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Pattern Transformations of the Single Walled Carbon Nanotube Bundle under External Stimuli

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Summary

Recently, much attention has been paid to the single walled carbon nanotube (SWCNT) bundle, which exhibits remarkable mechanical, chemical and electrical properties. Here, we present the pattern transformations of the SWCNT bundle under contraction and expansion. We first report three simple relations governing the geometry of the SWCNT bundle under no pressure. Then, due to the expansion of the bundle, a new hexagonal structure is found by using both the hybrid atom-continuum model and density functional theory. The results show that when the diameter of the nanotubes is larger than certain critical value, the nanotubes in the bundle will undergo three phase transformations. The corresponding critical size and the phase diagram of the bundle are also presented. Finally, the pattern transformations of the SWCNT bundle under hydrostatic pressure are calculated by density functional theory and the corresponding mechanisms of the pattern transformations are also investigated. The studies of the pattern transformations of SWCNT bundle can offer new understandings into the fabrication of novel materials and devices at the nano-scales.