Aspect Ratio Dependent Buckling Mode Transition in Single-Walled Carbon Nanotubes under Compression
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Introduction:
Most theoretical studies on buckling of single-walled carbon nanotubes (SWCNTs) under compression have focused on tubes with small aspect ratios. Buckling modes of SWCNTs with large aspect ratios remain poorly understood. We explore this issue using molecular dynamics simulations and unveil the underlying mechanism responsible for the aspect-ratio-dependant buckling mode transition.

For a bent SWCNT, the critical buckling curvature can be estimated as:

$$K_{C}^{shell} = \frac{bh}{d^2}$$

The relationship between the tube curvature and the compressive strain in a compressed SWCNT is:

$$R = \frac{1}{K} \alpha \frac{L}{\sqrt{\varepsilon}}$$

The critical strain for the secondary buckling strain can therefore be obtained:

$$\varepsilon_{cr} = C \left( \frac{1}{d^2} \frac{L}{d} \right)$$

The underlying mechanism for buckling mode transition can be understood from the responses of bond angles and bond lengths to strain. The definition of variables is shown in panel (A).

1. Responses of both bond lengths and bond angles contribute to the first column buckling, leading to the first drop in strain energy;
2. After the column buckling, variation of bond angles plays a more important role, which leads to the second strain energy release. The SWCNT is strongly curved before the second buckling.

From panel (C) one can see that the shell buckling comes from column-buckling-induced bending strain. Therefore we can develop a formula to predict this buckling strain based on bending buckling theory.

Simulated (dots) and predicted (curve) critical strain for the secondary buckling vs aspect ratio. Good agreement is achieved between the two sets of data.

References:

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