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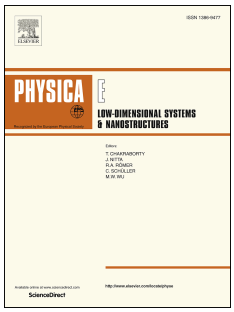

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Axial buckling behavior of single-walled carbon nanotubes: Atomistic structural instability analysis

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Abstract

To reveal the atomistic scale mechanism of buckling of single-walled carbon nanotubes (SWCNTs) under axial compression, we carried out molecular dynamics (MD) simulation and atomistic structural instability (ASI) analysis. The ASI analysis enables us to reveal the development of 'latent' instability modes until buckling of structure, which cannot be clarified with MD alone. Euler-type buckling was found in relatively thin and long nanotube models, while buckling triggered by change of cross-sectional shape (i.e., radial buckling) was found in thick and short models. With growing radius, a crossover between the Euler-type and radial buckling modes was clearly found in the ASI analysis. Even when the deformation behavior was apparently the same, the buckling can be triggered by different instability modes. We also analyzed the structural instability using the Flügge theory based on linear continuum mechanics (LCM) to compare the results with the ASI analysis. Initial eigenvalues and development of instability modes were different between the ASI and LCM results, leading to a significant deviation of buckling strain and instability crossover points. We investigated the effect of chirality of CNT which is difficult to explain by LCM.

Key words : Buckling; Structural instability; Deformation mode; Atomistic simulation; Carbon nanotube

Research highlights

- Atomistic origin of axial buckling mechanism of SWCNTs is investigated in detail through atomistic structural instability (ASI) analysis.
- Buckling deformation has three types; S-shaped Euler type buckling without kinks, Z-shaped with kinks and I-shaped with fin structures. The buckling type has little to do with ASI mode designating the motion of atoms at instability.
- As a result of atomistic model calculations, adjusted material parameters suitable for buckling analysis based on a continuum theory are proposed.
- Chiral SWCNTs exhibit peculiar, two-fold buckling mechanism, which has been revealed for the first time due to our ASI analysis.
- Chiral SWCNTs can present a characteristic shape with a spiral undulation prior to large buckling deformation, suggesting the possibility of peculiar physical properties emerging due to the undulated shape.