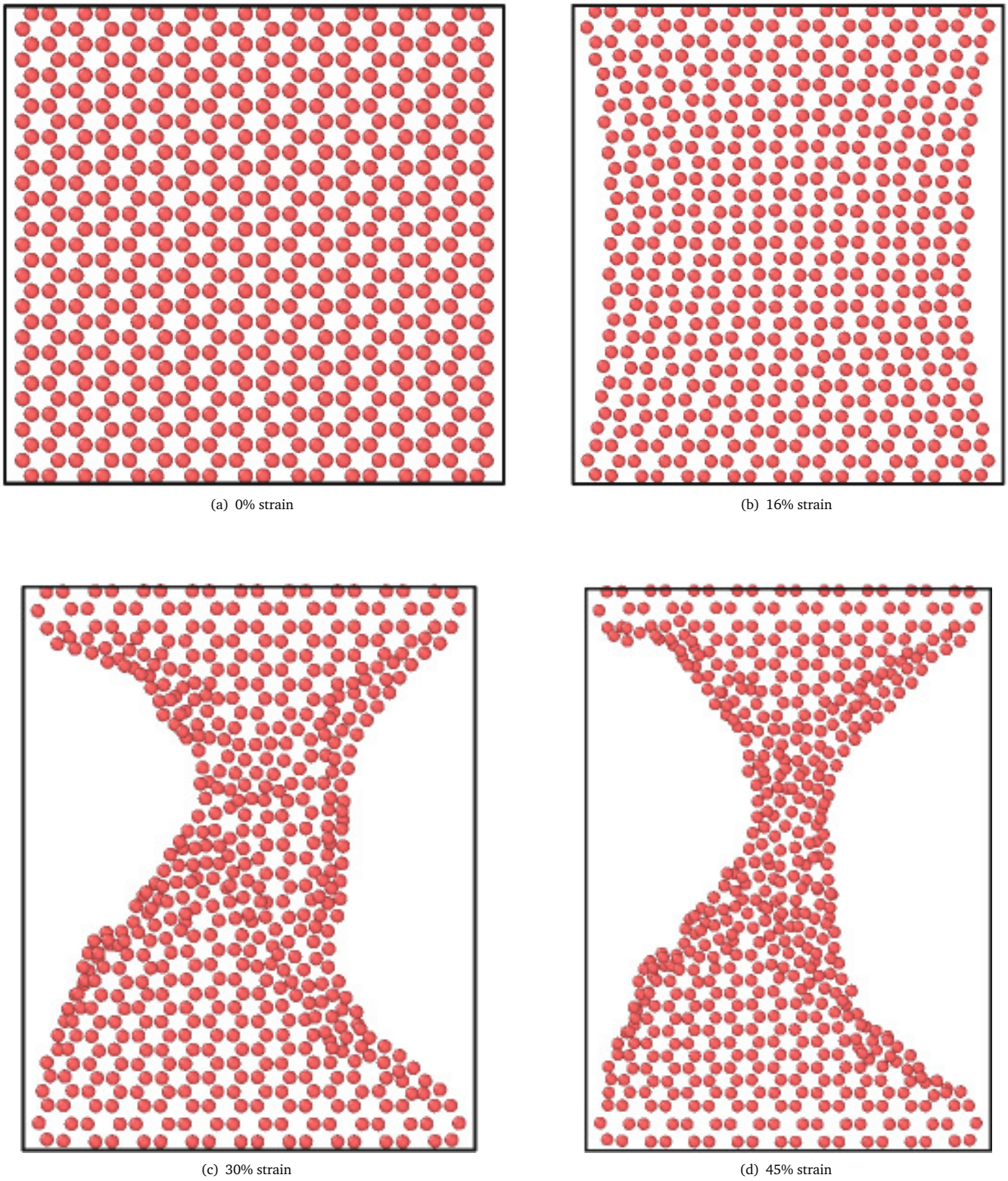
(a) Front view

(b) Lateral view

Fig. 1 Snapshots of atomic configurations of relaxed pristine silicene nanoribbon of 60 Å side at 300K.

Initial conditions for atoms are the positions of ideal low-buckled silicene NR. After relaxation, although atoms seem to have ideal positions on the plane (Fig. 1(a)), buckling is not uniform through the structure as seen Fig. 1(b).

In FIg. 2 we show snapshots that represent different points on the stress-strain curve. Fig. 2(a) shows the relaxed silicene structure, corresponding to zero deformation. Fig. 2(b) corresponds to the ultimate tensile strength, just before necking occurs. SNRs considered in this study show ductile behavior due to the formation of the necking before reaching its breaking point. Fig. 2(c) and Fig. 2(d) present the necking process of the silicene structure. The critical strains of SNRs are at 14.5% and 11.5% for zz and ach, respectively. As we can see, SNR's critical strains are smaller than those obtained for silicene sheets (19.5% for zz and 15.5% for ach)[63].



(a) 0% strain

(b) 16% strain

(c) 30% strain

(d) 45% strain

Fig. 2 Snapshots of atomic configurations of pristine silicene nanoribbon of 60 Å side, at different strains along zig-zag direction.

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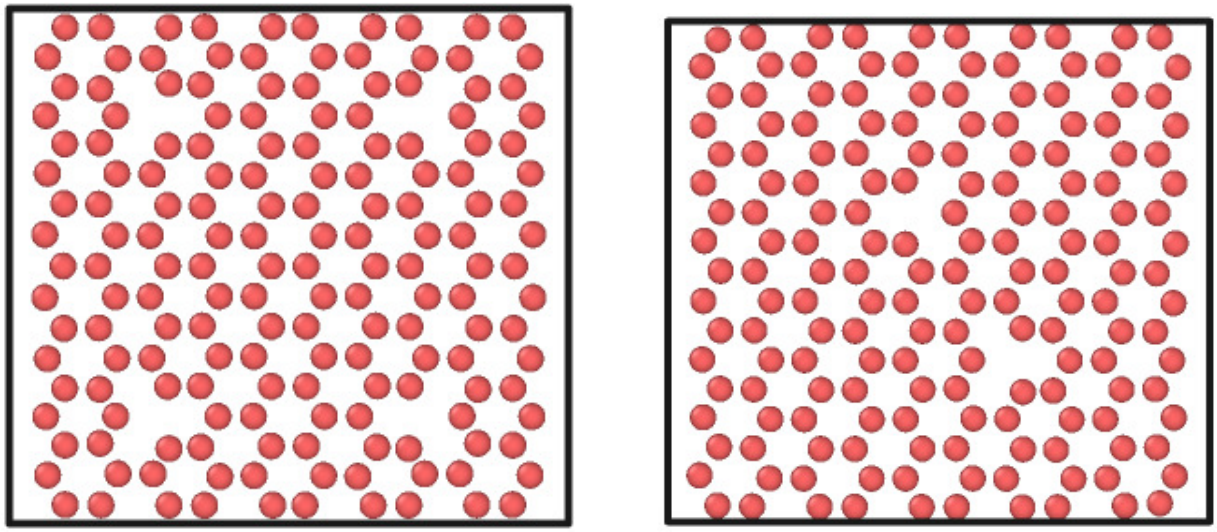
2 Vacancy self-healing



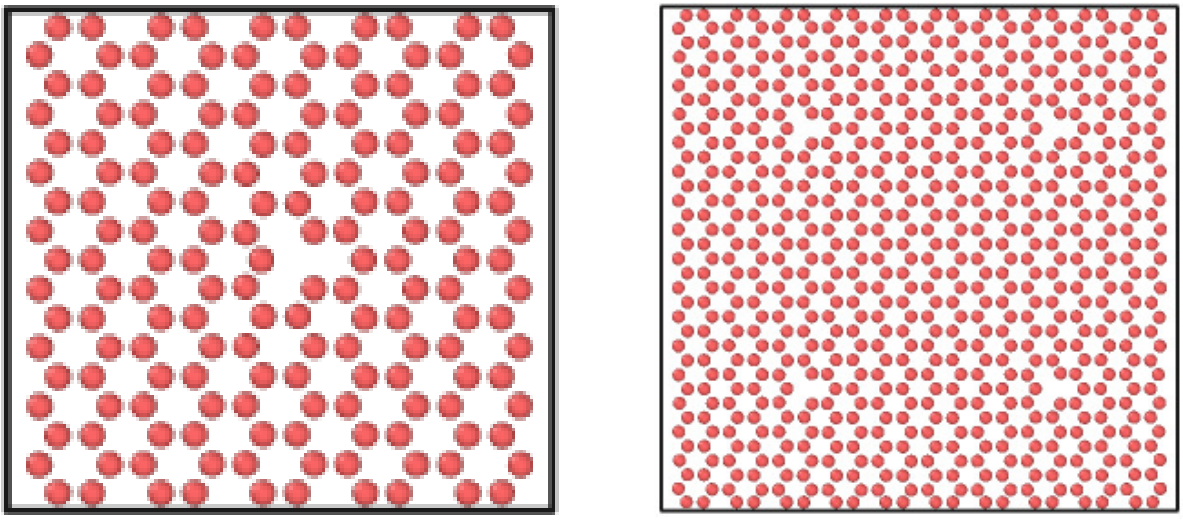
(a) Monovacancies close to the ribbon's boundaries (mve)

(b) Monovacancies close to each other

Fig. 3 Snapshots of atomic configurations of relaxed defective SNRs of 32 Å side.

Moonovacancy-defects do not coalesce into a multivacancy in the relaxed structures.

3 Density dependence



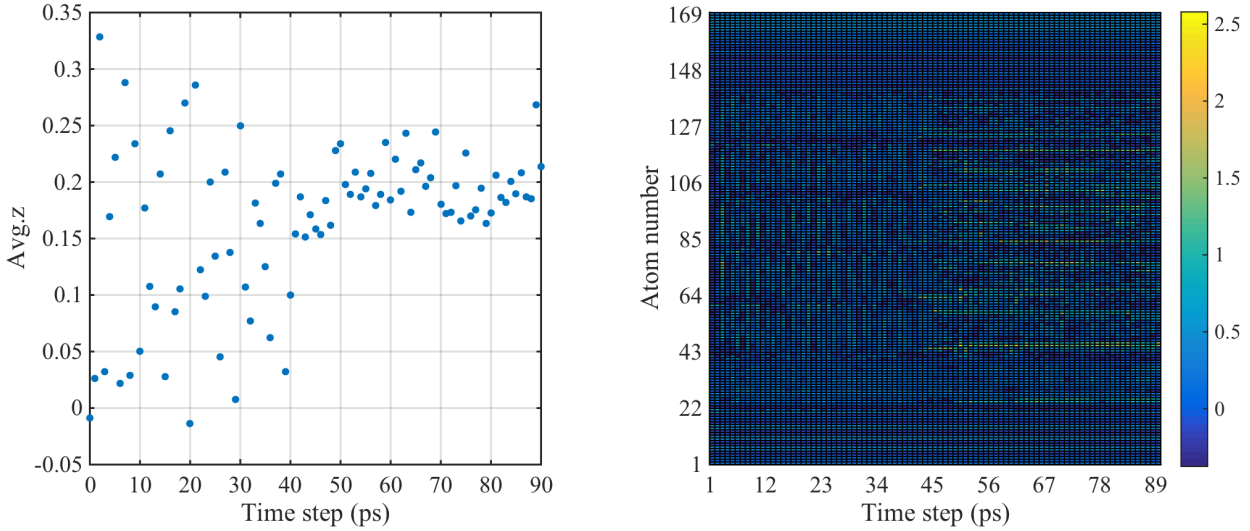
(a) Defective NR of length L

(b) Defective NR of length 2L

Fig. 4 Snapshots of atomic configurations of relaxed defective SNRs, whose length varies from L (32 Å) to 2L .

Both SNRs have the same density of defects, but different YM values.

4 Buckling



(a) Average buckling (b) Buckling position

Fig. 5 Buckling behaviour of the zz-SNRs under uniaxial tension.(a) shows the average value of $|z(t)| - z(t=0)$, over the total number of atoms. (b) Buckling position for each atom defined as $|z(t)| - z(t=0)$.

Notice that the average buckling amplitude changes importantly during the lineal regime and the plastic region. Around 40 ps the ultimate tensile strength (UTS) is reached. After that point the structure is in the necking region and the buckling dispersion decreases as a result of the applied tension, indicating that the structure tends to be planar. Atomic buckling, Fig. 5(b), also shows a change of regime at 40 ps.